TOWARDS HYBRID METHODS FOR SOLVING HARD COMBINATORIAL OPTIMIZATION PROBLEMS

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I certify that I have read this dissertation and that, in my opinion, it is fully adequate in scope and quality as a dissertation for the degree of Doctor of Philosophy.

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Abstract

Combinatorial Optimization is a branch of optimization in applied mathematics and computer science, related to operations research, algorithm theory and computational complexity theory that sits at the intersection of many fields, such as artificial intelligence, mathematics and software engineering. Combinatorial optimization problems commonly imply finding values to a set of variables which are restricted by a set of constraints, in some cases in order to optimize a certain function (optimization) and in others only to find a valid solution (satisfaction). Combinatorial optimization algorithms solve instances of problems that are believed to be hard in general by exploiting the usually large solution space of these instances. They can achieve this by reducing the effective size of the search space and by exploiting it efficiently.

In this thesis we focus on Combinatorial Optimization Algorithms which fall into the field of Artificial Intelligence (although the line that separates this field from Operations Research is very fine), instead of algorithms from the Operations Research field. Thus, methods such as Integer Programming (IP) or Branch and Bound (BB) are not considered. The goal of this thesis is to show that different approaches can be better suited for different problems, and that hybrid techniques which include mechanisms from different frameworks can benefit from their advantages while minimizing their drawbacks. All this is shown throughout this thesis by solving hard combinatorial optimization problems, such as quasigroup completion, social golfers, optimal Golomb rulers, using a variety of techniques, which lead to a hybrid algorithm for finding Golomb rulers that incorporates features of Genetic Algorithms, Local Search, Constraint Programming and even Clustering.

Resumen

La Optimización Combinatoria es una rama de la optimización en matemática aplicada y de la informática, relacionada con la investigación operativa, la teoría de algoritmos y la teoría de complejidad computacional, que se encuentra en la intersección de varios campos, tales como la inteligencia artificial, las matemáticas y la ingeniería del software. Los problemas de optimización combinatoria suelen consistir en encontrar valores para un conjunto de variables que estn restringidas por un conjunto de restricciones, en algunos casos para optimizar una función dada (optimización) y en otros tan solo para encontrar una solución válida (satisfacción). Los algoritmos de optimización combinatoria resuelven instancias de problemas considerados difíciles en general gracias a una exploración inteligente del espacio de búsqueda, en parte reduciéndolo, en parte recorriéndolo de una forma eficiente.

En esta tesis nos centramos en los algoritmos de optimización combinatoria que se consideran dentro del campo de la Inteligencia Artificial (aunque es cierto que la linea que lo separa del campo de la investigación operativa es muy fina), en vez de en algoritmos de investigación operativa. Así pues, métodos como la programación entera o el "Branch-and-Bound" no van a ser tratados. El objetivo de esta tesis es mostrar que diferentes técnicas pueden ser más adecuadas para diferentes problemas, y que técnicas híbridas que incluyen mecanismos de diferentes paradigmas se pueden beneficiar de las ventajas e intentar minimizar los inconvenientes de los mismos. Todo esto se muestra en esta tesis con la resolución de problemas difíciles de optimización combinatoria como completitud de cuasigrupos, golfista social, Golomb rulers, usando varias técnicas, que dan lugar al desarrollo de un algoritmo híbrido para encontrar Golomb rulers, que incorpora aspectos de algoritmos genéticos, búsqueda local, programación con restricciones e incluso clustering.

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Chapter 1

Introduction

Combinatorial Optimization is a branch of optimization in applied mathematics and computer science, related to operations research, algorithm theory and computational complexity theory that sits at the intersection of many fields, such as artificial intelligence, mathematics and software engineering. Combinatorial optimization problems commonly imply finding values to a set of variables which are restricted by a set of constraints, in some cases in order to optimize a certain function (optimization) and in others only to find a valid solution (satisfaction). Combinatorial optimization algorithms solve instances of problems that are believed to be hard in general (most of them are at least NP-complete [41]) by exploiting the usually large solution space of those instances. They are able to achieve this by reducing the effective size of the search space and by exploiting it efficiently.

1.1 Motivation

The goal of this thesis is to show that different approaches can be better suited for different problems, and that hybrid techniques which include mechanisms from different frameworks can benefit from their advantages while minimizing their drawbacks. All this is shown throughout this thesis by solving hard combinatorial optimization problems , such as quasigroup completion, social golfers, optimal Golomb rulers, using a variety of techniques, which lead to a hybrid algorithm for finding Golomb

rulers that incorporates features of Genetic Algorithms, Local Search, Constraint Programming and even Clustering. As can be seen from this enumeration, our focus is on algorithms that fall into the field of Artificial Intelligence (although the line that separates this field from Operations Research is very fine), instead of algorithms from the Operations Research field. Algorithms from Operations Research such as Integer Programming (IP) or Branch and Bound (BB), which have also been studied extensively for optimization problems are, however, not studied in this thesis.

The constraint paradigm is a useful and well-studied framework for expressing many problems of interest in Artificial Intelligence. The first research presented here deals with modelling *Constraint Satisfaction Problems* (CSPs), in particular for a well-known problem named *Quasigroup Completion Problem* (QCP). From this benchmark problem and comparing several modelling and solving methods we are able to yield important conclusions for a more general kind of problems, known as *Multiple Permutation Problems*. There has also been interest in the comparison between CSP and SAT techniques; discussing whether one can be more appropriate for a specific field or for another. We provide this comparison for this specific problem.

Local Search is known to be a powerful technique especially for dealing with optimization problems or problems with a significantly large search space. The second research work presented deals with modelling and solving social tournaments, in particular the Social Golfer Problem. The results presented here are significantly better than other complex approaches in the literature. It also raises the issue of symmetries in Local Search and presents a clever and simple heuristic to obtain initial solutions that boosts performance.

Genetic Algorithms are population based algorithms that mimic biological processes. Memetic Algorithms are hybrids that introduce Local Search to yield better results and converge to higher quality solutions. The next research work presented in this thesis deals with solving a very hard combinatorial optimization problem known as Golomb Ruler. The research developed here focuses on modelling and solving optimal and near-optimal Golomb Rulers, providing high quality results that are consistently superior to those presented in other Genetic Algorithms in the literature.

Finally, A Hybrid Memetic Algorithm known as Scatter Search is enriched with

Constraint Programming and Clustering techniques to further improve the results obtained in the previous research over the Golomb Ruler Problem as well.

In the next sections we introduce the problems dealt with troughout the whole research, we establish the boundaries of our work and present its main contributions.

1.2 Problems Addressed

Many real life problems fall into the category of Combinatorial Optimization Problems. In this thesis we solve different problems with different techniques and ultimately develop a hybrid that encloses them all.

The Quasigroup Completion Problem (QCP) is a very challenging benchmark among combinatorial problems, which has been the focus of much recent interest in the area of constraint programming [101]. It has a broad range of practical applications such as conflict-free wavelength routing in wide band optical networks, statistical design, and error correcting codes [101]; it has been put forward as a benchmark which can bridge the gap between purely random instances and highly structured problems [100]; and its structure as a multiple permutation problem [229, 118] is common to many other important problems in constraint satisfaction. Thus, solutions that prove effective on QCPs have a good chance of being useful in other problems with similar structure.

The social golfer problem has attracted significant interest since it was first posted on `sci.op-research` in May 1998. It is a highly combinatorial and symmetric problem and it is not surprising that it has generated significant attention from the constraint programming community (e.g., [72, 209, 178, 200, 199, 13, 184]). Indeed, it raises fundamentally interesting issues in modeling and symmetry breaking, and it has become one of the standard benchmarks for evaluating symmetry-breaking schemes. Recent developments (e.g., [13, 184]) approach the scheduling of social golfers using innovative, elegant, but also complex, symmetry-breaking schemes.

Finding Golomb rulers is an extremely challenging combinatorial problem which has received considerable attention over the last decades. Golomb rulers have applications in a wide variety of fields including radio communications ([27, 114]), x-ray

crystallography ([26]), coding theory ([56, 139]), and radio astronomy. Moreover, because of its highly combinatorial nature,[1] it has become a standard benchmark to evaluate and compare a variety of search techniques. In particular, genetic algorithms, constraint programming, local search, and their hybridizations have all been applied to the problem of finding Golomb rulers (e.g., [43, 76, 173, 176, 210, 213]).

In this thesis we are going to introduce pure approaches of dealing with combinatorial problems such as Constraint Satisfaction Problems (CSPs), The Satisfiability Problem (SAT), Local Search (LS) and Genetic Algorithms (GAs). We will also introduce hybrid approaches, namely CSP and LS, GA and LS (which is also known as Memetic Algorithms) and GAs that incorporate Constraint Satisfaction techniques. We are going to present research on these paradigms on different hard combinatorial optimization problems and finally develop a hybrid that incorporates them all and that yields results higher in quality for a hard combinatorial problem. We also include an appendix to briely describe some techniques used thorugh out the thesis, in particular Greedy Randomized Adaptive Search Procedures (GRASP) and Clustering.

1.3 Contributions

This research comes to prove that different techniques may be better suited for dealing with different combinatorial problems, and instead of devoting research on very specialized techniques within each field, we rather concentrate on problem solving, using whichever technique is most suited. We also aim to show that all these techniques can cooperate in a single algorithm to yield high quality results. Thus, the scope of this research is problem modelling, problem solving, and hybrid developing with CSP, LS and Genetic Algorithm's techniques.

The main contributions of our work, in that sense, are diverse. This thesis deals mainly with problem solving, and thus, every chapter reports top results in the literature for the various problems addressed. Also, a hybrid algorithm is presented as well, and altough it is problem oriented it can be easily generalized to deal with many

[1] The search for a 19-mark Golomb ruler took approximately 36,200 CPU hours on a Sun Sparc workstation using a very specialized algorithm [56].

different combinatorial optimization problems.

Therefore, the research presented in this thesis contributes to the state-of-the-art in presenting high quality results for the Quasigroup Completion Problem, the Social Golfer Problem and the Golomb Ruler Problem; as well as introducing an effective hybrid algorithm that within a Memetic Algorithm (MA) template introduces CSP and Clustering features. Thus, the main contributions are:

1.3.1 Quasigroup Completion with Systematic Search

First, we present several techniques that together allow us to solve significantly larger QCPs than previously reported in the literature. Specifically, [101] reports that QCPs of order 40 could not be solved by pure constraint programming approaches, but could sometimes be solved by hybrid approaches combining constraint programming with mixed integer programming techniques from operations research. We show that the pure constraint satisfaction approach can solve many problems of order 45 close to the transition phase, which corresponds to the peak of difficulty. Our solution builds upon some known ideas, such as the use of redundant modelling [36] with primal and dual models of the problem connected by channelling constraints [229], with some new twists. In addition, we present a new value ordering heuristic which proves extremely effective, and that could prove useful for many other problems with multiple models. Finally, we show how redundant constraints can be used to "compile arc consistency into forward checking", that is, to ensure that the latter has as much pruning power as the former but at a much lesser cost in constraint checks.

It is interesting to note that our approach involves only binary constraints, which seems to go against common wisdom about their limitations —when contrasted with the use of non-binary constraints such as alldiff [188]— in solving quasigroup completion problems [215].

1.3.2 SAT vs. CSP comparison

Second, we perform a systematic study of modelling choices for quasigroup completion, testing a variety of solvers and heuristics on various SAT and CSP encodings.

The clear winner is the SAT 3D-encoding, specially with the solver Satz [144], closely followed by the solver Satzoo [62] on the same encoding. As these two solvers are quite different (one uses a strong form of lookahead in its heuristic, but no back-jumping or learning, while the other relies heavily on the last two), the 3D encoding appears to be quite robust as a representation. On the other hand, CSP models perform significantly worse with the two solvers we tried, and standard SAT encodings generated from the CSP models are simply too large in practice. These results strongly suggest that the 3D encoding can turn out to be quite competitive in other permutation problems (many of which arise in quite practical problems [118]) when compared with the currently preferred channelling models.

The reasons for this appear to be twofold. First, we can show that the 3D encoding (which is basically the "SAT channelling model" of [118] extended to multiple permutations and dual models) exactly captures the channelling models of QCPs as defined in this thesis, but in a much more concise way, by collapsing primal and dual variables. Further, we can show that the 3D encoding captures the "support SAT encoding" of the channelling model, hence by results of [89], that unit propagation on the 3D encoding achieves the same pruning as arc consistency (MAC) in the CSP channelling model. These results appear easy to extrapolate to other permutation problems (or similar ones with "channelling constraints"), which have received a lot of recent attention [35, 229, 118]. Second, empirically, we identify Satz's UP heuristic as crucial to its success in this domain; as shown by the fact that, when importing the heuristic into our CSP solvers, we obtain significant improvements in their scalability.

1.3.3 Scheduling Social Golfers with Local Search

This research proposes a local search algorithm for scheduling social golfers, whose local moves swap golfers within the same week and are guided by a tabu-search meta-heuristic. The local search algorithm matches, or improves upon, the best solutions found by constraint programming on all instances but 3. It also found the first solutions to 11 instances that were previously open for constraint programming.[2]

[2]For the current statuses of the instances, see Warwick Harvey's web page at `http://www.icparc.ic.ac.uk/wh/golf`.

Moreover, the local search algorithm solves almost all instances easily in a few seconds and takes about 1 minute on the remaining (harder) instances. The algorithm also features a constructive heuristic which trivially solves many instances of the form $odd - odd - w$ and provides good starting points for others.

The main contributions of this chapter are as follows.

1. It shows that local search is a very effective way to schedule social golfers. It finds the first solutions to 11 instances and matches, all other instances solved by constraint programming but 3. In addition, almost all instances are solved in a few seconds, the harder ones taking about 1 minute.

2. It demonstrates that the local search algorithm uses a natural modeling and does not involve complex symmetry-breaking schemes. In fact, it does not take symmetries into account at all, leading to an algorithm which is significantly simpler than constraint programming solutions, both from a conceptual and implementation standpoint.

3. The experimental results indicate a nice complementarity between constraint programming and local search, as some of the hard instances for one technology are trivially solved by the other.

1.3.4 Finding Near-Optimal Golomb Rulers with a Hybrid Evolutionary Algorithm

This work proposes a novel hybrid evolutionary algorithm for finding near-optimal Golomb rulers in reasonable time. The algorithm embeds a local search into a genetic algorithm and outperforms earlier genetic algorithms, as well as constraint programming algorithms and their hybridizations with local search. In particular, the algorithm quickly finds optimal rulers for up to 13 marks and was able to find optimal rulers for 14 marks, which is clearly out of reach for the above mentioned algorithms. The algorithm also finds near-optimal rulers in reasonable time, clearly indicating the effectiveness of hybrid evolutionary algorithms on this highly combinatorial application. Of particular interest is the conceptual simplicity and elegance of the algorithm.

Even though there are solutions for higher number of marks for other complete search approaches, evolutionary algorithms have the advantage of providing good quality solutions in a short period of time. This is a main contribution of this research as well, providing high quality solutions (improving all previous evolutionary approaches) in a few seconds or minutes.

The main technical contribution of the novel hybrid evolutionary algorithm is its focus on feasibility. Indeed, the main step of the evolutionary algorithm is to find a Golomb ruler of a specified length (or smaller), using constraint violations to guide the search. Near-optimal rulers are obtained indirectly by solving a sequence of feasibility problems.

1.3.5 Scatter Search and Final Hybrid

We present a hybrid EA designed to find optimal or near-optimal Golomb Rulers. This algorithm makes use of both an indirect approach and a direct approach in different stages of the search. More specifically, the indirect approach is used in the phases of initialization and restarting of the population and takes ideas borrowed from the GRASP-based evolutionary approach published in [43]. The direct approach is considered in the stages of recombination and local improvement; particularly, the local improvement method is based on the tabu search (TS) algorithm described in the previous chapter. Experimental results show that this algorithm succeeds where other evolutionary algorithms did not. Our algorithm systematically finds optimal rulers for up to 13 marks. OGRs up to 15 marks (included) can now be found. Moreover, the algorithm produces Golomb rulers for 16 marks that are very close to the optimal value (i.e., 1.1% far), thus improving significantly the results previously reported in the EA literature.

At this point, we try to improve the performance of this algorithm in different ways:

- **Complete Search:** we use complete search techniques to combine the individuals in the population, using constraint programming features such as propagation. While this technique does not necessarily translates into the generation

of high quality individuals, it is nevertheless able to produce valid solutions and even optimal solutions.

- **Clustering:** this technique, on the other hand, is introduced in order to acquire a higher degree of diversity in the population. Instead of maintaining the best individuals in the population, we divide it into different clusters and then choose the best in each of the clusters.

These two techniques allow, first, to implement a novel hybrid algorithm which can be easily generalized to deal with several other problems, and second, to yield results that are even better in quality than the allready top results obtained with the Scatter Search alone.

The results are outstanding, we are now able to solve a 16 marks ruler and to consistently solve every 14 marks rulers. The algorithm is tested using different sets of parameters referred to the clustering mechansism and the results are consistently superior to the previous algorithm without the improvements.

1.4 Publications

Finally we present the main publications that this thesis yielded. We are going to classify them into the chapters to which the research is related. Also, the "Others" section indicates papers published during the Ph.D. time that are not included in this thesis; and "Under Submission" referres to papers that have been submitted to conferences from which we are awaiting the outcome.

CSP and SAT

- Carlos Ansótegui, Álvaro del Val, Ivń Dotú, Cesar Fernández y Felip Manya, "Modeling Choices in Quasigroup Completion: SAT vs. CSP". In AAAI'04 Proceedings, San José ,California, USA, July 2004.

- Iván Dotú, Álvaro del Val and Manuel Cebrián, "Redundant Modeling for the QuasiGroup Completion Problem". In CP'03 Proceedings, Kinsale, Ireland,

September 2003.

- Iván Dotú, Álvaro del Val and Manuel Cebrián, "Channeling Constraints and Value Ordering in the QuasiGroup Completion Problem". In IJCAI'03 Proceedings, pages 1372-1373, Acapulco, México, August 2003.

LS for Scheduling Social Tournaments

- Iván Dotú and Pascal Van Hentenryck, "Scheduling Social Tournaments Locally". To appear in AI Communications Special Issue on Constraint Programming for Planning and Scheduling, 2006.
- Iván Dotú, Álvaro del Val and Pascal Van Hentenryck, "Scheduling Social Tournaments". In Proceedings of CP-05, Sitges, Spain, October 2005.
- Iván Dotú and Pascal Van Hentenryck, "Scheduling Social Golfers Locally". In CPAIOR'05 Proceedings, Prague, May 2005.

Genetic Algorithms for the Golomb Ruler Problem

- Iván Dotú and Pascal Van Hentenryck, "A Simple Hybrid Evolutionary Algorithm for Finding Golomb Rulers". In IEEE CEC'05 Proceedings, Edimburgh, September 2005.

Scatter Search and Final Hybrid

- Carlos Cotta, Iván Dotú, Antonio J. Fernández and Pascal Van Henteryck, "A Memetic Approach for Golomb Rulers". To appear in Proceedings of PPSN'06, Reykjavik, Iceland, 2006.

Others

- Iván Dotú and Pascal Van Hentenryck, "A Note on Low Autocorrelation Binary Sequences". To appear in Proceedings of CP'06, Nantes, France, September 2006.

- Manuel Cebrián and Iván Dotú, "GRASP-Evolution for CSPs". To appear in Proceedings of GECCO'06, Seattle, USA, July 2006.
- Manuel Cebrián and Iván Dotú, "A simple Hybrid GRASP-Evolutionary Algorithm for CSPs". In Proceedings of LLCS'05 Workshop in CP-05, Sitges, Spain, October 2005.
- Iván Dotú, Juan de Lara, "Rapid Prototyping by Means of Meta-Modelling and Graph Grammars. An Example with Constraint Satisfaction". In Jornadas de Ingeniera del Software y Bases de Datos, JISBD-03. Alicante, Spain, November 2003.

Under Submission

- Carlos Cotta, Iván Dotú, Antonio J. Fernández and Pascal Van Henteryck, "Scheduling Social Golfers with Memetic Evolutionary Programming". Submitted to HM'06, Canary Islands, October 2006.

Introducción

La Optimización Combinatoria es una rama de la optimización en matemática aplicada y de la informática, relacionada con la investigación operativa, la teoría de algoritmos y la teoría de complejidad computacional, que se encuentra en la intersección de varios campos, tales como la inteligencia artificial, las matemáticas y la ingeniería del software. Los problemas de optimización combinatoria suelen consistir en encontrar valores para un conjunto de variables que están restringidas por un conjunto de restricciones, en algunos casos para optimizar una función dada (optimización) y en otros tan solo para encontrar una solución válida (satisfacción). Los algoritmos de optimización combinatoria resuelven instancias de problemas considerados difíciles en general gracias a una exploración inteligente del espacio de búsqueda, en parte reduciéndolo, en parte recorriéndolo de una forma eficiente.

Motivación

El objetivo de esta tesis es mostrar que diferentes enfoques pueden ser más adecuados para diferentes problemas, y que las técnicas híbridas que incorporan mecanismos de distintos paradigmas pueden beneficiarse de sus ventajas e intentar minimizar sus defectos. Todo esto se muestra en esta tesis con la resolución de problemas difíciles de optimización combinatoria como completitud de cuasigrupos, golfista social, Golomb rulers, usando varias técnicas, que dan lugar al desarrollo de un algoritmo híbrido para encontrar Golomb rulers, que incorpora aspectos de algoritmos genéticos, búsqueda local, programación con restricciones e incluso clustering. Como se desprende de esta enumeración, nuestro interés está en los algoritmos de optimización combinatoria que se consideran dentro del campo de la Inteligencia Artificial (aunque es cierto que la linea que lo separa del campo de la investigación operativa es muy fina), en vez de en algoritmos de investigación operativa. Así pues, métodos como la programación entera o el "Branch-and-Bound" que han sido ampliamente estudiados para problemas de optimización, no van a ser, sin embargo, estudiados en esta tesis.

El paradigma de la programación con restricciones es un marco muy útil y muy

estudiado para expresar muchos problemas de interés para la Inteligencia Artificial. El primer trabajo de investigación presentado aquí trata la modelización de problemas de restricciones (CSPs), en concreto para un problema muy concocido, llamado *Quasigroup Completion Problem* (QCP). Desde este problema y comparando varios modelos y métodos de resolución, somos capazes de extraer importantes conclusiones para un tipo de problema más general como es el de los problemas de permutaciones. También es sabido el interés en la comparación entre técnicas de CSP y de SAT; discutir cual es más adecuada para ciertos tipos de problema. Nosotros realizamos esta comparación para este problema en concreto.

La búsqueda local es conocida como una técnica poderosa para resolver, especialmente, porblemas de optimización, así como problemas con espacios de búsqueda significativamente grandes. El segundo trabajo presentado en la tesis aborda el modelado y resolución de calendarización de torneos sociales, más concretamente el "Social Golfer Problem". Los resultados aquí presentados son significativamente superiores a otros métodos complejos que se encuentran en la literatura. Además, motiva el tema de la simetría en la búsqueda local y presenta una heurística simple e inteligente para generar soluciones iniciales que mejora la eficiencia del algoritmo.

Los algoritmos genéticos son algoritmos basados en poblaciones que imitan procesos biológicos. Los algoritmos meméticos son híbridos que introducen búsqueda local para producir mejores resultados y converger a soluciones de mayor calidad. El trabajo de investigación en este caso trata de resolver un problema de optimización combinatoria muy difícil conocido como Golomb Ruler. La investigación desarrollada aquí se centra en el modelado y resolución de Golomb Rulers óptimos y cuasi-óptimos, y produjo resultados de gran calidad que son consistentemente superiores a los producidos por otros algoritmos genéticos que se encuentran en la literatura.

Finalmente, enriquecemos un algoritmo memético conocido como Scatter Search con la introducción de técnicas de programación con restricciones y clustering para mejorar todavía má sa los ya de por sí buenos resultados de la investigación anterior sobre el Golomb Ruler Problem.

En las próximas secciones introducimos los problemas estudiados en esta tesis, establecemos los límites de la misma y presentamos sus contribuciones principales.

Problemas estudiados

Muchos problemas de la vida real se encuentran dentro de la categoría de problemas de optimización combinatoria. En esta tesis resolvemos diferentes problemas con diversas técnicas y finalmente desarrollamos un híbrido que las engloba a todas ellas.

El problema de completitud de cuasigrupos (QCP) es uno de los más competitivos problemas de combinación, y ha sido el centro de reciente interés dentro del área de la programación con restricciones [101]. Tiene una ancho rango de aplicaciones prácticas como el enrutado de longitud de onda libre de conflictos en redes ópticas de ancha banda, diseño estádistico, códigos de corrección de errores [101]; se ha considerado un problema que puede estar en un lugar entre las instancias puramente aleatorias y los problemas con gran estructura [100]; su estructura de problema de múltiples permutaciones [229, 118] es común a muchos otros problemas de satisfacción de restricciones. Así pues, soluciones que resulten efectivas para QCPs tiene muchas posibilidades de ser útiles en otros problemas de estructura similar.

El problema del "Social Golfer" ha atraido un interés significativo desde que se incluyó en `sci.op-research` en Mayo de 1998. Es un problema altamente combinatorio y simétrico, y no es sorprendente que haya atraido tanta atención en la comunidad de la programación con restricciones (e.g., [72, 209, 178, 200, 199, 13, 184]). De hecho, destapa aspectos fundamentalmente interesantes en modelización y rotura de simetrías, y se ha convertido en un problema estándar para evaluar métodos de rotura de simetrías. Recientes investigaciones [13, 184]) se acercan al problem del "Social Golfer" usando esquemas innovadores, elegantes, pero también complefos, de rotura de simetrías.

Encontrar "Golomb rulers" es un problema combinatorio extremadamente complicado que ha recibido una atención considerable en las últimas décadas. Este problema tiene aplicaciones prácticas en gran variedad de campos incluyendo radiocomunicaciones ([27, 114]), cristalografía de rayos X ([26]), teoría de códigos ([56, 139]), y radio- astronomía. Además, debido a su extrema naturaleza combinatoria[3] ha llegado a ser un problema estándar para evaluar y comparar una gran variedad de

[3]La búsqueda de un "Golomb ruler" para 19 marcas tardó aproximadamente 36,200 CPU horas en una Sun Sparc workstation usando un algoritmo muy especializado [56].

métodos de búsqueda. En concreto, algoritmos genéticos, programación con restricciones, búsqueda local, y sus hibridizaciones han sido aplicados a este problema (e.g., [43, 76, 173, 176, 210, 213]).

En esta tesis vamos a introducir métodos puros para la resolución de problemas de combinatoria tales como los problemas de satisfacción de restricciones (CSPs), el problema de la satisfacibilidad (SAT), la búsqueda local (LS), y los algoritmos genéticos (GAs). También introduciremos métodos híbridos, como CSP y LS, GA y LS (conocido como algoritmos meméticos) y GAs que incorporan técnicas de programación con restricciones. Vamos a presentar trabajos de investigación en éstos paradigmas para resolver problemas de combinación difíciles, para finalmente desarrollar un híbrido que incorpora todas esas técnicas para producir resultados de gran calidad para uno de éstos problemas. También incluimos un apénice donde introducimos brevemente dos técnicas que se usan en el último híbrido desarrollado, en concreto "Greedy Randomized Adaptive Search Procedures" (GRASP) y Clustering.

Contribuciones

Este trabajo de investigación intenta demostrar que diferentes técnicas pueden ser más adecuadas para diferentes problemas ed combinación, y, en vez de centrar tanto esfuerzo en desarrollar técnicas muy especializadas en cada campo, es preferible concentrarnos en la resolución de problemas con la técnica que sea más adecuada. También nos interesa mostrar como todas esas técnicas puede cooperar en un único algoritmo para producir resultados de gran calidad.

Las principales contribuciones de este trabajo son varias. Esta tesis trata de resolver problemas, y en ese sentido cada capítulo presenta resultados líderes en calidad en la literatura para varios problemas. Además, presentamos también un algoritmo híbrido que, aunque esta orientado al problema que tratamos, es fácilmente generalizable para poder ser aplicado a diferentes problemas de combinatoria.

Por lo tanto, el trabajo presentado en esta tesis contribuye al estado del arte al presentar resultados de gran calidad para el problema de completitud de cuasigrupos, el Social Golfer y el Golomb ruler; también es una contribución el desarrollo de un

algoritmo híbrido que introduce aspectos de CSPs y de clustering en el esquema de un algoritmo memético. Así pues, las contribuciones principales de esta tesis son:

Completitud de Cuasigrupos con búsqueda completa

Primero, presentamos varias técnicas que conjuntamente nos permiten resolver QCPs significativamente más grandes que los presentados previamente en la literatura. En concreto, [101] afirma que QCPs de orden 40 no se pueden resolver con técnicas puras de programación con restricciones, pero sí con técnicas híbridas que combinen la programación con restricciones co la programación entera de investigación operativa. Aquí mostramos que un método puro puede resolver varios problemas de orden 45 cercanos a la fase de transición, que corresponde con el pico de dificultad. Nuestro método está construido sobre conceptos como el del modelado redundante [36] con modelos primal y dual y restricciones de canalización para unirlos [229], pero con algunas modificaciones innovadoras. Adicionalmente presentamos una nueva heurística de ordenación de valores que resulta muy efectiva, y que podría serlo también para muchos otros problemas de permutaciones múltiples. Finalmente, mostramos como cierta restricciones redundantes se pueden utilizar para compilar arco consistencia en "forward checking", lo que significa asegurar que el último tendrá el mismo poder de propagación que el primero pero con menos chequeos de consistencia.

Es interesante recalcar que nuestro modelo no sólo incluye restricciones binarias, lo que parece ir en contra del conocimiento común acerca de sus limitaciones —al contrastar con el uso de restricciones no binarias como alldiff [188]— en este problema [215].

Comparación SAT vs. CSP

En segundo lugar, realizamos un estudio sistemático de las opciones de modelado para la completitud de cuasigrupos, probando una gran variedad de resolutores y heurísticas en diversas codificaciones SAT y CSP. La clara ganadora es la codificación 3D de SAT, especialmente con el resolutor Satz [144], seguido del resolutor

Satzoo [62] en la misma codificación. Debido a que estos dos resolutores son bastante diferentes, la codificación 3D aparece como muy robusta. Por otro lado, los modelos CSP son muy inferiores en los dos resolutores probados, y los modelos SAT generados de manera estándar a partir de los modelos CSP son sencillamente demasiado grandes en la práctica. Todo esto sugiere que la codificación 3D puede ser muy competitiva para otros problemas de permutación (muchos de los cuales aparecen en problemas prácticos [118]) si los comparamos a los habitualmente preferidos modelos de canalización.

Parece que hay una doble explicación para lo anterior. Primero, podemos demostrar que la codificación 3D (que es básicamente el "SAT channelling model" de [118] extendido para permutaciones múltiples y modelos duales) capturar exactamente los modelos de canalización de QCPs definidos, pero de una forma mucho más concisa: colapsando variables primales y duales. Además, podemos demostrar que la codificación 3D captura la codificación SAT de soportes del modelo de canalización, y, por lo tanto, por el resultado de [89], la propagación unitaria en 3D consigue el mismo nivel de poda que la arco-consistencia en el modelo de canalización CSP. Parece que estos resultados son fácilmente extrapolables a otros problemas de permutación que han recibido gran atención reciéntemente ([35, 229, 118]). En segundo lugar, hemos identificado empíricamente la importancia crucial de la heurística de Satz para su eficacia en este dominio; lo cual se demuestra por el hecho de que, al importar esta heurística a los resolutores de CSP, se obtienen mejoras significativas.

Resolviendo el Problema del Golfista Social con Búsqueda Local

Este trabajo propone un algoritmo de búsqueda local para generar un calendario para golfistas sociales, cuyos movimientos consisten en intercambiar golfistas en la misma semana, y esta guiado por una metaheurística de tipo tabu. El algoritmo empata o mejora todas las soluciones encontradas mediante programación con restricciones para todas excepto 3 instancias. También encuentra nuevas soluciones para 11 instancias

que estaban abiertas para la programación con restricciones.[4] Además, el algoritmo resuelve prácticamente todas las instancias en pocos segundos y tarda alrededor de un minuto en las instancias restantes. También se incorpora una heurística constructiva que resuelve de forma trivial muchas instancias del tipo $impar - impar - w$, y constituye un buen punto de partida para el resto.

Las principales contribuciones de este trabajo son:

1. Muestra que la búsqueda local es un método muy efectivo para el problema del golfista social. Encuentra la primera solución para 11 instancias, y empata con la mejor solución en el resto excepto por 3 instancias. Además, casi todas las instancias se resuelven en apenas unos segundos.

2. Demuestra que el algoritmo de búsqueda local usa un modelo natural del problema sin esquemas complejos de rotura de simetrías. De hecho, no tiene para nada en cuenta las simetrías, dando lugar a un algoritmo mucho más simple que los desarrollados dentro de la búsqueda completa para CSPs, desde ambos, el punto de vista conceptual y el de la implementación.

3. Los resultados experimentales indican cierta complementariedad entre la búsqueda completa y la búsqueda local dentro de la programación con restricciones, ya que unas instancias difíciles para una tecnología son fáciles para la otra.

Encontrando "Golomb Rulers" Cuasi-Óptimos con un Algoritmo Evolutivo Híbrido

Este trabajo propone un nuevo algoritmo evolutivo híbrido para encontrar "Golomb rulers" cuasi-óptimos en un tiempo razonable. El algoritmo incorpora una búsqueda local dentro de un algoritmo genético, y sobrepasa a algoritmos genéticos anteriores, así como a algoritmos de programación con restricciones híbridos de búsqueda completa y local. En concreto, el algoritmo encuentra reglas de hasta 13 marcas

[4]Para el estado actual de las distintas instancias, véase la página web de Warwick Harvey `http://www.icparc.ic.ac.uk/wh/golf`.

rápidamente, y también fue capaz de encontrar el óptimo para 14 marcas, lo que estaba fuera del alcanze de los mencionados algoritmos. El algoritmo también encuentra reglas cuasi-óptimas en un tiempo razonable, indicando la efectividad de los agoritmos evolutivos híbridos en esta aplicación altamente combinatoria. Es de particular interés la simplicidad conceptual y la elegancia del algoritmo.

A pesar de que hay soluciones de mayor número de marcas con otros enfoques de búsqueda completa, los algoritmos evolutivos tiene la ventaja de generar soluciones de alta calidad en poco tiempo. Esta es también una de las mayores contribuciones, generar soluciones de gran calidad (mejorando los resultados de otros enfoques evolutivos anteriores) en pocos segundos o minutos.

La mayor contribución técnica radica en un nuevo híbrido que se centra en la validez. De hecho, el paso principal del algoritmo evolutivo es encontrar reglas de una longitud específica (o menor) usando violaciones de restricciones para guiar la búsqueda. Las reglas cuasi-óptimas se encuentra resolviendo una secuencia de problemas de satisfacción.

Scatter Search y el Híbrido Final

Aquí presentamos un algoritmo evolutivo híbrido para encontrar "Golomb rulers" óptimos o cuasi-óptimos. Este algoritmo usa un enfoque indirecto y uno directo en diferentes etapas de la búsqueda. Más concretamente, el enfoque indirecto se usa en las fases de inicialización y re-inicialización de la población, haciendo uso de ideas prestadas del enfoque basado en GRASP publicado en [43]. El enfoque directo se usa en las etapas de recombinación y mejora local; en concreto, el método de mejora local está basado en una búsqueda tabu. Los resultados experimentales muestran que este algoritmo es capaz de encontrar reglas óptimas hasta 13 marcas sistemáticamente. Ahora se encuentran reglas óptimas de hasta 15 marcas (incluida). Además, el algoritmo genera reglas de 16 marcas que son muy crecanas al óptimo (1.1% lejos), así pues, mejorando sensiblemente el estado del arte.

En este momento, intentamos mejorar la eficacia del algoritmo de diferentes maneras:

- **Búsqueda Completa:** usamos técnicas de búsqueda completa para combinar individuos de la población, haciendo uso de mecanismos de la programación con restricciones tales como la propagación. Esta técnica no implica necesariamente que se generen individuos de gran calidad, pero si es, sin embargo, capaz de producir soluciones válidas e incluso óptimas.

- **Clustering:** esta técnica se introduce en este caso para conseguir mayor diversidad en la población. En vez de mantener los mejores individuos en la población, dividimos ésta en distintos clusters y elegimos los mejores individuos de cada cluster.

Estas dos técnicas introducidas nos permiten, por una parte, crear un novedoso algoritmo híbrido que es fácilmente generalizable para resolver muchos otros problemas de combinatoria, y, por otra parte, conseguir resultados de mayor calidad a los presentados antes de dichas incorporaciones, que ya eran resultados de máxima calidad para este dominio.

Los resultados son verdaderamente sobresalientes, ahora somos capaces de resolver reglas de 16 marcas, y encontrar el óptimo para hasta 14 marcas sistemáticamente. Además, el algoritmo se ha probado usando distintos conjuntos de parámetros referentes al clustering y los resultados son consistentemente superiores a los del algoritmo previo sin mejoras.

Publicaciones

Finalmente presentamos las principales publicaciones que ha generado esta tesis. Las vamos a clasificar en los distintos capítulos a los que pertenecen dentro de la tesis. Además, se aade una sección de "Otros" en la que se incluyen otras publicaciones obtenidas durante el tiempo de doctorado que no han sido finalmente reflejadas en esta tesis y otra de "Esperando Notificación", para artículos que han sido enviados a conferencias y se está esperando la notificación.

CSP y SAT

- Carlos Ansótegui, Álvaro del Val, Ivń Dotú, Cesar Fernández y Felip Manya, "Modeling Choices in Quasigroup Completion: SAT vs. CSP". In AAAI'04 Proceedings, San José ,California, USA, July 2004.

- Iván Dotú, Álvaro del Val and Manuel Cebrián, "Redundant Modeling for the QuasiGroup Completion Problem". In CP'03 Proceedings, Kinsale, Ireland, September 2003.

- Iván Dotú, Álvaro del Val and Manuel Cebrián, "Channeling Constraints and Value Ordering in the QuasiGroup Completion Problem". In IJCAI'03 Proceedings, pages 1372-1373, Acapulco, México, August 2003.

Búsqueda Local para Torneos Sociales

- Iván Dotú and Pascal Van Hentenryck, "Scheduling Social Tournaments Locally". To appear in AI Communications Special Issue on Constraint Programming for Planning and Scheduling, 2006.

- Iván Dotú, Álvaro del Val and Pascal Van Hentenryck, "Scheduling Social Tournaments". In Proceedings of CP-05, Sitges, Spain, October 2005.

- Iván Dotú and Pascal Van Hentenryck, "Scheduling Social Golfers Locally". In CPAIOR'05 Proceedings, Prague, May 2005.

Algoritmos Evolutivos para el "Golomb Ruler Problem"

- Iván Dotú and Pascal Van Hentenryck, "A Simple Hybrid Evolutionary Algorithm for Finding Golomb Rulers". In IEEE CEC'05 Proceedings, Edimburgh, September 2005.

Scatter Search y el Híbrido Final

- Carlos Cotta, Iván Dotú, Antonio J. Fernández and Pascal Van Henteryck, "A Memetic Approach for Golomb Rulers". To appear in Proceedings of PPSN'06, Reykjavik, Iceland, 2006.

Otros

- Iván Dotú and Pascal Van Hentenryck, "A Note on Low Autocorrelation Binary Sequences". To appear in Proceedings of CP'06, Nantes, France, September 2006.

- Manuel Cebrián and Iván Dotú, "GRASP-Evolution for CSPs". To appear in Proceedings of GECCO'06, Seattle, USA, July 2006.

- Manuel Cebrián and Iván Dotú, "A simple Hybrid GRASP-Evolutionary Algorithm for CSPs". In Proceedings of LLCS'05 Workshop in CP-05, Sitges, Spain, October 2005.

- Iván Dotú, Juan de Lara, "Rapid Prototyping by Means of Meta-Modelling and Graph Grammars. An Example with Constraint Satisfaction". In Jornadas de Ingeniera del Software y Bases de Datos, JISBD-03. Alicante, Spain, November 2003.

Esperando Notificación

- Carlos Cotta, Iván Dotú, Antonio J. Fernández and Pascal Van Hentenryck, "Scheduling Social Golfers with Memetic Evolutionary Programming". Submitted to HM'06, Canary Islands, October 2006.

Part I

Formal Preliminaries

Chapter 2

Pure Approaches

In this chapter we are going to introduce the main frameworks this thesis deals with: Constraint Satisfaction Problems (CSPs) and the algorithms to solve them both Complete Search (CP) and Local Search (LS), the Satisfiability Problem (SAT) and Evolutionary Computation (EC). Note that the SAT problem will not be part of the final hybrid presented in this thesis, however, it is important for its relevancy within the CSP framework, and also because it has been used in preliminary work for this thesis. This chapter is thus devoted to the introduction of pure approaches.

2.1 CSPs

We now review the framework of *Constraint Satisfaction Problem* (CSP) and some of the main available search methods and techniques.

2.1.1 Definitions

Definition 2.1. A Constraint Satisfaction Problem (CSP) $P = (X, D, C)$ is defined by a set of variables $X = \{x_1, ..., x_n\}$, a set of n finite value domains $D = \{D_1, ..., D_n\}$, and a set of c constraints or relations $C = \{R_1, ..., R_c\}$.

Definition 2.2. A constraint R_x is a pair $(vars(R_x), rel(R_x))$ defined as follows:

- $vars(R_x)$ is an ordered subset of the variables, called the constraint *scheme*. The size of $vars(R_x)$ is known as the *arity* of the constraint. A *binary* constraint has arity equal to 2; a *non-binary* constraint has arity greater than 2. Thus, a *binary CSP* is a CSP where all constraints have arity equal or less than 2.

- $rel(R_x)$ is a set of tuples over $vars(R_x)$, called the constraint *relation*, that specifies the allowed combinations of values for the variables in $vars(R_x)$. A *tuple* over an ordered set of variables $X = \{x_1, ..., x_k\}$ is an ordered list of values $(a_1, \ldots, a_k)$ such that $a_i \in dom(x_i), i = 1, \ldots, k$.

Solving a CSP means finding an assignment for each variable that does not violate any constraint.

Definition 2.3. A constraint graph associates a vertex with each variable and has an edge between any two vertices whose associated variables are related by the same constraint.

Definition 2.4. An assignment of values to variables is a set of individual assignments, $\{X_i \leftarrow v_i\}$, where no variable occurs more than once.

An assignment can be either *partial*, if it includes a proper subset of the variables, or *total*, if it includes every variable.

Definition 2.5. We say that an assignment is consistent if it does not violate any constraint.

A *solution* to a CSP is then a total consistent assignment. Thus, the task of finding a solution to a CSP or proving that it does not have any can be referred as the task of *achieving total consistency*.

Example 1. *The n-queens problem is usually expressed as a CSP. The problem consists on placing n queens on an $n \times n$ chess board, in such a way that no two queens attack each other. It can be naturally expressed as a binary CSP where each variable is associated with a board row, and its assignment denotes the board column where the queen is placed. Constraints restrict the valid positions for each pair of queens:*

two queens cannot be placed in the same column nor in the same diagonal (note that they cannot be placed in the same row either, although this is already guaranteed by the representation).

2.1.2 Constraint Optimization Problems

With this same technology we can model constraint optimization problems. These are constraint satisfaction problems where not only we search for a solution but for the one that optimizes a given criterion:

Definition 2.6. A Constraint Optimization Problem $P = (X, D, C, f)$ is defined by a set of variables $X = \{x_1, ..., x_n\}$, a set of n finite value domains $D = \{D_1, ..., D_n\}$, a set of c constraints or relations $C = \{R_1, ..., R_c\}$, and a function f to be optimized (minimized or maximized).

Note that the function f represents an optimization criteria, it referres to the quality of the solution. Sometimes, it can be presented as a *soft* constraint which the solution can violated but that decreasing its violations increases the quality of the solution. However, we are going to assume that the criterion is a function f without loss of generality.

2.1.3 Constraint algorithms: Complete Search

Once a problem of interest has been formulated as a *constraint satisfaction problem*, a solution can be found with a general purpose constraint algorithm. CSPs are NP-complete [84]. Many constraint algorithms are based on the principles of search and deduction. Complete Search stands for the fact that the search covers the whole search space, and thus, it is guaranteed to find a solution. The most effective constraint satisfaction algorithms are based on:

Search based backtracking

The term *search* is used to characterize a large category of algorithms which solve problems by guessing an operation to perform or an action to take, possibly with the

help of a heuristic. A good guess results in a new state that is nearer the goal. If the operation does not result in progress towards the goal, it can be retracted and another guess made. For CSPs, search is exemplified by the backtracking algorithm. Backtracking search assigns a value to an uninstantiated variable, thereby extending the current partial solution. It explores the search space in a depth-first manner. If no legal value can be found for the current variable, the previous assignment is retracted, which is called a *backtrack*. In the worst case, the backtracking algorithm requires exponential time in terms of number of variables, but only linear space. The backtracking algorithm was first described more than a century ago, and since then it has been reintroduced several times [24].

Consistency based algorithms

Other kinds of algorithm to solve a CSP rely on applying reasoning that transforms the problem into an equivalent but more explicit form. The most frequently used type of these algorithms is known as constraint propagation or consistency enforcing algorithms [148, 81]. These procedures transform a CSP problem by deducing new constraints, tightening existing constraints, and removing values from variable domains. In general, a consistency enforcing algorithm will extend some partial solution of a subproblem to some surrounding subproblem by guaranteeing a certain degree of local consistency, defined as follows.

Definition 2.7. A CSP problem is 1-*consistent* if the values in the domain of each variable satisfy all the unary constraints.

Definition 2.8. A problem is *k-consistent*, $k \geq 2$, iff given any consistent partial instantiation of any $k-1$ distinct variables, there exists a consistent instantiation of any single additional variable [80].

The terms *node-*, *arc-*, and *path-consistency* [148] correspond to 1-, 2-, 3-consistency, respectively.

Definition 2.9. Given an ordering of the variables, a problem is *directional* k-consistent iff any subset of $k-1$ variables is k-consistent relative to every single variable that succeeds the $k-1$ variables in the ordering [52].

A problem that is k-consistent for all k is called *globally* consistent.

The complexity of enforcing i-consistency is exponential in i [42]. Considering this high cost, there is a trade-off between the effort spent in pre-processing (enforcing local consistency at each search node) and the time savings that it may produce.

Regarding CSPs (and also binary CSPs), arc-consistency –or weaker forms of arc-consistency– are commonly used to detect and remove unfeasible values before and during the search. Their interest is due to having low time and space requirements.

Look-ahead Algorithms

Search algorithms can be combined with consistency enforcement algorithms detecting dead-ends at earlier levels in the search tree. The idea is to enforce local consistency at each node during the search. If the current node is in a dead-end and the search does not detect it, achieving some level of consistency may lead to its discovery, saving the search from visiting unsuccessfully deeper nodes of the current subtree. This process is generally called *lookahead* or *propagation* of the current assignment.

In practice, algorithms that perform a limited amount of propagation are among the most effective. *Forward Checking* (FC) [110] is a simple, yet powerful algorithm for constraint satisfaction. It propagates the effect of each assignment by pruning inconsistent values from future variables[1]. When a future domain becomes empty, FC backtracks because there is no value for one (or more) future variable consistent with the current partial assignment.

On the other hand, there is an algorithm that maintains arc-consistency during search (denoted MAC [195]) which requires more computational effort than FC at each search state. MAC filters arc-inconsistent values simplifying the search space, and if this propagation process causes an empty domain, then the subproblem is unsolvable. Given that MAC can prune more values than FC, it has better dead-end detection capabilities. This means that MAC can backtrack in nodes where FC would continue searching at deeper levels. In general, MAC is not the most effective algorithm on easy problems because tree reduction does not pay off the computational

[1]Future variable is the term we use to denote a variable that has not been instantiated yet at a given search node, while past variable is a variable that has already been instantiated

overhead, while on hard problems, maintaining arc-consistency is often cost effective.

Look-back Algorithms

There are some other ways in which the basic *Backtracking* (BT) strategy can be improved by keeping track of previous phases of search (for this reason they are known as look-back algorithms):

Backmarking (BM) [86] avoids the repetition of some consistency checks. When BT assigns the current variable it checks the consistency of this assignment with past variables. If any of these tests fails, BM records the point of the failure in a *maximum check level* array. Suppose that the algorithm backtracks up to some variable, then deepens in the tree and attempts again to assign the same variable. In this situation it is known that the current assignment is consistent with past variables up to the *maximum check level* as far as their assignment has not been changed. BM avoids the repetition of these already performed checks.

Backjumping (BJ) [87], improves BT by making a more suitable decision of which variable has to backtrack to. BJ only differs from BT at those nodes where a dead-end is detected. Instead of backtracking to the most recently instantiated variable, BJ *jumps* back to the deepest past variable that the current variable was checked against, which corresponds to the earliest constraint causing the conflict. When the current variable is not responsible for the dead-end detection, no jump is done. In that case BJ backtracks chronologically.

Conflict-Directed Backjumping (CBJ) [183] improves BJ by following a more sophisticated jumping strategy. The conflict set of a variable is formed by past variables with which a consistency check failed with some value of the considered variable. When all the values have been attempted for the current variable, CBJ jumps to the deepest variable in its conflict set. This variable is removed from the conflict set of the current variable, and this new conflict set is added to the conflict set of the variable it jumps to. With this approach, jumps can be done at those nodes where backtracking occurs not because a dead-end is detected, but because all values have already been attempted. In addition, more than one jump can be done along the same path from a detected dead-end to the root.

Learning Algorithms

There are other algorithms that use a technique called constraint recording or *learning*.

An opportunity to learn new constraints is presented whenever the backtracking algorithm encounters a dead-end. Had the problem included an explicit constraint prohibiting this conflict set, the dead-end would have never been reached. The learning procedure records a new constraint that makes explicit an incompatibility that already existed implicitly in a given set of variable assignments. Note therefore that nothing *new* is learnt, except information that logically follows from the specification of the problem. These new constraints are usually called *nogoods* .

In learning algorithms, the savings from possibly reducing the amount of search by finding out earlier that a given path cannot lead to a solution must be balanced against the cost of processing at each search node a more extensive database of constraints.

Learning algorithms may be characterized by the way they identify smaller conflict sets. Learning can be *deep* or *shallow*. Deep learning records only the minimal conflict sets. Shallow learning allows nonminimal conflict sets to be recorded as well. Learning algorithms may also be characterized by how they bound the arity of the constraints recorded. Constraints involving many variables are less frequently applicable, require additional memory to store, and are more expensive to consult than constraints having fewer variables. The algorithm may record a single nogood or multiple nogoods per dead-end, and it may allow learning at leaf dead-ends only or at internal dead-ends as well.

Heuristics

If backtrack is used to solve CSPs, then another issue is the order in which variables are considered for instantiation. There is overwhelming evidence that the ordering in which variables are chosen for instantiation can have substantial impact on the algorithms' efficiency (see e.g. [51]). The same happens with the order in which an algorithm tries the domain values for the current variable. Heuristics for variable or value ordering can be grouped into two categories:

- Static orderings: A static heuristic establishes an ordering before search starts, and maintains this ordering throughout all of the search.
- Dynamic orderings: A dynamic heuristic makes selections dynamically during search.

A well-known static heuristic involves ordering variables by their degree in the constraint graph. The idea is to consider first the most constrained variables (those with more edges in the constraint graph) because they are likely to be more difficult to assign. Inconsistencies are expected to be found at early tree levels, where recovering from mistakes is less costly. Variables with few constraints have more freedom in the values they can take, so it is easier to find a good value for them. With this heuristic their assignment is delayed to deep tree levels. This static variable ordering is denoted *maximum degree ordering heuristic*.

Dynamic variable orderings are generally much more effective than static ones, since they can take into account the current state of the search to decide what to do next. The most popular variable ordering heuristic selects the variable with the minimum number of values in its current domain [110]. This heuristic, denoted *minimum domain* (MD), is usually applied with look-ahead algorithms, because the actual size of domains is available to the heuristic at no additional cost.

The performance of MD is often improved with the addition of some information from the graph topology. For instance, [83] breaks ties among variables in the MD heuristic by using a *graph degree*. [22] select the variable having the lowest ratio *domain cardinality divided by degree* in an attempt to combine both dynamic and static information. Other approaches also consider *dynamic* degree information, as the constraint graph is simplified as search proceeds.

Value ordering has not attracted the attention of the CSP community as much. It is generally believed that good values are those which are more likely to participate in solutions. This idea is developed in [52] where they propose a value ordering heuristic which relies on a tree-relaxation of the problem to estimate the goodness of a value.

A different approach for value ordering is followed in [138, 88, 83]. Within the context of look-ahead algorithms, values are ordered by the pruning effect that they

have on future domains. This approach requires the propagation of each possible assignment to obtain the size of the resulting domains.

While there are quite successful domain-independent variable ordering heuristics, the current state of research suggest that good value ordering heuristics are likely to be highly problem-specific.

Optimization Techniques

Solving Optimization Problems with complete search techniques usually implies borrowing techniques from Operations Research (OR) such as Branch-and-Bound (BB) to intertwin them with constraint algorithms.

We are not going to give a comprehensive review of these techniques since it is not the focus of this thesis (hybrid optimization methods will be described in the next chapter), but we are going to present some of the most popular techniques in the literature.

Optimization problems can be solved using a number of different techniques within the constraint satisfaction paradigm. Full lookahead ([110]) is popular because it is easy to implement and works on a large variety of problems. Essex algorithms ([220]), which are a variation on Freuder's solution synthesis techniques[2] ([80]), significantly ouperform lookahead algorithms on the N-Queens problem. Of special interest is the technique presented in ([17, 16]) where constraint satisfaction, branch-and-bound and solution synthesis techniques are integrated.

[2]Solution synthesis is a method used to generate all solutions to a CSP. That is, all assignments of values to variables that satisfy the problem's constraints produced by a solution synthesis algorithm. Often, this set of solutions can be further judged according to some separate criteria to obtain the optimal solution.

2.1.4 Local Search

Local search is a different paradigm for solving combinatorial optimization problems. It differs from the constraint satisfaction techniques that perform a complete search in the way in which the search is performed. We can say it sacrifices completeness in return for better performance in a number of problems. Instead of performing a complete search of the search-tree which guarantees finding the optimal, it explores local neighborhoods to find near optimal solutions fast. In some problems it can reach the optimum although it cannot be proven by the mechanism itself. It is usually well-suited for large-scale problems and for optimization problems, rather than for satisfiability.

Local Search evolved on its own but it was quickly incorporated as a class of algorithm to solve CSPs. We now review the main aspects of this framework:

The LS Algorithm

A typical LS algorithm starts with an initial solution (either randomly or heuristically generated) and it moves to neighbooring solutions in order to optimize the value of a function f. This function f measures the quality of a solution. In constraint satisfaction it is usually the number of constraint violations; thus, the algorithm will try to minimize f, reaching a solution when $f = 0$ (no constraint violations). In optimization problems it is usually the function to be optimized, although it can be mixed with constraint violations if we allow the algorithm to move through unfeasible solutions.

The main operation of a LS algorithm is *moving* from a solution s to one of its neighbors. This new solution s' to which the algorithm will move, can be found within the set of neighbors $N(s)$ called *neighborhood* of s. Sometimes, a legality of a move might be defined. In that case, the LS algorithm will identify which moves are legal at a certain time, and then choose one of them as the new solution. Thus, the algorithm selects (S selection operator) a legal neighbor (L legality operator) from the neighborhood $N(s)$ of s.

Figure 2.1 depicts a generic LS algorithm. The search starts from an initial state

```
1.   function GenericLocalSearch()
2.       s ← InitialSolution();
3.       s* ← s;
4.       k ← 0;
5.       while k ≤ maxIt
6.           if satisfiable(s) and f(s) < f(s*) then
7.               s* ← s;
8.           s ← S(L(N(s), s), s);
9.           k++;
10.      return s*;
```

Figure 2.1: A Generic Local Search Algorithm

in line 2, and performs a certain number of iterations (line 5). Lines 6 and 7 are used to keep track of the best solution found so far, and line 8 performs the move to the new solution.

Formalizing LS Concepts

In this section we are going to summarized some concepts within the LS framework. We have already explained that LS evolved independently from CSPs and so we are going to give introduce some general concepts.Let us assume that we have a combinatorial optimization problem $\mathcal{P}$ of the form:

$$\begin{aligned} &\text{minimize } f(\vec{x}) \text{ subject to} \\ &C_1(\vec{x}) \\ &\vdots \\ &C_m(\vec{x}) \end{aligned}$$

where $\vec{x}$ is a vector of n decision variables, f is the objective function that represents the quality of a solution, and $C_1, \cdots, C_m$ are the constraints to which the variables

are subject. Based on all that we can now define:

Definition 2.10. A *solution* to $\mathcal{P}$ is an assignment $\hat{x}$ of all the variables in $\vec{x}$. The set of solutions is denoted by $\mathcal{L}_{\mathcal{P}}$.

Definition 2.11. A *feasible solution* to $\mathcal{P}$ is a solution $\hat{x}$ that satisfies the constraints $C_1, \cdots, C_m$. The set of feasible solutions is denoted by $\tilde{\mathcal{L}_{\mathcal{P}}}$.

Definition 2.12. The set of *optimal solutions* to $\mathcal{P}$, denoted by $\mathcal{L}^*_{\mathcal{P}}$ is defined as

$$\mathcal{L}^*_{\mathcal{P}} = \{s \in \tilde{\mathcal{L}_{\mathcal{P}}} \mid f(s) = \min_{k \in \tilde{\mathcal{L}_{\mathcal{P}}}} f(k)\} \tag{2.1}$$

Note that in this case we use the term solution to name a complete assignment of values to variables, and feasible solution to a solution that satisfies the constraints. Rembember than in the constraint satisfaction framework a solution corresponds to a feasible solution here.

Definition 2.13. A *search space* for $\mathcal{P}$ is a set $\hat{\mathcal{L}_{\mathcal{P}}}$ such that $\mathcal{L}_{\mathcal{P}} \subseteq \hat{\mathcal{L}_{\mathcal{P}}} \subseteq \mathcal{N}^n$.

Note that the search space may vary from one algorithm to the other. It is part of the modeling of the problem, in some cases we might want to move within the space of feasible solutions, where $\hat{\mathcal{L}_{\mathcal{P}}} = \tilde{\mathcal{L}_{\mathcal{P}}}$; or we might want to enforce some constraints and leave others to be part of the objective function f, i.e. permit violations of those constraints and try to minimize them during search. For a constraint satisfaction problem, when violations are non-existent, it means we have a solution; for constraint optimization problems it means that we have found a $feasible$ solution.

Definition 2.14. A *neighborhood* is a pair $\langle \hat{\mathcal{L}_{\mathcal{P}}}, N \rangle$ where $\hat{\mathcal{L}_{\mathcal{P}}}$ is a search space and N is a mapping $N : \hat{\mathcal{L}_{\mathcal{P}}} \longrightarrow 2^{\hat{\mathcal{L}_{\mathcal{P}}}}$ that defines set of reachable solutions $N(s) \subseteq \hat{\mathcal{L}_{\mathcal{P}}}$ from solution s.

Definition 2.15. A *solution* s is *locally optimal* with respect to $\mathcal{L}_{\mathcal{P}}$ if

$$f(s) \leq \min_{i \in N(s)} f(i)$$

The set of local optimal solutions is denoted $\mathcal{L}^+_{\mathcal{P}}$.

Escaping from *local optima* is one of the issues that has been getting the most attention within this framework, and it is the cause of LS algorithms introducing interesting legality and selection criteria.

Definition 2.16. A *neighborhood* is a pair $\langle \hat{\mathcal{L}_\mathcal{P}}, N \rangle$ where $\hat{\mathcal{L}_\mathcal{P}}$ is a search space and N is a mapping $N : \hat{\mathcal{L}_\mathcal{P}} \longrightarrow 2^{\hat{\mathcal{L}_\mathcal{P}}}$ that defines set of reachable solutions $N(s) \subseteq \hat{\mathcal{L}_\mathcal{P}}$ from solution s.

Definition 2.17. A *legality condition* L is a function $(2^{\hat{\mathcal{L}_\mathcal{P}}} \times \hat{\mathcal{L}_\mathcal{P}}) \longrightarrow 2^{\hat{\mathcal{L}_\mathcal{P}}}$ that filters sets of solutions from the search space.

Definition 2.18. A *selection rule* $S(\mathcal{M}, s)$ is a function $(2^{\hat{\mathcal{L}_\mathcal{P}}} \times \hat{\mathcal{L}_\mathcal{P}}) \longrightarrow \hat{\mathcal{L}_\mathcal{P}}$ where $\mathcal{M} = L(N(s), s)$, that chooses an element s_i from $\mathcal{M}$ and decides whether to accept it or to keep the current solution s.

Definition 2.19. A *local search algorithm* for $\mathcal{P}$ is a succession of solutions

$$s_0 \rightarrow s_1 \rightarrow \ldots \rightarrow s_k$$

such that

$$s_{i+1} = S(L(N(s_i), s_i), s_i) \;\; (1 \leq i \leq k) \tag{2.2}$$

It is very common that such a local search algorithm produces a final solution s_k that belongs to $\mathcal{L}^+_\mathcal{P}$. In the next section we are going to introduce *heuristics* and *metaheuristics*, whose role is to direct the search towards high-quality local optima, and specially those in $\mathcal{L}^*_\mathcal{P}$ if possible.

Heuristics

All the heuristics here are based on the template depicted in figure 2.1, and assuming that it receives the parameters f, N and the *legality* and *selection* rules L and S. We are also going to assume that we are always dealing with minimization problems, so that the goal is to minimize f.

Heuristics typically choose the next neighbor based on local information, basically the current solution and its neighborhood, which translates into providing different

selection mechanisms and different legality conditions. For example, we can define three different legality conditions, where N is assumed to be the neighborhood of S:

1. **function** *L-Improvement*(N, s)
2. **return** $\{n \in N \mid f(n) < f(s)\}$;

which only allows to move to a neighbor with a strictly superior quality.

1. **function** *L-ImprovementAndWalk*(N, s)
2. **return** $\{n \in N \mid f(n) \leq f(s)\}$;

which allows moves where the value of the objective function is the same.

1. **function** *L-All*(N, s)
2. **return** N;

or the last case in which any kind of move is allowed.

Systematic Heuristics This type of heuristic performs an exploration of the neighborhood in order to decide which neighbor is going to become the next solution. The main relevant ones being:

Best Neighbor: this heuristic chooses the neighbor with the best value of the objective function:

1. **function** *S-Best*(N, s)
2. $N^* \leftarrow \{n \in N \mid f(n) = \min_{s \in N} f(s)\}$;
3. **return** $\{n \in N^*\}$;

where n can be chosen randomly with probability $\frac{1}{|N^*|}$, where $\mid N^* \mid$ is the number of elements in N^*. A Best-Improvement LS algorithm can thus be specified by instantiating the generic local search in the following manner:

1. **function** *BestImprovement*(s)
2. **return** *GenericLocalSearch*$(f, N$,*L-Improvement,S-Best*$)$

First Neighbor: sometimes, the search space is too large to completely scan it in order to find the best neighbor. The First-Neighbor heuristic chooses the first neighbor which improves the value of the objective function. It assumes a function $lex(n)$ that specifies the lexicographic order of a neighbor n when scanning the neighborhood:

1. **function** *S-First*(N, s)
2. **return** $\{n \in N\}$ **minimizing** $lex(n)$;

A First-Improvement LS algorithm can thus be specified by instantiating the generic local search to use the first-neighbor heuristic as selection rule:

1. **function** *FirstImprovement*(s)
2. **return** *GenericLocalSearch*(f, N,*L-Improvement,S-First*)

Random Walks The Random Walks heuristic randomly selects a candidate from the neighborhood and decide whether to select it or not (instead of performing an exploration of the neighborhood).

Random Improvement: this is the simplest example of a random walk, it consists on accepting a neighbor if it improves the current solution:

1. **function** *S-RandomImprovement*(N, s)
2. **select** $\{n \in N\}$;
3. **if** $f(n) < f(s)$ **then**
4. **return** n;
5. **else** 6. **return** s;

In line 2, n can be randomly selected with probability $\frac{1}{|N|}$, where $\mid N \mid$ is the number of elements in N. Note also that in line 6 the current solution is returned, which means that s is implicitly part of the neighborhood. The random nature of this approach seems critical in some applications ([6]). A RandomImprovement LS algorithm can thus be specified by instantiating the generic local search in the following manner:

1. **function** *RandomImprovement*(s)
2. **return** *GenericLocalSearch*(f, N,*L-All,S-RandomImprovement*)

The Metropolis Heuristic: is a variant of Random Walks that allows occassional degradation of the value of the objective function. It selects a random candidate, if it does not degrade the objective function the candidate is returned, if it does, then it is accepted with a small probability

$$exp(frac{-(f(n) - f(s))}{t})$$

that depends on the distance between the objective functions, and on a parameter t called temperature. Assuming a function $True(f(n), f(s), t)$ that checks this probability, the Metropolis heuristic can be specified by:

```
1.  function Metropolis(N, s, t)
2.      select {n ∈ N};
3.      if f(n) ≤ f(s) then
4.          return n;
5.      else if True(f(n), f(s), t)
6.          return n;
7.      else
6.          return s;
```

Again, n can be randomly selected with probability $\frac{1}{|N|}$, where $\mid N \mid$ is the number of elements in N.

Metaheuristics

The heuristics presented in the previous section aim exclusively at choosing the next solution within the neighborhood in order to provide high quality local optima. But local optima are not necessarily global optima, and thus, some mechanism is needed to escape from them. These mechanisms are known as metaheuristics.

All the metaheuristics here are also based on the template depicted in figure 2.1, and assuming that it receives the parameters f, N and the *legality* and *selection* rules L and S. We are also going to assume that we are always dealing with minimization problems, so that the goal is to minimize f.

In the following we will present some of the most characteristic metaheuristic that can be found on the literature:

Iterated Local Search The idea behind this metaheuristic is to iterate a specific local search from different points in the search space. Sometimes, the starting points can be generated from the last local minima reached on the previous iteration.

```
1.  function IteratedLocalSearch(f, N, L, s)
2.      s ← InitialSolution();
3.      s* ← s;
4.      for k = 1 to maxSearches do
5.          s ← LocalSearch(f, N, L, s);
6.          if f(s) < f(s*) then
7.              s* ← s;
8.          s ← GenerateNewSolution(s);
9.          return s*;
```

Figure 2.2: Iterated Local Search

```
1.  function SimulatedAnnealing(f, N)
2.      s ← InitialSolution();
3.      t_1 ← InitialTemperature(s)
4.      s* ← s;
5.      for k = 1 to maxSearches do
6.          s ← LocalSearch(f,N,L-All,Metropolis(t_k), s);
7.          if f(s) < f(s*) then
8.              s* ← s;
9.          t_{k+1} ← UpdateTemperature(s, t_k);
10.         return s*;
```

Figure 2.3: Simulated Annealing

Figure 2.2 depicts the outline of this algorithm. In line 2 an initial solution is generated and a certain number of iterations are performed (lines 5-8). Each iteration consists of a call to a Local Search procedure (which could be any of the metaheuristics presented in this section) and the generation of a new solution that can be produced either through some kind of transformation of the current solution s or from scratch.

Simulated Annealing This is a very popular metaheuristic that is based on the Metropolis heuristic presented in the previous section. The key feature is the parameter t or temperature. Different temperatures produce different trade-offs between the

```
1.   function GuidedLocalSearch(f, N, L, S)
2.       s ← InitialSolution();
3.       f_1 ← f
4.       s* ← s;
5.       for k = 1 to maxSearches do
6.           s ← LocalSearch(f_k, N, L, S, s);
7.           if f(s) < f(s*) then
8.               s* ← s;
9.           f_{k+1} ← UpdateObjectiveFunction(s, f_k);
10.          return s*;
```

Figure 2.4: Guided Local Search

quality of the solution and the execution time. The idea behind this metaheuristic is to iterate the Metropolis algorithm with a sequence of decreasing temperatures.

$$t_0, t_1, \ldots, t_k \;\; (t_{k+1} \leq t_k)$$

The results is to allow many moves initially, and progressively reduce the number of allowed moves, converging thus toward random improvement with the hope of high-quality local optima when $t_i \to 0$.

Figure 2.3 depicts the Simulated Annealing template. There are, however, two critical decisions to take: the initial temperature (line 3) and the cooling mechanism (line 9). Both of these can be chosen experimentally or can be derived systematically for specific instances ([1],[126])

Guided Local Search This metaheuristic is based on the recognition that a local optima s for an objective function f might not be locally optimal to a different objective function f'; thus, using f' will drive the search away from s. As a consequence, the key idea is to use a sequence of objective functions $f_0, f_1, \ldots, f_k$ to direct the search towards different areas of the search space.

Figure 2.4 depicts the Guided Local Search algorithm, whose embedded local search is generic. The key feature is the updating mechanism for the objective function

```
1.  function GenericLocalSearch()
2.      s ← InitialSolution();
3.      s* ← s;
4.      τ ← ⟨s⟩;
5.      k ← 0;
6.      while k ≤ maxIt
7.          if satisfiable(s) and f(s) < f(s*) then
8.              s* ← s;
9.          s_{k+1} ← S(L(N(s_k), τ), τ);
10.         k++;
11.         τ ← τ + s_{k+1};
12.     return s*;
```

Figure 2.5: The Generic Local Search Revisited

(line 9), which can be done in terms of the previous objective function or from scratch.

Tabu Search This is a very popular and effective metaheuristic that mixes a great variety of techniques. In order to better understand it we are going to extend the generic local search presented earlier. The new idea is to maintain a sequence

$$\tau = \langle s_0, s_1, \ldots, s_k \rangle$$

of solutions explored so far. Figure 2.5 depicts the new local search procedure.

As a first approximation, given a sequence $\langle s_0, s_1, \ldots, s_k \rangle$, tabu search selects s_{k+1} to be the best neighbor in $N(s_k)$ that has not yet been visited.

As a consequence, tabu search can be viewed as the combination of a greedy strategy with a definition of legal moves ensuring that a solution is never visited twice:

```
1.  function TabuSearch(f, N, s)
2.      return LocalSearch(f, N,L-NotTabu,S-Best)
```

where

1. **function** *L-NotTabu*(N, τ)
2. **return** $\{n \in N \mid n \notin \tau\}$;

There are two interesting features to highlight here. First, there are no references to the objective function in the legality conditions, which means that degrading moves are allowed, which can translate into escaping from local minima. Second, its greedy nature ensures that the quality is not going to degrade too much at any step, since the best neighbor is always chosen.

Tabu List is the name of the structure where tabu search stores the sequence of visited solutions. However, memory space constraints limit the stored information. Often, only characteristics of the move are recorded, rather tha the complete solutions. Thus, the tabu list usually stores limited aspects of the solutions which do not fully characterize them, but can also consider non visited solutions with the same characteristics. As a consequence, solution aspects are only stored temporarily, and are freed at some point. The number of steps during which the chosen features of a solution are stored is called the *tabu tenure*. Thus, the election of the aspects of a solution to store, and the value of the tenure are key assets in the algorithm's performance.

Aspiration is a mechanism related to the partiality of the stored information. It allows choosing a solution in the tabu list when it is better than the current best solution. The resulting legal moves are specified as

1. **function** *L-NotTabu-Asp*(N, τ)
2. **return** $\{n \in N \mid n \notin \tau \ \vee f(n) < f(s^*)\}$;

Long-Term Memory: we know that the tabu list abstracts a small suffix of the solution sequence, and cannot capture long-term information. As a consequence, tabu search cannot ensure that the search will not focus on low quality solutions, or that it will spend too much time on the same region of search space. Thus, tabu search algorithms typically implement two different mechanism to avoid the previous problems:

- *Intensification* consists on storing high-quality solutions during the search and returning to them periodically, thus, allowing a more extensive exploration of the regions where the best solutions have been found.
- *Diversification* provides a means to explore more diverse regions of the search space. There are many ways to achieve this goal, such as using iterated local search to perturb or to restart the search, or using strategic oscillation, which consists of changing the objective function in order to balance the time spent in the feasible and infeasible regions ([6]).

There are other more complex metaheuristics in the literature such as Variable Neighborhood Search (VNS) [161] or Ant Colony Optimization (ACO) [57]. Also, hybrid evolutionary approaches are sometimes considered as metaheuristic, but we will explore such methods in the next chapter.

Most of the figures and templates in this section can also been found with higher detail in [115].

2.2 SAT

Consider the following problem:

Example 2. *I'm hungry and I would like something to eat. My father says I must eat meat or else don't eat fish. My mother says I must eat fish, vegetable or both. My girlfriend asks me not to eat either vegetables or meat or both. What can I eat?*

This problem can be represented as a propositional satisfiability problem. We can express the three constraints by means of a propositional formula,

$$(M \vee \neg F) \wedge (F \vee V) \wedge (\neg V \vee \neg M)$$

where M, F and V are Boolean variables which are true if and only if I eat respectively, Meat, Fish, and Vegetables. A solution to the problem is a satisfying assignment, an assignment of truth values to the Boolean variables that satisfies the propositional formula. In this case, there are just two satisfying assignments (out of eight possible). These either assign M and F to true and V to false, or assign M and F to false and V to true. That is, I can either eat both Meat and Fish, and not Vegetables, or I can eat only Vegetables and neither Meat nor Fish.

Whilst propositional satisfiability is a very simple problem, it is a cornerstone in the theory of computational complexity. Propositional satisfiability was the first problem shown to be NP-complete [41].

2.2.1 Satisfiability

Propositional satisfiability (SAT) is the problem of deciding if there is an assignment for the variables in a propositional formula that makes the formula true. Many AI problems can be encoded quite naturally into SAT (*eg.* planning [137], constraint satisfaction, vision interpretation [189], diagnosis,hardware verification and design, ...).

Much research into SAT considers problems in *conjunctive normal form* (CNF). A formula is CNF if and only if it is a conjunction of clauses; a clause is a disjunction of literals, where a literal is a negated or un-negated Boolean variable. A clause containing just one literal is called a unit clause. A clause containing no literals is called the empty clause and is interpreted as false. k-Sat is the class of decision problems in which all clauses are of length k. k-SAT is NP-complete for any $k \geq 3$ but is polynomial for $k = 2$ [84]. Other polynomial classes of SAT problems exist including Horn-SAT (in which each clause contains no more than one positive literal), renamable Horn-SAT and several other generalizations.

2.2.2 Complete procedures

There are different approaches to solve a SAT problem, such as complete procedures, approximation algorithms, mixed techniques, etc. We are now going to focus in complete procedures, explaining the algorithms and some basic features.

Davis-Putnam procedure

Despite its simplicity and age, the Davis-Putnam procedure remains the core of one of the best complete procedures for satisfiability [61]. Davis, Logemann and Loveland changed the original procedure by adding a splitting rule which divides the problem into two smaller subproblems [49]. In much of the literature, this later procedure is rather inaccurately called "Davis-Putnam" or "DP" procedure.

Procedure DP(Σ)
(Sat) **if** Σ empty **then return** satisfiable
($Empty$) **if** Σ contains an empty clause **then return** unsatisfiable
($Tautology$) **if** Σ contains a tautologous clause c **then return** DP($\Sigma - \{c\}$)
($Unitpropagation$) **if** Σ contains a unit clause l **then**
return DP(Σ simplified by assigning l to $True$)
($Pureliteraldeletion$) **if** Σ contains a literal l but not the negation of l **then**
return DP(Σ simplified by assigning l to $True$)
($Split$) **if** DP(Σ simplified by assigning l to $True$) is satisfiable **then**
return satisfiable
else return DP(Σ simplified by assigning the negation of l to $True$)

Figure 2.6: The Davis-Putnam procedure.

After applying the splitting rule, the algorithm simplifies the set of clauses by deleting every clause that contains the literal l assigned to *True* (often called unit subsumption) and deleting the negation of l whenever it occurs in the remaining clauses (often called unit resolution).

Branching heuristics

The DP algorithm is non-deterministic as we can choose the literal upon which to branch. A popular and cheap branching heuristic is MOM's heuristic. This picks the literal that occurs most often in the minimal size clauses. Ties are usually broken with a static random ordering.

The Jeroslaw-Wang heuristic [129] estimates the contribution each literal is likely to make in order to satisfy the clause set. Each literal is scored as follows: for each clause c the literal appears in, $2^{-|c|}$ is added to the literal's score, where $|c|$ is the number of literals in c. The split rule is then applied to the literal with the highest score.

Hooker and Vinay, after investigating the Jeroslaw-Wang score function ([120]) claimed for a "simplification hypothesis", that it is best to branch into simpler subproblems with fewer and shorter clauses after unit propagation. The simplification hypothesis suggests a "two-sided" Jeroslaw-Wang rule which performs better than the original.

There more recently proposed branching heuristics [3], like the Variable State Independent Deacying Sum (VSIDS) heuristics found in Chaff solver [165]. Some of its features are:

- Choose the literal that has the highest score to branch.
- Initial score of a literal is its literal count in the initial clause database.
- Score is incremented by 1 when a new clause containing that literal is added.
- Periodically, divide all scores by a constant.

Intelligent backtracking and learning

The standard DP procedure performs chronological backtracking, exploring one branch of the search tree completely before backtracking and exploring the other. We can

[3] See http:// research.microsoft.com/users/lintaoz/SATSolving/satsolving.htm for a good SAT Solving Mini Course by Linato Zhang

```
1.  function StochasticLocalSearch(φ, maxTries, maxSteps)
2.      for k = 1 to maxTries do
3.          s ← InitRandomAssignment();
4.          for l = 1 to maxSteps do
5.              if s satisfies φ then
6.                  return s;
7.              else
8.                  x ← chooseVariable(s, φ);
9.                  s ← s with truth value of x flipped;
10.     return no solution.
```

Figure 2.7: Stochastic Local Search. ϕ is the input formula

improve upon this by adapting some of the well-developed techniques from the constraint satisfaction community like conflict-directed backjumping and nogood learning (in fact, nogood learning has developed much more efficiently in the SAT framework). Conflict-directed backjumping backs up the search tree to the cause of failure, skipping over irrelevant variable assignments. Nogood learning records the cause of failure to prevent similar mistakes being made down other branches. Bayardo and Schrag have described how both of these mechanisms can be implemented within the DP procedure [15], and are now a standadr feature of all state-of-the-art SAT solvers.

Early mistakes

The problem with a complete procedure like DP is that an early mistake can be very costly. Gomes, Selman and Kautz have shown that a strategy of randomization and rapid restarts can often be effectively used at tackling such early mistakes [99]. Meseguer and Walsh show that other modifications of the depth-first search strategy like limited discrepancy search and interleaved depth-first search can also help avoiding early mistakes [154].

2.2.3 Local Search-based Procedures

Our focus in this thesis is not on Local Search methods for the SAT paradigm. Several hybrid methods are, nontheless, introduced in the next chapter. Here, we are going

to give a brief set of references to pure Local Search solvers and methods for the SAT framework.

Stochastic Local Search (SLS) can be interpreted as performing biased random walk in a search space which, for SAT, is given by the set of all complete truth assignments. A general outline of a SLS algorithm for SAT is given in Figure 2.7.

SLS algorithms differ mainly in the heuristic for choosing the variable to flip in each search step. WalkSAT algorithms (citeSelman96) use a two-step variable selection process: first, one of the clauses which are violated by the current assignment is randomly chosen; then, according to some heuristic, a variable occurring in this clause is flipped using a greedy bias to increase the total number of satisfied clauses. Variants of this technique are WalkSAT with Tabu ([153]) and the Novelty versions ([153, 121, 47]). WalkSAT is similar to GSAT ([60]) but the former introduces the notion of *noise parameter*.

A rather comprehensive review of Complete and Local Search (WalkSAT-like) review can be found in [122], and an empirical comparison of LS methods in [123].

2.3 Evolutionary and Genetic Algorithms

An Evolutionary Algorithm (EA) indicates a subset of Evolutionary Computation, which specializes in solving combinatorial optimization problems. EAs are categorized as a kind of Evolutionary Computation, being the latter a broader term which includes metaheuristic optimization algorithms. Some of these techniques have been mentioned in the previous section, such as ant colony optimization (which is sometime included in the Local Search paradigm), or others such as particle swarm optimization ([37]).

EA is thus a term to define any population-based techniques which implements certain mechanisms such as reproduction, mutation, recombination and natural selection, all of them inspired by biological evolution. EAs can be also viewed as a form of Local Search, where there are multiple complete assignments instead of just one, and where richer methods of moving across the search space are provided. A broad classification of EAs would be the following:

- **Genetic Algorithms:** the most popular kind of EA, it looks for a solution within a population of strings of numbers which evolves through recombination methods that include mutation and selection operators.
- **Evolutionary Programming:** it consists on fixing the structure of the program and letting the parameters evolve during time.
- **Genetic Programming:** here the solutions are in the form of computer programs which fitness corresponds to the ability of solving a computational problem.
- **Evolution strategy:** which maintains a representation of vectors of real numbers and typically includes self-adaptive mutation rates.
- **Learning classifier system:** instead of a fitness function they implement a rule utility decided by a reinforcement learning technique.

This categorization is neither extensive nor exclusive, and its only pretension is to introduce the subfield of the Evolutionary Algorithms. To learn more about EAs and Evolutionary Computation conslut [69]. In the next subsections we are going to focus on Genetic Algorithms (GAs).

2.3.1 Genetic Algorithms

Everybody seems to agree on the fact that Holland was the father of the GAs. His early works (in 1962) on adaptive systems laid the foundation for latter developments. Moreover, his book *Adaptation in Natural and Artificial Systems* ([119]) was the first to present the concept of adaptive digital systems using mutation, selection and crossover as a problem-solving strategy. However, this research was conceived by Holland as a means of studying adaptive behavior and not as a function optimization method. To learn more about the history of GAs consult [96].

```
1.  function GenericGeneticAlgorithm()
2.      pop ← InitialPopulation();
3.      Evaluate(pop);
4.      while not Termination()
5.          parents ← selectParents(pop);
6.          descendants ← Combine(parents);
7.          Mutate(descendants);
8.          pop ← SelectPopulation(pop, descendants);
```

Figure 2.8: A Generic Genetic Algorithm

The Algorithm Template

Figure 2.8 shows the generic GA template. The population *pop* is initialized in line 2 and evaluated in line 3. Then, a certain number of iterations is repeated until a termination criteria is reached (line 4). During these iterations the individuals are selected (line 5) to be combined (line 6) and their descendants are mutated (line 7). Afterwards, a new population is generated from the previous one and the descendants, although sometimes, the previous population is completely forgotten and only new individuals are considered for the next iteration.

In the next sections we are going to review each one of these steps.

2.3.2 Representation

This is an issue that is prior to the development of the algorithm. Typically, GA use a string of number as a representation, and very often it is only a binary string. However, we should not forget that choosing the right representation of a problem is key to the algorithm's performance. Thus, it is well worth to devote some time to representation.

The first issue which arises in some GAs is to link the real problem to the problem representation. This mimics biology where a *genotype* encodes the information that yields a *fenotype* which is the natural transformation of that information.

Sometimes, this distinction does not appear if the information and the representation are one and the same thing, which happens often. However, as we will latter see, it is important to explicitly make this distinction since the *genotype* is used for individuals interaction, but the *fenotype* is needed to calculate the real value of the evaluation function. Every unit of information stored in the *genotype* is typically named *gene*.

The second issue is what kind of structures do we need to use to represent our *genotype* and/or *fenotype* (Note that, many times, the fenotype is not actually implemented, and it might be only calculated when the evaluation function needs it). In general, we can distinguish several types of representation:

- **Binary Representation:** this is the simplest representation we can find. It consists on a binary sequence, i.e., a sequence of 1's and 0's. While this technique is very commonly used, it is not always the best suited approach. Its main drawback is based on the genotype-to-fenotype mapping. For example, when the 1's and 0's represent boolean variables, the genotype-to-fenotype mapping is direct: a 1 represents a true variable and a 0 represents a false one. Instead, if for example, we are representing numbers with binary sequences, we can encounter problems derived from the fact that the distances between the numbers and between their representations do not match. Observe that the distance between 3 and 4 is only 1, while if we are representing the numbers as a 4-bits sequence, the distance between 0011 and 0100 is not 1 anymore. Here, as in the next types of representation, we have to decide the length of the string.

- **Integer Representation:** to avoid problems like the one previously stated, we can safely represent the individuals as sequences of integers. This is probably a better suited representation for complex problems. The only issue here would be to decide whether those integers can be finite or infinite.

- **Real or Floating-Point Representation:** which consists of a string of real values. This approach is typically better suited for genes that come from a continuous distribution.

There are other more complex representations such as: strings of letters (which is basically equivalent to that of a finite integer representation) and permutation representations (see [69], p. 41–42).

2.3.3 Evaluation Function

Closely related to the representation, the issue of the evaluation function arises. This function associates a value to every individual in the population, and corresponds to the quality of that individual. Thus, different representations of the same problem may have different evaluation functions, since this is typically calculated from the values of the genes of each individual and through the genotype-to-fenotype mapping.

The evaluation function is often referred to as *fitness function* in the Evolutionary Computation field.

2.3.4 Initial Population

Once the representation is fixed, the first issue in developing the algorithm is that of the initial population. This is typically performed by randomly generating individuals so that the population can cover wider areas of the search space.

Nonetheless, there are other more specialized methods. A very common approach is to generate the individuals in a greedy manner, which means that every individual is constructed in a way such that at every time, the next gene is given the value that optimizes the evaluation function for that individual. Occasionally, the solutions may be somehow seeded in areas where solutions are likely to be found.

2.3.5 Parent Selection

Selection is the method through which certain elements in the population are chosen to be combined. This selection mechanism tries, in general, to choose parents that are likely to produce a high-quality descendant. Typically, two individuals are chosen two reproduce and yield descendants. Different kinds of selection mechanism are:

- **Fitness Proportional Selection:** consists of giving a certain probability to be chosen for every individual. This probability depends directly on the absolute fitness of the individual ([119]). The main drawback of this mechanism is that the best candidates are very likely to take over the whole population very quickly. This method is often called *roulette-wheel selection*.

- **Ranking Selection:** this method is very similar to the previous one. The difference is that, in this case, the individuals are ranked according to their fitness, and then probabilities are given based on the ranking rather than on the fitness itself ([11]).

- **Tournament Selection:** this is may be the simplest mechanism, and also the least time-consuming. It consists on choosing k individuals completely at random, and then selecting the two individuals with highest fitness function. Obviously, the complexity of this method depends on the value of k.

There are many other methods, mainly variations of the ones described above. Again, the reader is referred to [69] for more details.

Multiparent Selection Is to worth mentioning that some algorithms implement a multiparent selection scheme. This means that, independently of the selection method they use, more than two parents are selected for combination. We detail the kind of combination methods for this type of selection in the next section.

2.3.6 Reproduction

This operator is in charge of combining the parents in such a way that a high quality individual (descendant) will be obtained. This mechanism is also known as *crossover*. In some GAs, this operator is able to generate more than one descendant (usually two), but we will assume from now on that only one descendant is going to be generated. Thus, different crossover operators are:

- **One point crossover:** this is the most popular method. It consists on choosing a point randomly, and copying the genes of a parent, from the beginning

until this point, to the descendant, and the genes of the other parent from that point till the end.

As an example, imagine we have two parents of the form:

$$\sigma_1 = \langle\ 0\ 1\ 0\ 0\ 1\ 1\ 1\ 1\ 0\ \rangle$$
$$\sigma_2 = \langle\ 0\ 0\ 0\ 1\ 1\ 0\ 1\ 0\ 0\ \rangle$$

and $k = 5$ is the crossover point, the descendant would either be

$$\langle\ 0\ 1\ 0\ 0\ 1\ /\ 0\ 1\ 0\ 0\ \rangle$$

or

$$\langle\ 0\ 0\ 0\ 1\ 1\ /\ 1\ 1\ 1\ 0\ \rangle$$

Note that extending this operator to generate two descendants is trivial.

- **Multiple point crossover:** is based on the previous operator, and its only difference is that instead of 1 point, several k points are chosen randomly. Then, to generate a descendant it would copy the genes of each parent in turns after each crossover point.

- **Uniform crossover:** is slightly different than the previous one. It treats each gene independently and decides from which parent it is going to be inherited (typically with the same probability).

These methods are the most common ones in the literature. Other more complex ones can also be found. It is also very common to implement a type of uniform crossover where instead of proabilities, the decision criteria is based on the fitness of the descendant.

Multiparent Combination

As we mentioned in the previous subsection it is also possible (although not very common) to implement a multiparental combination. Instead of 2 parents, k parents are selected and combined. Thus, combination methods for this option tend to be

different from those of the traditional scheme. These methods can be categorized as follows:

- Generalizing uniform crossover ([166]).
- Generalizing multiple point crossover ([64]).
- Generalizing arithmetic combination operators ([221]).

To know more about the efficiency and suitability of this type of combination on certain structures of the search space (landscapes) consult [68].

2.3.7 Mutation

This operator is the source of great diversity. It is based in the biological fact that some genes can mutate for different reasons, and thus, the descendant can acquire genes that are from neither of its parents. The most common ones are:

- **Random bit modification:** consists on changing the value of some bits with a given probability. The operator changes the value of every bit in the sequence with a certain probability. If the representation is binary, the effect is that of *flipping* a bit, either from 0 to 1 or from 1 to 0.
- **Swap mutation:** simply selects two genes (at random) in the sequence and swaps their values. Imagine the individual:

  $\langle$ 0 [1] 0 [0] 1 0 1 0 0 $\rangle$

  and the swapping genes 1 and 3, the mutated individual would be

  $\langle$ 0 [0] 0 [1] 1 0 1 0 0 $\rangle$

- **Insert mutation:** chooses two genes at random and moves the second one next to the first. Again, if we have the individual

  $\langle$ 0 [1] 0 0 [1] 0 1 0 0 $\rangle$

and the inserting genes 1 and 4, the mutate individual would be

⟨ 0 [1] [1] 0 0 0 1 0 0 ⟩

- **Scramble mutation:** selects a region in the sequence and randomly scrambles its values. For example,

  ⟨ [0 1 0 0] 1 0 1 0 0 ⟩

  and the region from 0 to 3, a possible mutate individual would be

  ⟨ [1 0 0 0] 1 0 1 0 0 ⟩

Note that all these operators can be applied to any kind of representation, even though the illustrations assume a binary representation.

Many other complex and specialized mutation operators can be found in the literature, including the ones where the mutation is not random but biased by the subsequent value of the fitness function of the individual.

2.3.8 Selection of the New Generation

As we have previously introduced, this is the mechanism that replaces the last population by a new one. In order to do so, some algorithms completely replace the previous population for the new set of descendants or *offspring*. However, this is usually not a very effective technique, and GAs normally implement mechanism to generate the new population from both, the previous one and the offspring. Among these mechanism we can distinguish:

- Fitness based: selection focuses on keeping the individuals with higher fitness for the next generation.

- Generations based: selection takes into account the number of generations passed since its creation, and replaces then those individuals which have been in the population for a larger amount of generations.

- Replace Worst: some techniques tend to replace the worst x individuals in each step. Many of these techniques do not present a generational model as shown in figure 2.8, but a different model explained in section 2.3.10.

A technique associated with this operator (independent of the mechanism type) is to *always* maintain the highest quality individual in the population. This technique is usually referred to as *elitism*.

2.3.9 Termination

The termination condition indicates when it is time for the algorithm to stop. At this point, the algorithm will usually return the best individual according to its fitness function. We can distinguish two kinds of termination condition:

- **Objective reached:** when a GA is implemented to reach a certain goal (i.e., a solution of a certain quality), reaching that goal should be the indication for the algorithm to stop.
- **External conditions:** However, the previous case is very rarely achieved, due to the stochastic nature of these algorithms. Therefore, a different criteria must be used. Different conditions include:
  - Fixed number of generations reached.
  - Maximum time allowed reached.
  - Fitness improvement does not occur for a certain period of time/generations.
  - Manual inspection.
  - A combination of the above.

2.3.10 Evolutionary Models

This last issue deals with the structure of the algorithm rather than with the nature of its operators. There two well-known kinds of evolutionary models:

- **Generational Model:** this is the model corresponding to figure 2.8. In each generation a set of parents are selected to generate a new population of the same size as the previous one. This new population is often called *offspring*. The old population will be replaced by the new one (offspring) or by a combination of both (as explained in section 2.3.8).

- **Steady State Model:** in this model the population is not replaced at once. Instead, only a certain number λ of old individuals is changed. The percentage λ/γ (where γ is the size of the population) of replaced solutions is called the *generational gap*. This technique was introduced in [232] and has been widely studied and applied since then ([228, 193]).

For a more technical point of view on Evolutionary Computation and Evolution strategies consult [23].

Chapter 3

Hybrid Approaches

Our final hybrid incorporates features from Constraint Programming, Local Search and Genetic Algorithms. Since hybrids incorporating these three techniques are almost non-existent, we are going to review some state-of-the-art approaches that combine these techniques two by two. Thus, in this chapter we are going to review different hybrids divided into three sections:

- Constraint Programming and Local Search hybrids, including SAT procedures.
- Memetic Algorithms which introduce Local Search in Genetic Algorithms.
- Genetic Algorithms and Constraint Programming hybrids.

3.1 CP and LS

Many combinatorial problems can be represented and solved within the general framework provided by Constraint Satisfaction Problems (CSP), which allows a very natural modeling of many practical applications, such as planning, scheduling, time tabling, vehicle routing, etc.

Search algorithms for solving CSPs are usually categorized into local search and systematic search algorithms. Since both approaches have their own advantages, combining them appears very promising. As a result, there is a growing interest in the development of new hybrid algorithms that combine the strength of both techniques.

3.1.1 A general view

Let us review the definition of a *Constraint Satisfaction Problem*; a CSP $P = (X, D, C)$ is defined by a set of variables $X = \{x_1, ..., x_n\}$, a set of n finite value domains $D = \{D_1, ..., D_n\}$, and a set of c constraints or relations $C = \{R_1, ..., R_c\}$. A constraint R_x is a pair $(vars(R_x), rel(R_x))$ defined as follows:

- $vars(R_x)$ is an ordered subset of the variables, called the constraint *scheme*. The size of $vars(R_x)$ is known as the *arity* of the constraint. A *binary* constraint has arity equal to 2; a *non-binary* constraint has arity greater than 2. Thus, a *binary CSP* is a CSP where all constraints have arity equal or less than 2.

- $rel(R_x)$ is a set of tuples over $vars(R_x)$, called the constraint *relation*, that specifies the allowed combinations of values for the variables in $vars(R_x)$. A *tuple* over an ordered set of variables $X = \{x_1, ..., x_k\}$ is an ordered list of values $(a_1, \ldots, a_k)$ such that $a_i \in dom(x_i), i = 1, \ldots, k$.

Solving a CSP means finding an assignment for each variable that does not violate any constraint.

Algorithms for solving CSPs fall into one of two families: systematic algorithms and local search algorithms.

Systematic algorithms typically start from an empty variable assignment that is extended in a systematic way by adding individual tentative assignments until either a solution is found or the problem is detected inconsistent (there is no solution for the problem). Crucial to the efficiency of these methods is that each decision (branch) is immediately propagated by local consistency techniques which prune the search space (mainly, though not only) by deleting values from variables' domains. Backtracking occurs when a dead-end is reached, typically because the propagation mechanism made a variable's domain empty (produced a *domain-wipeout*, as it is called). The biggest problem of this approach is that it requires an important computational effort and therefore it encounters some difficulties with large scale problems; it also might suffer from early mistakes in the search which can cause a whole subtree to be explored with no success. These methods are usually improved by adding specific techniques

such as look-back enhancements (backjumping, learning) or look-ahead mechanisms (filtering techniques, variable or value ordering heuristics).[1] Thus, we can say that these algorithms are complete, systematic, and they search through the space of partial assignments.

Local search algorithms mainly rely on the use of heuristics to efficiently explore interesting areas of the search space. They typically start from a complete variable assignment and perform an incomplete exploration of the search space by repairing unfeasible complete assignments. Local search algorithms are capable of following a local gradient in the search space. Even though these methods can better deal with large-scale problems of certain kinds, their main drawbacks are that they are not guaranteed to find a solution even if there is one, cannot collect all solutions, and cannot detect inconsistency. Thus, we can say that these algorithms are incomplete, non-systematic (they usually follow a local gradient which does not ensure exhaustive exploration), and they search through the space of complete assignments, moving from one to another according to certain predefined rules of "neighbourhood".

In terms of the field terminology, local search stands for the simple strategy of performing local changes to a starting solution in order to decrease a given cost function. The special heuristics that guide this process, mainly to avoid or escape local minima are called "meta-heuristics". However, for simplicity, we will refer to them as local search algorithms through all the review. If the reader is interested in meta-heuristics we recommend [159] for an extensive review.

A promising idea for producing more efficient and robust algorithms consists in combining these paradigms in order to take advantage of their respective assets. Many existing proposals provide different forms of hybridization between both methods, but they often deal with very specific classes of problems and also mix satisfaction and optimization. We are going to categorize those hybrid approaches into three different branches:

1. The loosest form of integration is to use both local and systematic search,

[1] Industrial applications of constraint modeling, in particular, have proved the importance of specialized filtering techniques for predefined *global constraints*, e.g. that some variables have all different values, or cardinality constraints such as "each machine can have at most k shifts" that arise frequently in practice.

but separately, e.g. perform local search after or before systematic search, interleaved or in parallel. Portfolio or time-slicing techniques may for example allocate time and processing power to each of a variety of solvers, which may be local or systematic, according to various strategies. While there are often computational advantages to be gained from this approach, it does not represent a real degree of integration, and is therefore left outside the scope of this chapter.

2. Perform systematic search improved by local search. We distinguish three directions within this category:

   - Over complete assignments. Typically for optimization or repair-like techniques.
   - Over partial assignments. In construct and repair approaches.
   - Over global constraints. Local search is basically used to prune support values in global constraints.

3. Perform local search improved by complete search. We can distinguish three different branches within this category:

   - Use complete search to explore the neighborhood.
   - Use consistency techniques to prune the search space.
   - Record nogoods (learnt constraints that represent an explanation of domain wipe-outs found during search) in order to achieve completeness.

It is also worth mentioning a recently proposed general framework to enclose all these methods: PLM, which stands for Propagation, Learning and Move. The authors claim that any algorithm can be decomposed in these three components. Thus, any method could be implemented by specifying each of these three elements.

The chapter is organized as follows. Section 2 and 3 review hybrid approaches from the second and third categories respectively. Section 4 describes the PLM framework. Section 5 introduces hybrid methods for the SAT problem which we also found interesting to address. A necessary discussion about hybridization (what has been

done and what we believe should be pursued in the future) is presented in section 6. Finally, section 7 is dedicated to conclusions and future work.

3.1.2 Local Search enhancements for Complete Search

Complete search and constraint programming algorithms have been the most used methods for solving constraint satisfaction problems. After the proved superiority of local search methods in many problem instances, trying to incorporate features from local search into complete search was a goal that seemed worth pursuing. As introduced in the previous section we will distinguish among three different branches within this hybridization category.

Local search over complete assignments

This type of method is particularly suited for optimization purposes. It is very straightforward to perform local search from an initial solution obtained by systematic search to improve its fitness. Usually, in the constraint programming framework, this issue would be tackled using branch and bound techniques. However, this can result in a useless exploration of the search space where visiting different branches will not lead to a substantial change in the cost function. Thus, it seems very promising to introduce local search mechanisms to more efficiently explore the neighborhood of the constructed solution.

Local search can also be applied to a set of global search generated solutions. Global search will only be used as a way to produce several initial solutions on which a local search improvement phase is performed. In this context, it is important to generate starting solutions that are diverse enough for the later exploration. Limited Discrepancy Search ([112]) is an interesting way of generating a diversified initial set of solutions.

We will not further explore this branch of hybrid algorithms since it does not represent a clear effort for integration. Local search is typically performed over constructed solutions, thus, both methods can even share the same information structure. A more interesting idea is to perform local search at internal nodes of the search tree,

i.e. local search over partial assignments, an idea we tackle in the next subsection.

Local search over partial assignments

This is a very interesting kind of hybridization because the degree of integration achieved is more sophisticated. These methods typically perform an iterative extension of a consistent partial assignment until all problem variables are instantiated. If the tentative extension reaches a dead-end, it is necessary to backtrack and produce alternative instantiations. At this point we can find methods which perform a reparative stage, while others introduce the local search like techniques to remove inconsistent variables instead of backtracking. Also, some methods implement a CP-like search (instead of a greedy construction) to extend the consistent partial assignment and to prune the search space as well.

A construction and repair approach Merging constructive and reparative features into hybrid search has been investigated in different ways. Distinguishing among these various forms of hybrid search is a matter of stating the degree of integration between the two approaches. We can find methods where the integration is loose, different constructive and reparative modules exchange information while operating independently ([168],[236]). In other approaches we encounter a higher degree of integration, where the reparative process employs constructive methods to explore the neighborhood ([197],[194]).

A Construction and Repair approach with a higher degree of integration is presented in [34]. They introduce a general hybrid method named CR, and then proceed to specify it in order to provide a fully operational search method called CNR.

CR is a generic search framework which integrates both constructive and reparative features as operators. Search is then performed in two alternating stages. A construction stage where a consistent partial assignment is iteratively extended until inconsistency or complete consistency is proved. And a repair stage which modifies the current inconsistent assignment until it becomes consistent.

CNR stands for Construction and Neighborhood Repair search, and it represents an instantiation of the CR framework described above. In the constructive stage,

an implementation of the **extend** function is provided. It includes both variable and value ordering heuristics, as well as a **consistency** function which performs a modified version of arc-consistency. In the reparative stage a neighborhood of an assignment is specified. At each time, a member of the neighborhood will be selected greedily according to a cost function f. This cost function evaluates partial assignments taking into account not only the number of variables with empty domains but also how *constrained* the assignment is. They also provide different repair operators which give rise to different neighborhoods.

The experimental results shown in [34] correspond to the *open-shop* scheduling problem. The algorithm is tested on three sets of benchmarks from the literature: Taillard instances ([217]), Brucker instances ([29]) and Guéret & Prins instances ([105]). The algorithm's performance is compared against five different methods: the genetic algorithm of Prins ([182]), the Tabu Decision-Repair algorithm of Jussien and Lhomme ([133]), two Tabu search methods of Alcaide ([5]) and Liaw ([146]), and the Branch-and-Bound algorithm of Guéret and Prins ([104]). Authors assure that their algorithm outperforms all these methods in every instance except for a single 9X9 one; and it also yields strictly better solution quality for every 10X10 instance.

Improving The Scalability of Backtracking Other methods aim at improving the scalability of backtracking through the integration of local search techniques. An early example is based on dynamic backtracking [92], an "intelligent" backtracking technique able to backtrack to a variable without removing the remaining assignments, while dynamically reorganizing the search tree. Partial Order Dynamic Backtracking ([93]), improves the scalability of Dynamic Backtracking without sacrificing completeness. The main feature that introduces with respect of DB is the allowance of greater flexibility in the choice of the backtracking variable.

Another hybrid approach is to use systematic backtracking techniques in a non-systematic ways. In [143], Iterative Sampling is introduced. It simply consists of restarting a constructive search every time inconsistency is proved. However, this approach requires a lower degree of integration. It is nonetheless worth mentioning that variations on this approach have been shown to outperform both local search

and backtracking methods on certain problems ([46],[99]).

A new approach called Incomplete Dynamic Backtracking (IDB) is described in [177]. IDB is inspired by Dynamic Backtracking and Partial Order Dynamic Backtracking, and is able to jump back to an earlier variable without removing the remaining assignments. It allows total flexibility in the choice of the variable to backtrack with, and it also records no information about the visited search space, thus sacrificing completeness. The authors claims that this form of backtracking is indeed a local search in a space of consistent partial assignments.

IDB's schema is quite simple: it proceeds by randomly selecting unassigned variables, and assigning values to them following a certain value ordering heuristic; when a dead-end is reached it backtracks by randomly removing several assignments. Termination is only guaranteed when a solution is found.

More specifically, IDB implements forward checking as a form of constraint propagation. It is thus important to adapt this consistency technique to a random unassignment of variables, since it has to be capable of leaving the state of those variables as if forward checking had been only applied to the currently assigned variables. It also implements a minimum-domain (MD) heuristic for variables selection, while values are only selected if they do not generate any conflicts and if propagating them causes no domain wipeout. Among these allowed values, the one that was assigned the last, is selected where possible. However, IDB attempts to use a random different value for one variable every time a dead-end is reached.

Another issue is how to unassign variables when inconsistency has been proven. IDB provides a heuristic that consists of selecting variables with the largest current domain, breaking ties randomly.

Finally, in order to adapt this schema to optimization problems, ideas from the Constraint Programming framework are borrowed. It simply restarts the search after each solution until the first dead-end occurs, reusing then as many assignments from the previous solution as possible.

The approach is tested through several known problems: the n-queens, the Golomb ruler and the maximum cliques problem. The n-queens problem is used mainly to

introduce the algorithm; on the Golomb ruler it improved the scaling of constrained-based approaches and achieved better solutions than genetic algorithms. On maximum cliques, it outperformed many different algorithms and was only inferior to a sophisticated local search method ([14]).

Scheduling and Timetabling In many cases we find very specific approaches to deal with very specific problems. Some of them are easily extended to a general cases, while others introduce various problem-tailored rules that are very hard to generalize. Thus, it is interesting to study those methods within the context of the type of problems they focus on. In this particular subsection, many methods have been devoted to solving Scheduling and Timetabling problems.

Scheduling and Timetabling problems are often tackled with constraint programming techniques, and as in other application areas, hybridization appeared promising. Some of the approaches described next deal specifically with this application area, and are not always easy to extend to a more general domain.

In [214] authors employ a propose and revise rule-based approach to the course timetabling problem. Every time the construction reaches a dead-end a local change rule attempts to find a possible assignment for the unscheduled activity. They only perform a single step before restarting the construction, and their aim is only to accommodate the pending activity.

Another approach is to use a heuristic constructive mechanism in order to find an initial solution, and then apply a local search technique to improve it. In [235], authors implement an algorithm to solve a timetabling problem by means of combining an arc-consistency based construction and a min-conflict hill climbing stage. The construction phase accepts constraint violations, and when a complete solution is produced, the hill-climbing phase reduces the overall penalty.

A very interesting algorithm is described in [197]. It is similar to the other techniques introduced above, i.e., it constructs a tentative solution until a dead-end is reached, and then it performs a local search phase over the partial instantiation reached. However, it has two new features:

1. It performs a full run of local search, instead of a fixed number of local changes.

It also relies on well-studied local search algorithms, instead of implementing a set of problem specific moves.

2. It introduces a look-ahead factor that adds information to the cost function, in order to provide a better guidance towards more promising areas in the search space, not only taking into account feasibility but also possibility of the partial solution to be completed. This look-ahead factor is based in the min-conflicts heuristic, which counts the number of uninstantiated values for every uninstantiated variable.

This approach features the possibility to be applied to both search and optimization problems. This is achieved due to the flexibility of the score function which allows different combinations of weights to take into account feasibility, optimality (if necessary) and look-ahead in many proportions. Depending on the weights given to each aspect the search would be directed towards different regions: for example, a high weight for feasibility would direct the search towards feasible regions (which authors argue not to be efficient due to the extreme risk to get trapped on local minima).

This technique is applied to solve the course timetabling problem. The author implemented three different versions: with random hill climbing, steepest hill climbing and min-conflict hill climbing ([160]). The results show that combined methods perform better than pure local search methods, and the best of them is the one that introduces min-conflict hill climbing. The algorithm is also applied to tournament scheduling yielding results that confirm the same conclusion.

Unfortunately, a considerable amount of research is devoted to algorithms specifically tailored to the problem at hand. Even though it can result in a very effective algorithm that outperforms previous works, it is hard to extract conclusions from it.

A very specific approach for a timetabling problem is presented in [48]. This paper describes an algorithm for an examination timetabling problem used at the "Ecole des Mines de Nantes".It is a constraint-based approach that introduces local repair techniques. An extra feature that this problem presents is that the timetable has to be generated in less than 1 minute.

The problem it tackles consists of scheduling examinations composed of four subjects. For every day, for every subject, every candidate has to be assigned to one examiner during one period.

The algorithm solves the problem in two consecutive steps:

1. A first step called preassignment that reduces the domains of the variables making them consistent with a defined set of required constraints.

2. A second step called final assignment which assigns a period to every candidate from the preassigned domains.

In the preassignment step the domains of the variables are reduced following this criteria:

- Every examiner should have the same number of candidates.

- Each candidate takes an exam in the language he chooses.

- No candidate should meet an examiner who comes from the same school.

- All candidates are then preassigned each to four examiners (one for each subject).

In the final step the algorithm searches for a solution. The method attempts to assign every variable following a smallest domain heuristic. When a dead-end is reached, several specific local repair techniques are applied: free assigned candidates that would be consistently assigned in the current state to the current examiner; extend the previous technique to other examiners; swap already assigned examiners and check the consistency of the resulting instantiation; and finally, swap examiners without checking.

The program was validated on fifty hand-made instances plus thirteen real ones. Since the problem is very specific they do not provide any comparison. However, they are able to solve instances in less than a second (for the real ones), and eight seconds at most for the hand-made ones.

Over Global Constraints

In the last years, the constraint programming community has shown a great interest in global constraints. CP models have become more and more focused on a few number of global constraints. For instance, the Travelling Salesman Problem (TSP) has been centred on one single TSP constraint ([19]). Moreover, Knapsack constraints ([219],[73]), or flow constraints ([28],[21]) have lately been developed.

Constraint propagation on these global constraints is usually improved by a specialized filtering algorithm. These algorithms are usually based on Operation Research polynomial algorithms. Well known global constraints such as *AllDifferent* and *Cardinality Constraints* have been thoroughly studied as well ([188],[227],[185]).

Consequently, some effort has lately been centered on developing local search techniques as filtering algorithms for global constraints. Thus, global constraints for local search rise as a compromise between the generality of low-level CSP-based local search and the efficiency of problem-tailored local search encodings.

A very straightforward approach for the Dynamic Job-Shop Scheduling problem is introduced in [167]. A global search control selects among a set of global constraints that implement their selection of heuristic, their improvement heuristic and their update functions; variables employ a common interface that links all the global constraints and permits updating their states.

Results for the dynamic job-shop scheduling are provided as well. Based on these experimental results, authors intend to boost performance by implementing various extra features: randomization to escape local minima and plateaus; random walks (random moves in the search space which disregard the cost function value) that can be included by allowing a second improvement heuristic for each constraint that performs the mentioned variation of a random variable; a taboo list is used for the global search control's constraint selection. They also provide different heuristics (using more knowledge or being more offensive) and show a comparison among them.

Another interesting approach is described in [20]. Authors implement a *Branch and Move* technique which consists of using the support of the main global constraint of the problem as a guide for the branching strategy.

The approach divides the problem into several global constraints. It selects the

main global constraint of the problem and an element of its support (a variable-value pair which is consistent with the current domains). This element has associated a function that signifies the distance to the current support with respect to all other constraints. This distance is a measure of the quality of the pair, i.e. how far is the pair from being consistent to each constraint; if the function is null it means the element is a solution, otherwise the algorithm selects a constraint with maximum value for the mentioned function, and then the algorithm branches on a constraint whose support set does not include the element. The search proceeds by successively considering sub problems (including the branching constraint and including the complementary decision).

Local search is introduced before each element's choice. A descent procedure is applied to a neighborhood structure for the main constraint.

Authors also provide an empirical comparison for the TV-break problem. The algorithm is compared against other CP, LS and Mixed Integer Programming (MIP) methods. It is claimed that the approach finds good solutions very quickly, and it is always better than the other approaches except for a few instances where the CP approach is equal or better.

3.1.3 Introducing Complete Search mechanisms in Local Search

Alternatively to the approaches discussed in the previous section, where complete search is enhanced through local search, one might try instead to introduce complete search characteristics into local search. This might be motivated by efficiency reasons and also as a way to address the lack of completeness of local search. In this case we differentiate three different branches:

CP for neighborhood exploration

In the last years, local search techniques have been more and more directed towards the use of larger and more complicated neighborhoods. However, the standard way of searching the best neighbor is to iterate over the neighborhood, testing its fitness and/or its feasibility. Moreover, real world problems usually require several side

constraints, which yield a smaller feasible space. Thus, getting stuck on local minima is more likely to happen, and exploring those neighborhoods by simple enumeration becomes ineffective.

A very referenced work ([204]) introduces a new search method named Large Neighborhood Search (LNS). LNS is a hybrid approach for solving vehicle routing problems. It explores a large neighborhood which consists of removing and re-inserting visits using a constraint based tree search. Also, it uses Limited Discrepancy Search (LDS [112]) to re-insert visits. It is basically a technique that moves through the search space in a local search fashion, but that uses constraint propagation to evaluate the cost and legality of the move.

The algorithm is basically a process of continual relaxation and re-optimization. It achieves this through a technique of relaxing and re-inserting visits. The re-insertion process makes use of the full power of constraint propagation and heuristics. A branch and bound technique is used to examine the whole search tree for the re-insertion of minimum cost. Variable ordering heuristics reduce the size of the search tree, while value ordering heuristics guide the search towards a solution. Finally, in order to explore the search tree, the algorithm includes LDS which directs the search towards an increasing number of *discrepancies* (i.e. number of branches taken against the value ordering heuristic).

The algorithm is then applied to solve the capacitated vehicle routing problem and the same problem with time windows. LNS is compared against the best methods implemented in the field of Operations Research, and it is extremely competitive: both in its average performance and in terms of its ability to produce new best solutions.

CP for search space pruning

A way of pruning or reducing the search space is to add symmetry constraints to a symmetric problem. However, this has lately been proved as an inefficient technique for local search ([179]).

Many local search approaches implement a technique to reduce the search space, mainly for optimization problems: limit the neighborhood to only feasible assignments ([107]). Others ([6]) feature a strategy which consists of allowing unfeasible navigation

but only for a given number of steps.

However, in [171] we find an interesting approach that combines CP models of the neighborhood and powerful propagation techniques. As the authors argue, the paper proposes a novel way of looking at local search algorithms for combinatorial optimization problems. The approach introduces a neighborhood exploration used instead of performing branch and bound search.

This adaptation of local search to the constraint programming framework relies on a particular neighborhood structure. Local search will iterate a branch and bound like search on a different search space. The exploration of the branch and bound strategy is translated to an examination of the neighborhood of a solution. Moreover, modeling constraints and lower bounds will help prune the search space over the whole neighborhood.

The approach is called branch and bound because it branches on a certain variable and it also bounds the cost of partially constructed neighborhoods. Recording the cost of the best neighbor found so far and computing lower bounds for partial neighbors is therefore a way to reduce the unexplored neighborhood.

This technique is very interesting because it implies the description of two different models: a CP model of the problem and a neighborhood model of a solution. There exists a one-to-one mapping between the set of solutions of the CP model and the set of neighbors which communicate through *interface constraints*. Local search is then formulated as a sequence of CP tree searches on auxiliary problems.

While the algorithm is searching for a neighbor the original model is also active, which can result in a propagation that can also reduce the search space. Thus, constraints are used not only for testing feasibility but also for removing sets of infeasible neighbors during search. Ultimately, the neighborhood exploration will tend to find the neighbor that optimizes a given cost function.

In order to evaluate the approach, it is tested on the Traveling Salesman Problem with Time Windows (TSPTW), with instances from the literature and the model described in ([172]). The resulting observations are vague, though the authors claim that the pruning yields savings on the number of neighbors.

This type of approach has a clear advantage: there is a clear separation between

problem modeling and problem solving which facilitates the addition of side constraints, very common in real-life problems.

Nogood recording to achieve completeness

There are not many approaches that attempt to implement a complete local search algorithm. Furthermore, apart from tabu search, most of the local search approaches are memoryless. However, we will see in the SAT section that this goal has been pursued in that field.

Nonetheless, we can find a complete local search approach in the local search literature ([91]). This method introduces a new neighborhood search heuristic which, making effective use of memory structure, achieves completeness. The approach called complete local search with memory (CLM) keeps track of the visited solutions in order to prevent the search from exploring them again at later stages. *Memory* stands for a special space for storing solutions generated by the heuristics; its size is the number of solutions that it can store.

The algorithm is based on maintaining three different lists of solutions:

- A LIVE list which contains available solutions.
- A DEAD list which stores solutions that were LIVE at some stage.
- and A NEWGEN list for new solutions that are generated by the heuristic during the current state.

The method starts with initial solution which is stored in LIVE. Then, iterates by choosing and exploring a given number of solutions from LIVE, transferring them to DEAD; at the same time good quality neighbors are generated. These neighbors are checked for membership in any of the three lists, if non of the lists contains them they are stored in NEWGEN. After all solutions have been explored, they are transferred from NEWGEN to LIVE.

Different stopping rules are studied in the paper. Whenever one of them is reached a generic local search is applied to every solution in LIVE and the optimal solutions

are added to DEAD. Finally, the heuristic returns the best solution found in DEAD. The choice of the stopping rule will substantially perturbate algorithm's performance.

The experimental setting is designed to compare the algorithm against tabu search on the traveling salesman problem (TSP) and the subset sum problem (SSP). After some parameter tuning effort, the algorithm yielded better quality solutions than tabu search and took less time for the TSP; however, for the SSP, tabu search was slightly slower but achieved marginally better results on the average.

Another very promising approach is that of Weak-commitment search ([233]). Even though it might not fit in this category, it represents an effort in developing complete local search algorithms. Weak-commitment search is able to revise bad decisions without exhaustive search, while maintaining completeness and featuring the possibility of introducing various heuristics to operate once a consistent partial solution is constructed.

It is a very special technique where two parallel sets of variables are maintained: *vars-left* and *partial- solution*. *Vars-left* is initialized to a tentative solution while *partial-solution* is assigned to an empty set. The algorithm will proceed by moving variables from one set to the other, while recording abandoned partial solutions as nogoods. The search iterates the following steps:

1. Check if all variables in *vars-left* are consistent with the nogoods. If so, the current assignment is a solution.

2. Choose a variable and value pair in *vars-left* that violates some constraints and create a set with the values that are consistent with *partial-solution*.

3. If the set is empty and *partial-solution* is also empty, it means that there exists no solution; if *partial-solution* is not empty, it is added as a nogood and all its elements transferred to *vars-left*.

4. If the set of consistent values is not empty, the variable and value pair is removed from *vars-left* and a value that minimizes the number of constraint violations with *vars-left* is assigned to the variable and both added to *partial-solution*.

The author provides a comparison of the algorithm against the min-conflict backtracking and the breakout algorithm ([162]), on problems such as the n-queens, the graph-coloring and the 3-SAT problem. An extensive discussion of the performance of the methods on every domain is provided as well. As a summary, it is enough to say that weak-commitment is 3 to 10 times more efficient than both other approaches.

3.1.4 The PLM Framework

In this section we describe the PLM framework which was introduced in [134] and [135]. As we have mentioned before, the authors claim that any algorithm (either systematic or local) can be decomposed into three components: a Propagation component, a Learning component and a Moving component. They also show that this generic framework is a useful basis for new search algorithms that combine constraint programming and local search; yielding a family of algorithms which they call the *decision-repair* family.

The Three Components

We are going to briefly summarize the three different search components:

- **The Propagation** component is used to propagate information when a decision is made during search. They divide this component into two operators: a *filtering* operator which removes parts of the search space that do not contain any feasible solutions, and a *checking* operator which checks if a solution can exist.

- **The Learning** component is used as a mechanism to avoid the exploration of states that have been proved not to contain a solution. This component also has two operators: *recording* and *forgeting*.

- **The Moving** component, whose aim is to explore the search space. There are two moving operators as well: a *repair* operator to be used when a dead-end is reached and a *extend* operator which incorporates new information when

not enough information about the existence of a solution, or lack thereof, is provided.

They also provide a taxonomy of search algorithms introduced to characterize any given technique using different values for the three components.

The Propagation component Its filtering operator can take different values such as: a simple consistency check, forward-checking, arc-consistency, bound-consistency, etc.

Its checking operator can be non-existent or pragmatic (as in [131]).

The Learning Component This component is only characterized by the lifetime of the recorded information: not used, single use, time-bounded use, size-bounded use, etc.

The Moving Component In this case two different types of movements can be achieved: a backtrack-like type of move, and a jump-like move (which is the case of local search algorithms that jump from a given state to a neighboring one).

With this taxonomy authors provide a characterization of several known algorithms, such as BT, MAC, MAC-CBJ, GSAT, etc.

The Decision-Repair Family

In [135], the authors also present a new family of algorithms by specifying the three PLM components. It is based on the idea of combining the propagation-based nature of *mac-dbt* ([132]) and the freedom given by a local search algorithm such as *tabu search* ([95]).

In terms of the PLM framework, this family would be characterized by: starting with an empty set of decisions; using a standard filtering algorithm for reducing the variables domains; recording explanations for the encountered dead-ends and storing them in a tabu list; forgetting the oldest explanation when the tabu list is full; classically extending the information by adding new decisions (variable assignment,

domain splitting, etc.); and repairing by heuristically selecting a decision to undo from the last computed explanations.

A decision-repair algorithm (DS) is tested on the open-shop scheduling problem. Hard instances are generated using results presented in [105], and the algorithm is compared against an intelligent backtracker ([104]) and a genetic algorithm ([182]). DS is better than both approaches up to size 9X9, while for 10X10 instances it is still better than the backtracker but it is matched by the genetic algorithm.

3.1.5 The Satisfiability Problem (SAT)

The development of hybrid approaches for SAT is clearly of interest for the topic of this thesis. The time-line for hybrid SAT methods is similar to that for their analogues in constraint satisfaction. After the appearance of local search algorithms that outperformed complete search methods for certain instances, the need for hybridization raised as a great opportunity. The main direction initially followed was randomization techniques for complete search solvers. Afterwards, a new direction focused on developing a more sophisticated integration. We can distinguish two different branches:

- Adding new learnt clauses in order to achieve completeness and/or boost performance
- Improving stochastic local search on structured problems by efficiently handling variable dependencies.

We briefly review some of these methods in the next subsections.

Randomizing complete search solvers

The *heavy-tailed cost distribution* phenomenon is the cause of unpredictability in running times for complete search algorithms ([98]). Randomization is meant to eliminate heavy-tails and thus boost complete search methods performance. A few works have been centered on randomization; in [46], authors implement an algorithm that employs a variable order randomization and a restart strategy. However, it is not

until [98] when the first explanation for the potential success of this kind of strategy is provided.

The approach described in [99] is characterized by two different techniques:

Randomization In systematic procedures a consistent assignment is iteratively extended. A new unassigned variable is heuristically selected at each time. If different variables appear to be equally good, a fixed rule is applied to choose one of them. It is there, in that step of tie-breaking, where randomization is applied. It simply consists of choosing among the equally ranked choices at random.

However, it is possible that, for certain heuristic functions, no equally ranked variables appear. In order to deal with this, authors introduce a new parameter to the algorithm. It is meant to provide a certain percentage of the highest score to be considered equally good. This expands the choice-set for random tie-breaking.

With these features they ensure that each run of the algorithm on the same instance will differ in the order in which choices will be made. They claim it can be advantageous to terminate the search when it appears to be stuck. Therefore, they are forced to introduce a *cutoff* parameter to limit the search to a given number of backtracks.

Restarts After the mentioned cutoff, the search is *restarted* from scratch, i.e. restarting at the root of the search tree. Authors claim that this strategy clearly prevents the algorithm from getting trapped in the long tails on the right of the heavy-tailed distribution.

The performance of this technique is mainly determined by the value of the cutoff parameter. Authors argue that a low value could be used to exploit the left part of the distribution, and thus allowing the algorithm to solve several instances after a sufficient number of restarts. A thoroughly study of the impact of the cutoff value on the algorithm performance is provided as well.

Adding new clauses

After finding in the 90's that local search performs well for many SAT problems, the following approaches focused on developing a strategy for escaping local minima. A first approach was to dynamically increase the weights of clauses as search progresses ([162],[203]). However, a more powerful and promising technique was introduced in [33] and [234]. Both approaches suggested that adding implied clauses is explicitly better then adding duplicate clauses, and it also achieves the same effect as in clause weighing.

In [33], adding new clauses is viewed as a way to make the slope of the search space smoother than the simple weighting. Authors claim that this approach is roughly four to ten times faster than weighting in terms of the number of search steps, for the specific weighting scheme they use.

The algorithm (ANC) works as any local search algorithm with a weight strategy. Moreover, as authors have pointed out, increasing the weight of a clause can be seen equivalent to adding another equal clause to the formula. The only problems is how to find these new clauses. The solution adopted in this case is to select resolvents of two clauses, a widely used technique in nogood recording in systematic SAT solvers.

This method is compared against a similar approach (WEIGHT) developed by the same authors ([32]). They present different kinds of instance: a completely random kind of formula, a hard random-generated type that makes use of AIM Generators ([8]), and a few natural ones on fault diagnosis of VLSI design. ANC is significantly better than WEIGHT in terms of moves, but no time comparison is provided, and ANC is supposed to spend a larger amount of time per move.

Even though [162] argued that increasing the cost of visited local minima can eventually solve a satisfiable instance but cannot easily detect unsatisfiability, [75] showed that local search can become complete by adding new clauses and without embedding it in a tree-like framework.

Thus, how to generate new implied clauses is the key feature for achieving completeness in [75]. Authors ensure that no local minima are left after all possible implied clauses have been generated. It is clear that this approach can suffer from

worst-case exponential space complexity, but authors argue that, in practice, the algorithm usually either finds a satisfying assignment or generates the empty clause before that can happen.

The algorithm scheme resembles that of many local search algorithms for SAT. The search proceeds by iteratively changing the value of a single variable in the current assignment. Randomness is not fundamental, and therefore the search moves to a neighboring assignment only if it is strictly better. When this is not possible it means that a local minimum has been reached. At this moment, the clause generator must produce a new implied clause, and it is critical that this is achieved in finite time.

The clause generator provided is called Neighborhood Resolution. For each literal in every violated clause a different clause critically satisfied by the negation of the literal is searched; a new clause is generated by resolving the two clauses. If this new clause is not empty it is added to the formula. The authors develop several theorems to prove that this approach is complete.

Furthermore, several other features are discussed: unit propagation when a unite clause is generated; equivalent literal detection as a limited form of equivalence reasoning; a resolution between similar clauses, if they only differ on the polarity of a single literal; and appropriate data structures with the help of doubly-linked lists.

The empirical evaluation for this approach is one of the most complete we have seen. It is based on the instances and the protocol of the 2003 SAT Competition ([207], [124]). Thus, the algorithm is compared against many state-of-the-art solvers using a broad collection of 996 problems. Comparison demonstrates that Complete Local Search (CLS) is of practical interest. It is very competitive, and it yields close results (mostly better) to local search methods on problems where local search is more efficient, and relatively close results to complete search methods on handmade and industrial instances. Authors claim that had it entered the competition, it would have achieved the best solver on satisfiable random instances award. It is only outperformed by RSAPS ([127]) on few random series.

Another complete local search method for SAT is presented in [206]. It is based

on the approach described above, and it differs in the way they generate new implied clauses. It also uses a form of resolution but over an ordering of propositional variables, which potentially can greatly reduce the number of generated resolvents without sacrificing completeness.

Improving local search by handling variable dependencies

Stochastic local search approaches for SAT became prominent when independently Selman, Levesque, and Mitchell ([202]) as well as Gu ([103]) introduced algorithms based on hill-climbing. One form of improving stochastic local search is to efficiently handle variable dependencies, and it is also one of the ten challenges proposed by [201]. Combining systematic and stochastic search was suggested as a way to achieve it. GSAT ([202]), a local search algorithm for SAT was combined with dynamic backtracking ([92]) in [93]. TSAT ([55]) integrates the extraction of variable implications to a tabu search method.

Another interesting approach is described in [106]. The main idea is to use variable dependencies to construct implications and equivalences between literals. This is achieved by combining two well-known algorithms such as Walksat ([153]) and Satz ([145]). The algorithm proceeds by iteratively extending the current assignment using Satz. When a fixed depth in the search tree is reached it constructs the literal implication graph. The implication graph is reduced to its collapsed strongly connected components graph. Every component is viewed as an equivalence class which is represented by a single literal. Furthermore, the transitive closure of the implication is generated. Walksat is applied to the reduced formula along with a tabu list to forbid any cycling. The process continues until either a solution is found or a fixed depth of the Satz tree is reached.

The hybrid WalkSatz algorithm is then compared against Walksat and Satz on several problems: latin squares, DIMACS instances, superscalar processor verification, Beijing-Challenge benchmarks, and Kautz & Selman planning problems. In general, compared to Walksat, WalkSatz reduces the number of flips required to reach a solution, and presents a good behavior when solving hard instances. However, Satz seems to perform significantly better, at least in terms of computation time.

It is also worth mentioning UnitWalk ([117]), which combines local search and unit clause elimination as well. It is, indeed, based on Walksat and GSAT, mingling the ideas of both algorithms into a single one. UnitWalk has been one of the most successful algorithms for random instances in the past SAT competitions[2].

3.2 Memetic Algorithms

Memetic Algorithms (MAs) is a population-based approach for heuristic search in optimization problems. Some researchers view them as hybrid genetic algorithms. The first use of the term *Memetic Algorithm* in the literature was in 1989 in [163], where a heuristic that incorporated Simulated Annealing with a cooperative game between agents, and the use of a crossover operator was applied to the Traveling Salesman Problem.

It has been argued that it is essential to incorporate some form of domain knowledge into evolutionary algorithms in order to arrive at a highly effective search ([102, 79, 10]). In [156] an assumption is given to support this fact. We can see in figure 3.1 the possibility of combining problem-specific heuristics and an Evolutionary Algorithm (EA) into a hybrid algorithm. It is also assumed that the amount of problem-dependant information is variable and can be adjusted: the more information, the more the curve will resemble a problem-specific method, the less information the more it will approach to a EA method.

Sometimes, an EA is applied to a problem where there is already large amounts of information available. It seems a good idea to use this information to create specialized operators and/or good solutions. In these cases it is common knowledge that a hybrid EA performs better than any of the techniques it incorporates alone. Note that this is not reflected in figure 3.1.

Another issue which is often used as a motivation by researchers is Dawkins' idea of "memes" ([50]). These are viewed as *units of cultural transmission* rather than biological transmission (genes). These "memes" are also selected for reproduction based on some measure of quality (typically either utility or popularity). Since the

[2]http://www.satcompetition.org

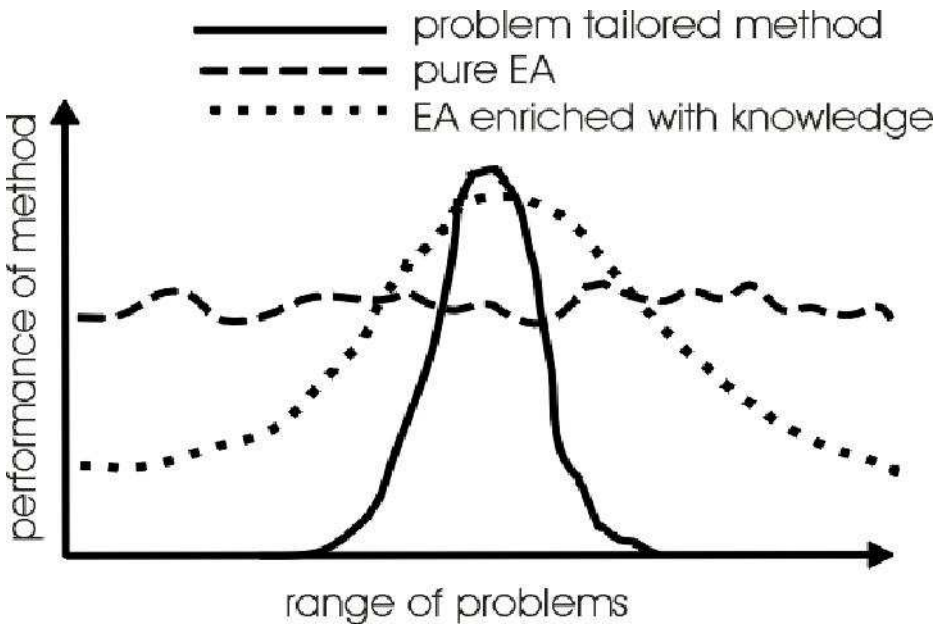


Figure 3.1: EA performance view from [156]

idea was created it has been extended by many authors ([25, 30]). We can view these "memes" from two different points of view: first, as agents that can transform a promising candidate solution; and second, as a learning phase where memes can influence genotypes.

3.2.1 Introducing Local Search

We have introduced the Local Search (LS) framework in the previous chapter. As we know, it is a heuristic technique for solving combinatorial problems by exploring neighborhoods of solution in order to optimize a given objective function. Introducing LS into a GA can be seen as an improvement or developmental learning phase within the evolutionary scheme. We have to consider then whether those changes (acquired traits) should be kept, or whether the improvement should be awarded to the individuals of the original population.

Lamarckianism and the Baldwin Effect

The issue of the inheritance of acquired traits (memes) was a major issue in the nineteenth century. Lamarck argued in favor, while the *Baldwin Effect* ([12]) suggested that favorable adaptation can be achieved without changes in the individuals. Modern theories of genetics strongly support the latter point of view.

However, working with computer algorithms we are not subject to those biological constraints, and thus, both schemes can be perfectly valid. In general MAs are called Lamarckian if the result of the local search phases replaces the original individual, and Baldwinian if the original solution is kept, but the result of its changes is somehow reflected in its fitness function (for example, after applying local search to a solution, maintain the original solution and incorporate the value of the resultant objective function in its fitness). There are many studies in the literature that have tried to extract the benefits from using one or the other ([125, 222, 230]). In the most recent work it seems that either pure Lamarckianism or a probabilistic combination of both are the preferred approaches.

3.2.2 A Memetic Algorithm

As we have seen so far, a Memetic Algorithms is a Genetic Algorithm that uses problem-specific knowledge or incorporates Local Search to any of its operators. Figure 3.2 shows all the places where these techniques can be introduced within a GA scheme (remember figure 2.8). In the following we are going to describe all these possibilities focusing mainly on the introduction of Local Search.

Initial Population

Typically, GAs generate their initial populations at random. However, it is very straightforward to introduce specific knowledge of the problem in this step. Although LS techniques are not usually applied at this point, it is precisely to them that GAs should pay attention: heuristic solutions that are known to be good as a seeding heuristic for a LS algorithm for a given problem can easily be adapted to generate an

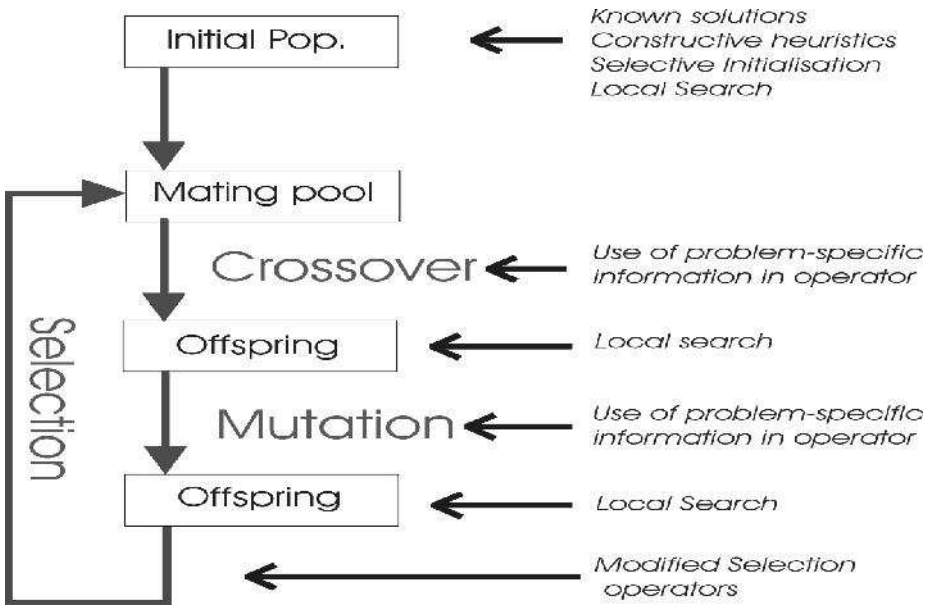


Figure 3.2: A GA scheme and possible ways of hybridization

equally good initial population for a GA.[3]

However, there are MA that incorporate LS as a pre-step to generate the initial population. Scatter Search ([142]), typically generates a set of individuals and then applies a form of LS to them in order to generate the initial population with the resultant solutions.

In any case, the purpose of this improvement is to have a high quality initial population. Nonetheless, in [216], the authors performed an examination of the effect of varying the proportion of the initial population of a GA that was derived from high quality solutions. Their conclusions were:

- Small proportions of derived solutions aided the GA.
- Average performance improves as proportion increases.
- The best performance is achieved from a more random initial population.

[3]Note that in this section we use the term GA instead of MA since we consider that these improvements are incorporated into a GA to yield a MA.

Thus, we can conclude that as the proportion increases, so does the average performance but at the same time, the variance in performance decreases.

Local Search as Crossover and/or Mutation

This idea is very straightforward: apply a certain LS technique as a Crossover or Mutation operator. Mutation and LS are intrinsically the same kind of technique, they change the genotype of the individuals. The difference is that mutation is random and LS is heuristic.

Some approaches in the literature report good results when introducing LS at this point. For example, in [223], a modified one point crossover operator used for protein structure prediction is introduced. The modified operator made use of some problem-specific knowledge by explicitly testing all the possible different orientations of the two fragments to recombine in order to find the most energetically favorable. If no feasible conformation was found, a different crossover point was chosen and the process repeated. This can be seen as a simple introduction of LS into the recombination operator.

In [130], the authors propose a simple *crossover hill-climber* in which all the possible offsprings arising from one point crossover are constructed and the best chosen.

In [82], a more complex approach is presented: a distance preserving crossover operator for the Traveling Salesman Problem (TSP). The intelligent part of the operator is based on a nearest-neighbor heuristic to join together the subtours inherit from the parents, thus, explicitly exploiting instance-specific edge length information.

Local Search applied to the outcome of recombination

The most common technique of hybridization of GAs is via the application of one or more steps of improvement to individuals of the population during the evolutionary cycle. LS is typically applied to whole solutions created by mutation or crossover.

Perhaps surprisingly, the effort to use GAs to evolve artificial neural networks gave a great deal of insight into the role of learning, Lamarckianism and the Baldwin effect

to guide evolution ([116, 125, 152, 231]). It also served to reinforce the opinion of several researchers of the usefulness of incorporating local search and domain-based heuristics.

It is of especial interest the formal proof in [141], which indicates that in order to reduce the worst-case run times, it is necessary to choose a local search method whose move operator is not the same as those of the crossover and mutation operators.

This is also a feature of the MA Scatter Search previously introduced. Not only applies local search to the pre-initial population, but also to every new generated individual after recombination.

Hybridisation during fenotype-to-genotype mapping

A widely used hybridization of GAs with other heuristics is during the genotype-to-fenotype mapping. Many approaches have been proposed in the literature for timetabling and scheduling problems ([111]) or for the vehicle routing approach ([218]).

([218]) presents a complex two-phase algorithm to solve the Vehicle Routing Problem with Time Windows (VRTW). The first phase is a GA and the second phase is a local post-optimization algorithm. In the GA the population is represented by sequences of offsets. The Genetic Sectoring method (as it is called in the paper) uses a genetic algorithm to adaptively search for sector rays that partition the customers into clusters served by each vehicle. This does not always yield feasible solutions, that is why it needs to be improved by means of a local optimization process that moves customers between clusters.

It is also interesting the approach presented in [43]. It introduces concepts from Greedy Randomized Adaptive Search Procedures (GRASP[4]) into the genotype-to-fenotype phase of a GA to solve the Golomb Ruler Problem. The genotype in this case is a vector of GRASP parameters that indicates which choice to make when assigning the next mark of the ruler during the genotype-to-fenotype mapping.

As it can be seen, there is a common thread in all these approaches, which is to

[4]GRASP is a metaheuristic that can be seen as a two step iterative process: construction an local search. Consult [190] and [175] for the related reactive GRASP.

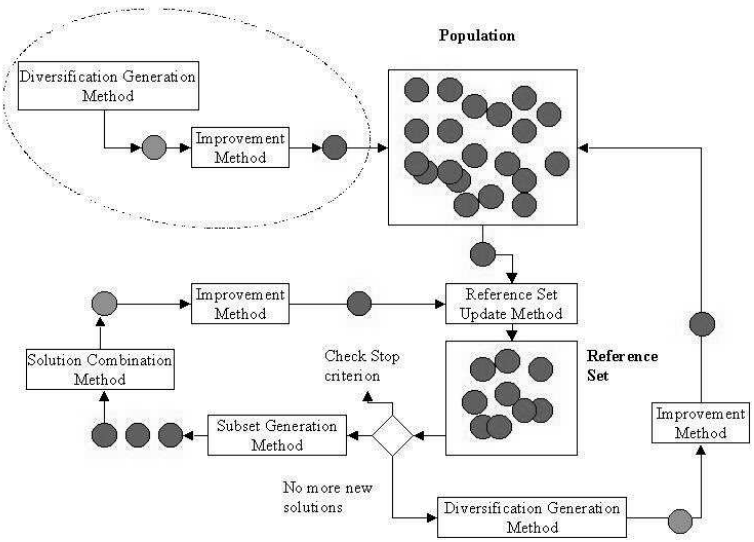


Figure 3.3: A generic SS algorithm diagram

make use of existing heuristics and domain specific knowledge.

3.2.3 Scatter Search: A Popular MA

We have previously mentioned the Memetic Algorithm known as Scatter Search. It is a generic template of a kind of MA which is thoroughfully described in [142]. It is of great importance for this research since the final hybrid is going to be based on this particular scheme.

Figure 3.3 shows the diagram of a generic Scatter Search Algorithm. It starts by generating the initial population and improving it by means of a heuristic procedure. From the population a high quality set of individuals is included in the Reference Set. From there the algorithm will select individuals to combine and improve the descendants as well. The Reference Set is then updated with the new individuals and the process is repeated until no more solutions can be added to the Reference Set, when some restarting mechanism is introduced, or finally, when some stopping criterion has been reached (typically max number of generations or time limit).

Let us review each of these steps more thoroughly:

Diversification Generation Method

In this step a starting set of solutions is generated. Through some mechanism, a certain level of diversity is guaranteed. This is usually achieved by generating high quality solutions and diverse solutions as separate goals. These solutions will now be improved in order to be transferred to the Reference Set.

Improvement Method

After the pre-initial population has been generated or whenever a new individual is created, an improvement method is applied to the solution. This method is usually a heuristic local search procedure such as tabu search or simulated annealing.

Reference Set Update Method

The Reference Set is now filled with the solutions with higher quality from the previous steps. The notion of quality here is not limited to the value of an objective function, diversity is a key factor to decide whether a solution must be kept on the reference set or not.

Subset Generation Method

This steps will define the subsets of individuals of the reference set to be latter recombined. These are the generic subsets to be generate:

- All 2-individuals subsets.
- 3-individuals subset generated from the 2-individuals subsets by adding the best solution not included in the subset.
- 4-individuals subsets generated in the same fashion from the 3-individuals subsets.
- The subsets consisting of the best n elements, being $n = 5$ to the size of the reference set.

Note that some subsets can be repeated, simple and efficient techniques to avoid that are presented in [94].

Solution Combination Method

This method consists of combining the individuals of the previously generated subsets. It is typically dependant of the specific problem. It can also generate one or more solutions depending on its implementation. It is also important that the new solutions are generated in a deterministic fashion; then, that will be recorded in order not to combine the same subsets in subsequent iterations.

3.3 Genetic Algorithms and CP

In this section we are going to review state-of-the-art approaches that introduce Constraint Programming techniques into GAs. Note that this section could fall into the category described in the previous section; these approaches can be seen as Memetic Algorithms, since they are GAs that incorporate problem-specific knowledge in some steps of the evolutionary scheme. In this case, this knowledge falls into the field of Constraint Programming, and thus, we have decided to separate it and describe it in a different section.

3.3.1 Handling Constraints

The first issue to describe is constraint handling. Remember that in a *constraint satisfaction problem* (CSP) we are given a set of variables, where each variable has a domain of values, and a set of constraints acting between variables. The problem consists of finding an assignment of values to variables in such a way that the restrictions imposed by the constraints are satisfied.

We can also define a CSP as a triplet $< X, D, C >$, where $X = \{x_1, \ldots, x_n\}$ is the set of variables, $D = \{D_1, \ldots, D_n\}$ is the set of nonempty domains for each variable x_i, and $C = \{C_1, \ldots, C_m\}$ is the set of constraints. Each constraint is defined over some subset of the original set of variables $\{x_1, \ldots, x_n\}$ and specifies the allowed

combinations of these variable values. Thus, solving the CSP is equivalent to finding a complete assignment for the variables in X with values from their respective domain set D, such that no constraint $C_i \in C$ is violated.

The issue is thus, how to handle these constraints: either directly or indirectly [63].

- **Direct handling** leaves the constraints as they are, and enforces them somehow during the execution of the algorithm; while,
- **Indirect handling** involves transforming the constraints into an optimization objective (included in the fitness function), which the EA will pursue.

Direct handling is not generally oriented for EA due to the lack of an optimization function in the CSP, which would result in no guidance towards the objective. Thus, indirect handling is the best suited approach for EA, although a mixed strategy where some constraints are enforced and some are transformed into an optimization criteria is suited as well.

Whenever a direct handling approach is chosen, the algorithm will have to face many problems, especially because the combination and mutation operators are blind to the constraints, and recombination of two feasible solutions can yield an infeasible one. Approaches to solve this are:

- Repair infeasible individuals.
- Eliminate infeasible individuals.
- Maintain feasiblity with special purpose operators.
- Transforming the search space.

Repairing infeasible solutions implies developing a repair operator which is very problem-dependant. If implemented properly can nontheless produce efficient results (see [158] for a comparative study). Eliminating infeasible individuals is not very efficient and hardly ever used. Maintaining feasiblity is also very problem-specific; note that in order to maintain this, the initial population needs to be feasible, which

is in itself NP-hard sometimes, and obviously not an option when dealing with constraint satisfaction problems[5]. Finally, transforming the search space can simplify the problem and allow an efficient GA. The new search space is decoded to create feasible solutions and it also allows a free search for the GA.

On the other hand, indirect constraint handling is typically performed by adding penalties to constraint violations. These penalties are incorporated into the objective function in order to drive the search towards a feasible solution. Constraint penalties represent distance to feasibility. This approach is usually the best suited for constraint satisfaction problems because it is general, and allows the problem to be transformed into an optimization problem. However, it is sometimes complicated to merge penalties with objective function. It is also known to perform poorly for sparse problems.

In the next sections we will review different GAs for solving constraint satisfaction problems, divided into three different groups:

- Heuristic based methods.
- Adaptive based methods.
- Memetic Algorithms for CSPs.

Note that all the techniques present either an indirect or a mixed direct and indirect constraint handling approach.

3.3.2 Heuristic based methods

The methods reviewed here have in common the fact that they all extract heuristic knowledge from the structure of the constraints to be incorporated in the GAs.

Heuristic Genetic Operators

This technique has been introduced in [65, 66]. It studies the possibility to incorporate exiting CSP heuristics into genetic operators. These operators are mutation and

[5]If we were trying to find a feasible solution for a problem and the initial population was feasible, then the problem would be already solved

multi-parent crossover, which are guided by the same heuristic: select the variables which appear in more constraint violations and instantiate them with the value that minimizes these violations.

Thus, the mutation operator will select a certain number of variables in the individual and will change their values so as to minimize the number of constraint violations. The multi-parent crossover will proceed similarly, only that in this case only the values found in any of the parents will be taken into consideration.

Knowledge Based Fitness

In this case, information about the constraint network is incorporated in the fitness function and in the genetic operators (see [191, 192]) as well.

The fitness function is called *arc-fitness* and it consists of the sum of the *error evaluations* of the violated constraints. The *error evaluations* of a constraint is the number of variables in its scope plus the number of variables conected to them in the constraint network.

The mutation operator (called *arc-mutation*) simply selects a variable randomly and instantiates it with the value that minimizes the sum of *error evaluations*. The crossover operator which is called *constraint dynamic adaptive arc-crossover* basically constructs a new individual by focusing on constraints and selecting the values of the variables in those constraints from one parent or the other in order to minimize the fitness function as well.

Moreover, it includes a heuristic parent selection mechanism that divides the population in three different groups, based on the value of their objective functions.

The Glassbox Approach

In [150, 151, 44] it is described a GA to solve CSPs based on pre and post-processing techniques. In particular, in [150], the algorithm developed relies on the transformation of the constraints into a canonical form. This rewriting of constraints is called *constraint processing* and is performed in two steps:

1. Elimination of functional constraints.

2. Decomposition of the CSP into primitive constraints in the form of inequalities.

With all the constraints in primitive form, a single repair-based heuristic is applied. This heuristic is called *dependency propagation* and it attempts to repair violated constraints in random order.

Note that at the end of the repairing process the individual might not be a feasible solution, since repairing violated constraints can produce other constraint violations.

Coevolutionary Approach with Heuristics

In [109, 108], we can find a coevolutionary algorithm where the host population is parasited on by a population of schemata. Schemata are individuals which have some of their variables instantiated with an unknown value. The interaction between the population is performed using two mechanisms:

- **Superposition:** a parasite finds a match in the host population and it simply instantiates the unknown variables with the values of its host. This is performed in order to calculate the fitness function of the parasite individuals.
- **Transcription:** it randomly chooses variables of an individual and replaces their values with the unknown values of the parasite population.

The host fitness function is not only based on constraint violations, but it is also normalized to a range from 0 to 1 taking into account the number of violated constraints versus the total number of constraints. The host mutation and crossover operators are standard (random mutation and one-point crossover).

Hybrid GRASP-Evolution

The method presented in [31] is slightly different from the rest of the approaches in this category. The algorithm does not present any specific-problem features, but it incorporates a novel genotype-to-fenotype mapping. The population is a set of GRASP parameter vectors as in [43]. In the same manner, the value of each parameter defines the exact candidate to select, instead of a range for a random selection as in the

general case in GRASP. This is due to the stochastic genotype-to-phenotype mapping that would yield, which will, thus, add a level of complexity in the algorithm.

The initial problem is transformed into that of finding an optimal ordering for the variables that will yield a feasible solution. Thus, the vector of GRASP parameters allows to choose, among the ranked variables, which one is going to be instantiated next.

The basic procedure for assigning a variable within the genotype-to-fenotype mapping is as follows:

1. Present the variables available for selection.
2. Apply the dom/degree heuristic to these variables.
3. Define the resultant Restricted Candidate List.
4. Select the candidate variable that the GRASP parameters vector indicates.
5. Instantiate the variable with the best value possible.
6. Reflect this selection and instantiation in the correspondant position of a vector that represents an actual tentative solution of the problem.

3.3.3 Adaptive based methods

All the methods included in this category share the common emphasis on adaptation features rather than on heuristic operators.

The Coevolutionary Approach

This approach has been tested on many different problems ([169, 170]). Interestingly, it has been aplied to solve CSPs in [71, 226]. It consists of two populations that evolve in a predator-prey model: a population of candidate solutions and a population of constraints.

The fitness of the individuals of both populations is based on a history of *encounters*. Encounters are matchings between constraint and individual which reward

the individual if it satisfies the constraint, or reward the constraint otherwise. This results in a higher fitness for constraints that are often violated, which means that the algorithm will focus on harder constraints.

Mutation and crossover are only performed in the population of candidate solutions. The crossover operator aims at generating diverse individuals.

Step-Wise Adpatation of Weights

The Step-Wise Adaptation of Weights (SAW) mechanism was introduced in [70, 225] as an improved version of the weight adaptation mechanism presented in [67]. The basic idea behind this mechanism is that constraints that are not satisfied and variables causing constraint violations after number of steps must be hard, and so they should be given higher weights.

This algorithm presents a steady state model with a representation based on permutation models. A permutation is transformed into a solution by a decoder that simply instantiates variables, in the order in which they occur in the chromosome, with the first feasible value; if this feasible value does not exist, the variable is then left uninstantiated. Uninstantiated variables are penalized and the fitness of a chromosome is the sum of all these penalties.

3.3.4 MAs for solving CSPs

We have separated these techniques because they not only introduce CSP like mechanisms but also Local Search. These are the most similar approaches to our final hybrid. They are, however, different in the sense that they only incorporate knowledge of the constraint network for solving a CSP, instead of actually including a CP-like procedure within the algorithm.

Genetic Local Search

A Genetic Local Search Algorithm for solving CSPs is presented in [151]. The basic scheme consists of the application of genetic operators to a population of local optima

produced by a LS algorithm. The process is iterated until either a solution is generated or the maximum number of generations is reached.

The LS algorithm used is a Repair and Improve heurisitic: it repairs the population by extracting and extending every candidate, and improves it by applying arc-consistency, deleting and extending.

Since the algorithm deals with feasible partial instantiations, in this case, the fitness functions corresponds to the number of instantiated variables on the individual.

Evolving Hill-Climbers

In [58, 59] we find a GA with a very small population (that is why it is called *micro-evolutionary*) whose population is a set of hill-climbers.

Every candidate solution contains four different fields:

- **Field 1:** is a chromosome containing each object.
- **Field 2:** is the fitness of the individual.
- **Field 3:** determines the heursitic-based mutation operator.
- **Field 4:** is the individual's family identification number[6].

The evaluation function determines the individual's fitness by substracting the weights of all violated constraints. The algorithm evolves the population using several crossover and mutation operators, and also applying an adaptation scheme that awards the operators that yield superior offsprings.

Most of these methods are compared using random binary CSPs in [45]. Other classifications are available in the literature ([157, 155]).

[6]Family or relatedness is a mechanism to reduce the number of duplicates within the population

Part II

Preliminary Work on Pure and Hybrid Approaches

Chapter 4

CP and SAT for the Quasigroup Completion Problem

The Quasigroup Completion Problem (QCP) is a very challenging benchmark among combinatorial problems, which has been the focus of much recent interest in the area of constraint programming. It has a broad range of practical applications [101]; it has been put forward as a benchmark which can bridge the gap between purely random instances and highly structured problems [100]; and its structure as a multiple permutation problem [229] is common to many other important problems in constraint satisfaction. Thus, solutions that prove effective on QCPs have a good chance of being useful in other problems with similar structure.

In this chapter, we present several techniques within the constraint programming and SAT frameworks that together allow us to solve significantly larger QCPs than previously reported in the literature. Specifically, [101] reports that QCPs of order 40 could not be solved by pure constraint programming approaches, but could sometimes be solved by hybrid approaches combining constraint programming with mixed integer programming techniques from operations research. We show that the pure constraint satisfaction approach can solve many problems of order 45 in the transition phase, which corresponds to the peak of difficulty. Our solution builds upon some known ideas, such as the use of redundant modeling [36] with primal and dual models of the problem connected by channeling constraints [229], with some new twists. For

example, we will consider models consisting of only channeling constraints, without any primal or dual constraints, and we demonstrate empirically for the first time the usefulness of channeling constraints linking several pairs of models of a problem, an idea that was considered, but only theoretically, in [35] and [212]. In addition, we present a new value ordering heuristic which proves extremely effective, and that could prove useful for many other problems with multiple models. The idea underlying this heuristic, which originates in the work of [35, 211] for single permutation problems, is that selecting a value for (say) a primal variable is in practice in the presence of channeling constraints also a choice of the dual variables corresponding to that value; therefore we can use *variable* selection heuristics on the dual variables to choose the *value* to assign to the previously chosen primal variable. Finally, we show how redundant constraints can be used to "compile arc consistency into forward checking", that is, to ensure that the latter has as much pruning power as the former but at a much lesser cost in constraint checks.

It is interesting to note that our approach involves only binary constraints, which seems to go against common wisdom about their limitations —when contrasted with the use of non-binary constraints such as alldiff [188]— in solving quasigroup completion problems [215]. It is certainly an interesting issue, which we plan to address in the future, whether the use of alldiff could yield even better results than our approach when coupled with other ideas in this work.[1]

The idea of redundant modeling was first introduced by [36]. The benefits of adding redundant constraints to some given model to improve pruning power were well-known in the literature, but [36] went a step further by considering the redundant combination of full models of a problem, where the models may involve different sets of variables. This combination is achieved by specifying how the various models relate to each other through *channeling constraints*, which provide a mapping among assignments for the different models. The combined model contains the original but redundant models as submodels. The channeling constraints allow the sub-models to cooperate during constraint-solving by propagating constraints among the problems,

[1] Besides the obvious computational limitations in running large experimental suites of hard QCP problems, we were limited in this aspect by the unavailability of open source alldiff code.

providing an extra level of pruning and propagation which results in a significant improvement in performance.

Another important modeling idea that we use is that of permutation problems (see e.g. [211, 229]). A constraint satisfaction problem (CSP) is a permutation problem if it has the same number of variables as values, all variables have the same domain and each value can be assigned to a unique variable. Thus, any solution can be seen as assigning a permutation of the values to the variables. In the same manner, a multiple permutation problem has some (possibly overlapping) sets of variables, each of which is a permutation problem. QCP is a paradigmatic example of a multiple permutation problem.

Moreover, we perform a systematic study of modelling choices for quasigroup completion, testing a variety of solvers and heuristics on various SAT and CSP encodings. The clear winner is the SAT 3D-encoding, specially with the solver Satz [144], closely followed by the solver Satzoo [62] on the same encoding. As these two solvers are quite different (one uses a strong form of lookahead in its heuristic, but no backjumping or learning, while the other relies heavily on the last two), the 3D encoding appears to be quite robust as a representation. On the other hand, CSP models perform significantly worse with the two solvers we tried, and standard SAT encodings generated from the CSP models are simply too large in practice. These results strongly suggest that the 3D encoding can turn out to be quite competitive in other permutation problems (many of which arise in quite practical problems [118]) when compared with the currently preferred channelling models.

The reasons for this appear to be twofold. First, we can show that the 3D encoding (which is basically the "SAT channelling model" of [118] extended to multiple permutations and dual models) exactly captures the channelling models of QCPs as defined in this thesis, but in a much more concise way, by collapsing primal and dual variables. Further, we can show that the 3D encoding captures the "support SAT encoding" of the channelling model, hence by results of [89], that unit propagation on the 3D encoding achieves the same pruning as arc consistency (MAC) in the CSP channelling model. These results appear easy to extrapolate to other permutation problems (or similar ones with "channelling constraints"), which have received a lot

of recent attention [35, 229, 118]. Second, empirically, we identify Satz's UP heuristic as crucial to its success in this domain; as shown by the fact that, when importing the heuristic into our CSP solvers, we obtain significant improvements in their scalability. Further, the improvements are much smaller if we only use lookahead to detect potential wipeouts (i.e. for "failed literal detection"), but choose variables instead by some other standard heuristic such as min-domain.

The rest of the chapter is organized as follows: first we introduce Quasigroups and the QCP problem, then we detail the modeling and heuristic used and give experimental results; Afterwards, we introduce SAT models and solvers, compare results against CSP solvers and introduce SAT features in our CSP solver to provide a new comparison. Finally, we present the lessons learnt from this research.

4.1 Quasigroups

A quasigroup is an ordered pair $(Q, \cdot)$, where Q is a set and $\cdot$ is a binary operation on Q such that the equations $a \cdot x = b$ and $y \cdot a = b$ are uniquely solvable for every pair of elements a, b in Q [101]. The order n of the quasigroup is the cardinality of the set Q. A quasigroup can be seen as an $n \times n$ multiplication table which defines a Latin Square, i.e. a matrix which must be filled with "colors" (the elements of the set Q) so that the colors of each row are all distinct, and similarly for columns.

Early work on quasigroups focused on quasigroup existence problems, namely the question whether there exist quasigroups with certain properties, solving several significant open mathematical problems [208]. We focus instead on the *quasigroup completion problem* (QCP), which is the (NP-complete [38]) problem of coloring a partially filled Latin square.

4.1.1 Quasigroup Completion Problem

Imagine you have an empty Latin square, and that you color some of its cells and left some others empty. Trying to extend that partial coloring to a solution (if possible) defines the *Quasigroup Completion Problem*.

QCP share with many real world problems a significant degree of structure, while at the same time allowing the systematic generation of difficult problems by randomly filling the quasigroup with preassigned colors. It is thus ideally suited as a testbed for constraint satisfaction algorithms [100]. Experimental studies of the problem have confirmed its interest for research, by for example helping to discover important patterns in problem difficulty such as heavy-tailed behavior [98].

Instances of QCP

It is also important to introduce types of instances for the *quasigroup completion problem*. Not only in order to establish a framework for the experiments, but also because the study of its hardness and its complexity are within the state of the art in this problem. There also a need of a source of satisfiable instances for the evaluation of some algorithms.

Under this perspective we can differentiate two kinds of instances for this problem:

QCP We have introduced the QCP problem in the initial sections, and it is an NP-complete problem [38] which has an interesting phase transition phenomenon with an associated easy-hard-easy pattern as a function of the fraction of number of preassigned colors. This kind of instances that we will refer to as QCP from now on, are generated in a way that can be solvable or not. This means that we cannot assure its solvability because of the way they are generated.

Within this kind we can distinguish between those instances which are *trivially* unsolvable, which means that the preassignment itself violates one ore more constraints; and those which we do not know its solvability until a complete algorithm terminates without finding a feasible solution.

QWH As mentioned above, there is a need for hard solvable instances, in order to have a source for evaluating for example local search algorithms. The *quasigroup with holes* (QWH) problem was proposed in [2] as a way to fill this need.

QWH instances are given this name because of the way they are generated [2]: (1) first generate a complete Latin square according to the Markov chain Monte Carlo approach proposed by Jacobson and Mathews [128]; punch a fraction p of "holes" in the Latin square in an uniformly distributed manner. The resulting partial Latin square is guaranteed to be solvable. We can also find two different types of instances within QWH:

Random This kind of instances are generated punching holes at random. This was the first kind of instances generated and studied, thus we know that its phase transition coincides with $\lceil 1.6 \times n^{1.55} \rceil$ holes for order n.

Balanced Lately, this kind of instances have been studied and it seems that they are much harder than random ones. They are generated in a way that the number of holes in each row and in each column is more or less the same.

4.2 Modelling and solving QCPs as a CSP

Our first step through improving efficiency solving QCPs is due to an effort to make competitive an initial implementation for this problem that yielded very poor results when compared with the literature. Guided by this objective and after studying some techniques and approaches applied to solve QCPs (those introduced in previous sections) we found an implementation and an heuristic that yields promising results.

4.2.1 Not-equal implementation

First of all we introduce the initial implementation of the problem, to which we will refer as the *primal model*.

This model represents cells of the Quasigroup as variables whose domains are the set of possible colors to be assigned:

[2] We thank Carla Gomes for providing us with the lsencode generator, which was used for generating satisfiable instances for the experiments that are presented in the next sections

$$x_{i,j} \in \{1,..,n\} \forall \quad i,j$$

$$x_{i,j} = k \quad \forall i,j \text{ such that } QCP_{i,j} = k$$

$$not-equal(x_{i,1}, x_{i,2}), not-equal(x_{i,1}, x_{i,3}), ..., not-equal(x_{i,1}, x_{i,n}) \quad \forall i$$

$$not-equal(x_{1,j}, x_{2,j}), not-equal(x_{1,j}, x_{3,j}), ..., not-equal(x_{1,j}, x_{n,j}) \quad \forall j$$

It is important to note that we first choose a not-equal implementation instead of an alldiff one. This election was maintained for all the experiments from now on.

4.2.2 Redundant models

Redundancy is a double-edged sword: it can help propagation by allowing more values to be pruned at any given point in the search, but it can also hinder it by forcing it to process a larger set of constraints. Fortunately, more fine grained distinctions are possible, as we might choose to combine only parts of various models. We could not speak of combining models if we don't use their respective sets of variables, but it will often be advantageous (as we will see) to drop some of the constraints from one or more models that become redundant when making the combination. If we do this, however, we must be careful to ensure the correctness and completeness of the combined model.

Several models can be defined for QCPs, as described next. While all models have the same logical status, it is common to distinguish between *primal* and *dual* models. The distinction is only a matter of perspective, specially in permutation problems, where variables and values are completely interchangeable.

Primal Model This is the model introduced before, and we will refer to it as `pr` model for short.

Row Dual Model There are different ways to formulate dual models for a multiple permutation problem. Here we consider dual models for each of the permutation subproblems (as opposed to a single dual model of the primal problem), and group

them by row and column, to obtain two complete models of QCPs. In the *row dual model*, the problem is reformulated as the question of which position (column) in a given row has a given color. The *row dual variables* are the set $R = \{r_{ik} \mid 1 \leq i \leq n,\ 1 \leq k \leq n\}$ where r_{ik} is the kth color in the ith row. The domain of each variable is again the set $D = \{j \mid 1 \leq j \leq n\}$, but now the values represent columns, i.e. the positions in row i where color k can be placed. The *row dual constraints* are similar to the primal constraints. There are n^2 constraints of the form $r_{ik} \neq r_{il}$, where $r_{ik}, r_{il} \in R$ and $l \neq k$, which means that two colors in the same row must not be assigned to the same column; and n^2 constraints of the form $r_{ik} \neq r_{jk}$ where $r_{ik}, r_{jk} \in R$ and $i \neq j$, which means that the same color in different rows must not be assigned to the same column. Alternatively, we could have *alldiff*$(r_{i1}, \ldots, r_{in})$ for every row i, and *alldiff*$(r_{1k}, \ldots, r_{nk})$ for every color k.

A simple symmetry argument shows that this model also fully characterizes the problem.

Column Dual Model The second dual model is composed of the set of dual models for each column permutation constraint, representing the colors in each column. The *column dual variables* are the set $C = \{c_{jk} \mid 1 \leq j \leq n,\ 0 \leq k \leq n\}$ where c_{jk} is the kth color in the jth column. All variables have domain $D = \{i \mid 1 \leq k \leq n\}$, where i represents the rows where color k can be placed in the jth column. Similar to the row dual model, we have *column dual constraints* of the form $c_{jk} \neq c_{jl}$ where $c_{jk}, c_{jl} \in C$ and $k \neq l$, which means that two colors in the same column must not be assigned to the same row; and of the form $c_{jk} \neq c_{lk}$ where $c_{jk}, c_{lk} \in C$ and $j \neq l$, which means that the same color in different columns must not be assigned to the same row.

This model also fully characterizes the problem. We refer to the combination of both dual models as the `dl` model.

4.2.3 Combining the Models

A *channelling constraint* for two models $M_1 = (X_1, F_1, C_1)$ and $M_2 = (X_2, F_2, C_2)$ is a constraint relating variables of X_1 and X_2 [36]. We will consider the following kinds of channelling constraint:

- *Row Channelling Constraints:* Constraints for the n row permutation constraints, linking the primal model with the row dual model:

$$x_{ij} = k \Leftrightarrow r_{ik} = j.$$

- *Column Channelling Constraints:* Corresponding to the n column permutation constraints, they link the primal and the dual column models:

$$x_{ij} = k \Leftrightarrow c_{jk} = i.$$

- *Triangular Channelling Constraints:* These constraints link both dual models, closing a "triangle" among the three models:

$$c_{jk} = i \Leftrightarrow r_{ik} = j.$$

Given two or more redundant, complete models, we can obtain a combined model by simply implementing all the models and linking them by channelling constraints. Thus the full combined model or `pr-dl-ch2-model` resulting from the above models is the model consisting of primal and dual variables and constraints, linked together by row and column channelling constraints.[3] More generally, as long as a combined model includes a complete model of the problem as a submodel, we are free to add any set of variables or constraints from other models, with the only requirement that in order to add a constraint all its variables must belong to the combined model. Thus, for example, given the primal variables and constraints, we may choose to add any number of dual and channelling constraints as long as the corresponding variables are also added. For example, we may decide to use only the row dual variables together with the row dual constraints and/or row channelling constraints. Nothing is lost by not including parts of the dual models, since all the necessary information is present in the primal model.

In fact we can take this as far as removing all primal and dual constraints! Walsh [229] shows that arc consistency on the channelling constraints for a permutation

[3]We don't consider adding the triangular constraints until later.

problem dominates in pruning power over arc consistency over the binary not-equal constraints. Intuitively, this means that nothing is gained by adding the not-equal constraints once we have the channelling constraints. Note that this doesn't prove the superiority of a model with only channelling constraints over, say, the primal model, as the former also has many more variables and constraints; this issue is empirically examined later. It is important however to show that the model consisting of primal and dual variables, with *only* row and column channelling constraints, but *without* the primal or dual constraints (i.e. alldiff or not-equal) is also a complete model of the problem. We refer to this model as the *bichannelling model* or `ch2`:

Proposition 4.2.3.1. The bichannelling model is equivalent to the primal model, hence it provides a full characterization of QCPs.

Proof. If the two models had the same set of variables and associated domains, we could define equivalence just as having the same set of solutions. Since that's not the case here, we need to provide instead a one-to-one mapping between solutions of either model.

Let us say that a primal assignment, or P-assignment for short, is an assignment of values to all the primal variables, and a PD-assignment an assignment to all primal and dual variables.

The proposition can then be phrased more exactly in terms of the following two claims.

Claim 1: Any P-assignment A which satisfies the (primal) alldiff constraints can be extended to a PD-assignment B which satisfies the channelling constraints. To extend A to B, we just pick each label $x_{ij} = k$ from A and set $r_{ik} = j$ and $c_{jk} = i$ in B. To see that B is well-defined, note that every r_{ik} gets assigned, since A must use all available colors in order to fill row i in accordance with the primal constraints; and that any given r_{ik} is assigned at most once, since otherwise we would have $x_{ij} = x_{ih}$ for distinct columns j and h, in contradiction with the fact that A satisfies the primal constraints. Similarly for any c_{jk}. Hence B is well-defined, and it satisfies the channelling constraints by construction.

Claim 2: Any PD-assignment B satisfying the row and column channelling constraints, is such that its primal subset A satisfies the primal constraints. Suppose not. Then B assigns the same value k to two primal variables x_{ij} and x_{ih} for $j \neq h$ (or the completely symmetric case where it is row indexes that vary). But since B satisfies the row channelling constraints, B should satisfy $r_{ik} = j$ and $r_{ik} = h$, which is impossible. □

Yet another combined model we will consider later is the *trichannelling model*, or `ch3` for short, which adds the triangular channelling constraints to `ch2`, but still keeps away from the primal and dual constraints. Given the above proposition, `ch3` is also a complete model, and redundantly so.

4.2.4 Variable and Value Ordering

It is well know that the order in which we make our choices as to which variable to instantiate, and with which value, can have a major impact in the efficiency of search. As already pointed out, all the results reported here use the *min-domain* variable ordering heuristic (often denoted `dom`), which at each search node chooses a variable with the smallest domain to instantiate. The reason for this is simply that we obtained better results with it than with other alternatives we tried. These included more fine-grained heuristics such as `dom+degree` and `dom/degree`, yielding further confirmation to previous results by [36] and [211] on simple permutation problems. These other heuristics would often make no difference with respect to `dom`,[4] but when they did it was most often to the worse. (We did not perform a systematic comparison, though.) We also considered a number of variants of the above which took into account the (primal or dual) model to which variables belong, e.g. selecting only among primal variables, or only among primal variables unless some dual variable had a singleton domain, etc. These variants would often significantly underperform the previous ones, so we didn't pursue them further.

[4]This is not much of a surprise, since the degree of a variable (number of constraints in which it is initially involved) cannot discriminate much among variables in a QCP; though this could also depend on details of implementation such as whether constraints are generated for variables that are explicitly or implicitly assigned by the initial coloring.

[35] introduced a *min-domain value ordering heuristic* to apply when dual variables are available during the search. The idea is to choose the value such that the corresponding dual variable has the smallest current domain. To generalize this idea to multiple permutation problems, we need a way to take into account the two dual models. The one that worked best is what we might call the *min-domain-sum value selection heuristic* (or more briefly `vdom+`, the 'v' standing for value). Once a primal or dual variable is selected, we need to choose a value for it. Since any such value corresponds to one specific variable from each of the two other models, we select the value whose corresponding two variables have a minimal "combined" domain. Specifically, say we have chosen x_{ij}. Then we choose a color k from its currently active domain for which the sum of the current domain sizes of r_{ik} and c_{jk} is minimal among the currently available colors for x_{ij}. Similarly, if the chosen variable is a dual one, say r_{ik}, we choose a column j for this variable as a function of the current domain sizes of the corresponding variables x_{ij} and c_{jk}.

4.2.5 First experiments on balanced instances

Our initial results on the various models were in fact quite favorable to the bichannelling model. In order to present them, we need to say a few words about the experiments in this section. First, in order to make our results comparable with others appearing in the literature, all instances were generated using the *lsencode* generator of QCPs. This generator begins by randomly coloring an empty quasigroup using a local search algorithm, and then randomly decoloring some cells. Hence all problems in our suites have a solution. All instances are of the "balanced" kind, which are known to be the hardest [101]; and most instances correspond to problems with 60% cells preassigned, which is close to the transition phase and corresponds to a peak in problem hardness. Second, all experiments here are run with a slightly optimized variant of van Beek's GAC library, which comes as part of the CSP planning system CPLAN [224], and which implements generalized arc consistency (though in our case we only need its binary version, which is equivalent to the MAC algorithm [22]). As discussed below, neither CBJ nor nogood learning seem to help in QCP, contrary to

% preassign →		20%		42%		80%	
order	% solved	mean	median	mean	median	mean	median
30	100%	0.94	0.93	0.43	0.25	0.03	0.02
35	100%	1.99	1.99	0.71	0.53	0.05	0.05
40	100%	4.98	4.98	2.51	1.09	0.08	0.08

	60% preassigned			
order	% solved	timeout	mean (solved)	median (all)
30	18%	100	48.74	100
35	22%	3600	903.07	3600
40	10%	3600	1751.90	3600

Table 4.1: Experimental results for the bichannelling model, MAC, no value ordering.

the experience in many other domains, hence they are disabled in our tests. Also, all experiments use the min-domain variable selection heuristic, which we found to be uniformly the best among the ones we tried (see also [36, 211] and the discussion in Section 4.2.4).

We can distinguish two different moments in these experiments:

Before applying our heuristic

In our initial tests, we found that the bichannelling model `ch2` could solve many problems that were out of reach for the other models, including many order 35 and some order 40 quasigroups with 60% preassigned cells. Table 4.1 shows mean time for solved instances and median time for the whole sample, both in seconds, and percent of solved instances within the given timeout (also in seconds) for sets of 50 instances of orders 30, 35 and 40, and 20, 42, 60 and 80% preassignment. (These results are also plotted in Figure 4.1 later.)

Our data confirm the existence of a peak of difficulty around 60% preassignment [101], whereas problems were trivially solvable with all other percentages we tried. Even though the results were promising, specially when compared with other models, they were also disappointing, in that the number of problems that we could solve in the transition phase was rather limited for various dimensions. (Note that in these

pr		pr-dl		pr-dl-ch2		ch2	
time	checks	time	checks	time	checks	time	checks
1.45	1.30	1.93	1.69	1.90	1.69	1	1

Table 4.2: Comparison of various models using MAC and no value ordering.

cases, median time is the same as timeout because less than 50% of instances were solved.) Nevertheless, we decided to pursue further the bichannelling model based on the somewhat anecdotal evidence of its clear superiority over other models. As the following sections show, we succeeded in this goal.

For the sake of a more systematic comparison, we present here a simple comparison of the various models. Due to limited available time, we chose the 29 easiest problems (as measured with the approaches developed later) for order 30 quasigroups with 60% preassignment. These are still relatively difficult problems close to the phase transition: the `ch2-model` took a total of 6624 seconds on the 19 problems (66%) in the sample that were solved with all tested models in less than 1800 seconds, yielding an average of 348.6 seconds per solved problem, and a mean (over the whole sample) of 574.16s. Table 4.2 shows the result of a comparison between various models on this sample. The table provides the ratios in the accumulated data in time and constraint checks over the solved problems, relative to the performance of `ch2`. Note that all models tried exactly the same number of assignments in all problems, empirically confirming the fact that arc consistency has identical pruning power in all four models.

We conjecture that these ratios will increase with problem difficulty. But there is little point on belaboring these data, as much better solutions are available, as discussed in the following sections.

Introducing value ordering

The results when the first combined model was used with the min-domain-sum value ordering heuristic were quite surprising, as it outperformed previous tests in three orders of magnitude in some cases. For example, for the instance bqwh-35-405-5.pls

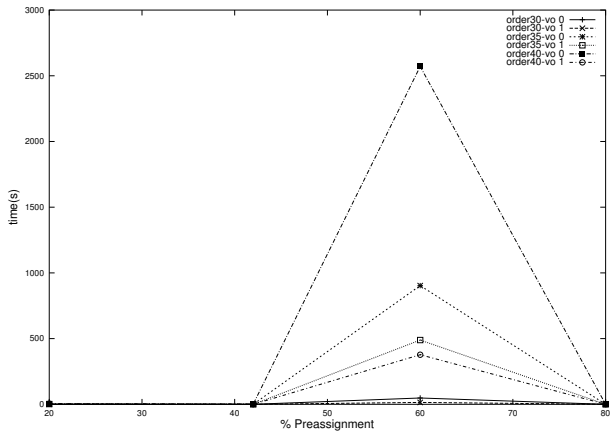


Figure 4.1: Mean solution time on QCPs of order 30, 35 and 40 with (vo1) and without (vo0) value ordering.

(balanced instance of order 35 and 60% preassigned cells) it took 2905 secs without value ordering and only 0.40 secs with it. For a more general picture, Figure 4.1 plots the data of Table 4.1, obtained with lexicographic value ordering, against the results over the same sample with `dom+` value ordering.

Encouraged by this performance, we generated a set of 100 balanced instances of orders 30, 35, 40 and 45, with 60% preassignment. Table 4.3 shows median and mean time in seconds (the latter taken only over solved instances), percent of solved instances and timeouts, in solving these instances with the new variable ordering heuristic.

order	mean	median	% solved	timeout
30	148.84	174.11	68%	1000
35	533.43	163.48	84%	3600
40	732.94	1010.82	68%	5000
45	1170.81	2971.40	56%	6000

Table 4.3: The min-domain value ordering heuristics at the phase transition, using MAC.

These results are significantly better than those previously found in the literature, as we can solve over 50% of balanced QCPs of order 45 at the phase transition. [101]

reports that pure constraint programming approaches, even when using specialized forms of arc consistency for non-binary alldiff constraints and a commercial solver, could not solve any problem of order 40 in the phase transition.

We considered other ways of combining domain sizes such as minimizing the product of the corresponding domain sizes (*min-domain-product* or `vdom*`), and their corresponding maximizing versions, without success. Perhaps there is no deep reason why `vdom+` was so clearly superior to `vdom*`. Maximizing versions were clear underperformers, and there is a reasonable explanation for it. For concreteness, consider choosing a value with the maximal combined domain of the corresponding variables, e.g. a value k for a primal variable x_{ij} such that *domain-size*(r_{ik}) + *domain-size*(c_{jk}) is maximal (over the colors available for x_{ij} at the current stage of search). While large domain sizes are usually indication of less tightness, and thus could be conjectured to capture the idea, often cited in connection with value ordering, of selecting a value which is "more likely to lead to a solution", in this case they have exactly the opposite effect. When $x_{ij} = k$ is the maximal labelling according to this criteria, the domains of r_{ik} and c_{jk} are immediately pruned into singletons. Hence a maximizing choice produces maximal pruning, which is the opposite of what is desired. And conversely, heuristics such as `vdom+` choose values that produce the least pruning.

4.2.6 Compiling AC to FC with redundant constraints

Our next and last step (in this subsection) in improving our solution derived from an examination of the pruning behavior of the bichannelling model with arc consistency. Suppose x_{ij} is assigned k at some point during the search. The GAC implementation of CPlan begins by checking arc consistency for constraints with a single uninstantiated variable, i.e. doing forward checking, which forces the domains of r_{ik} and c_{jk} to become the singletons $\{j\}$ and $\{i\}$ respectively, and also prunes, for each $h \neq k$, j from r_{ih}, and i from c_{jh}. Arc consistency will further discover (if not already known at this stage of the search):

- $x_{ih} \neq k$ for any column $h \neq j$, since otherwise $r_{ik} = h \neq j$;
- hence also $c_{hk} \neq i$ for any column $h \neq j$, since otherwise $x_{ih} = k$;

- similarly, $x_{hj} \neq k$ for any row $h \neq i$, since otherwise $r_{ik} = h \neq j$;
- hence also $r_{hk} \neq j$ for any row $h \neq i$, since otherwise $x_{hj} = k$;

It is not difficult to show that GAC cannot prune any more values as a result of an assignment to a primal variable, unless one of the listed prunings reduces a domain to a singleton. All these are useful prunings, but GAC does much more work than needed to obtain them. Each one of the pruned values – one for each $x_{ih}, x_{hj}, c_{hk}, r_{hk}$, potentially $4(n-1)$ pruned values and variables from a single assignment – requires GAC to check all the constraints in which the corresponding variables are involved, namely $2(n-1)$ or $(n-1)$ constraints for, respectively, the primal and dual pruned variables (further, in the CPlan implementation all affected variables have *all* their values tested, even if at most one will be pruned). This is wasted effort, as no additional pruning is achieved. One can however observe that most of the pruning power can be derived simply by assigning the variables whose domain became singletons (either directly through channelling constraints or indirectly when pruning a single value results in a singleton) and doing forward checking on them. To see that the remaining values pruned by GAC (namely the second and fourth items above) are also pruned by FC with the trichannelling model, observe that $c_{hk} \neq i$ since otherwise $r_{ik} = h \neq j$ using the corresponding triangular channelling constraint, and similarly $r_{hk} \neq j$ since otherwise $c_{jk} = h \neq i$.

We remark that the same effect can be achieved in different ways, e.g. the bichannelling model supplemented with the dual not-equal constraints also allows forward checking to derive the same consequences.

Results with the trichannelling model Table 4.4 compares the bichannelling model `ch2`, using only row and column channelling constraints with GAC, versus the trichannelling model `ch3` with the three kinds of channelling constraints using only FC, in both cases with the min-domain-sum value ordering. Each sample consists again of 100 balanced instances with 60% preassignment;the accumulated values are over the problems solved by both approaches within the given timeout. The median times are on the other hand over the whole sample. Accumulated times are in seconds

while the other accumulated values are in millions of checks and tried assignments respectively.

	ch3-fc			ch2-ac			ratios	
order	acc. time	median	solved	acc. time	median	solved	acc. time	median
30	6445.44	153.04	78%	9557.83	174.11	68%	1.48	1.14
35	29691.18	152.16	86%	45341.22	163.48	85%	1.53	1.07
40	33015.14	637.18	73%	48682.04	1010.82	68%	1.47	1.59
45	38569.95	1650.52	59%	61469.78	2971.40	56%	1.59	1.80

	checks			visits		
order	ch3-fc	ch2-ac	ratio	ch3-fc	ch2-ac	ratio
30	29886	80206	2.68	431	658	0.15
35	114572	279003	2.44	1617	218	0.13
40	205247	445790	2.17	2769	331	0.12
45	108276	321632	2.97	1489	236	0.16

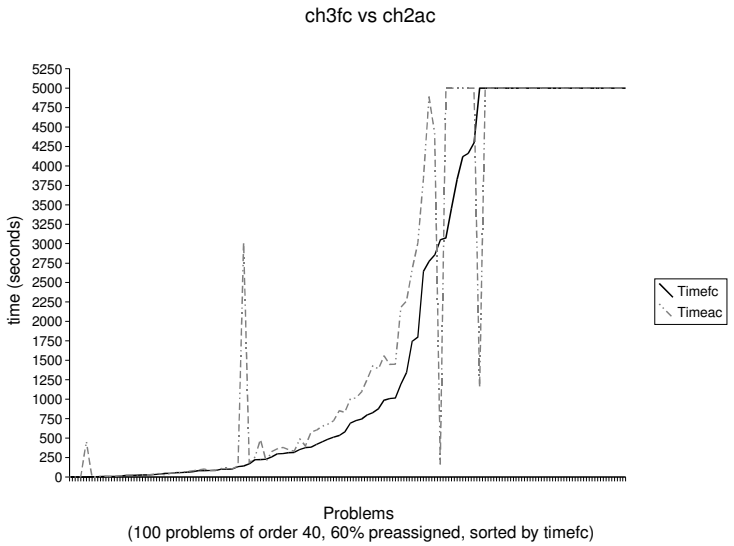
Table 4.4: The ch3 and ch2 models compared, with value ordering.

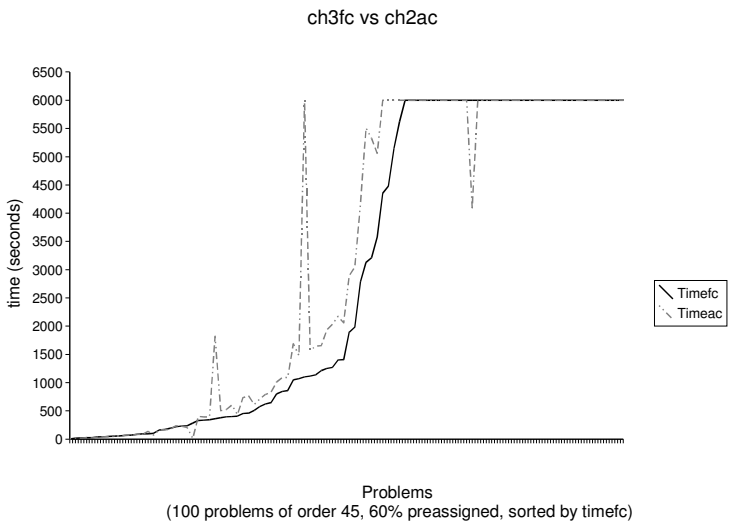
These tables show that there is a significant improvement in time with the `ch3` model using only FC, and this can be traced to the large savings in number of checks. On the other hand, `ch3` with FC tries almost one order of magnitude more assignments, which arise from the fact that it must instantiate the variables associated to a given assignment made in the search tree in order to extract the same consequences as AC with `ch2`; these added tried assignments do not however translate into any more checks or more true backtracking.

The results in this table are not however as straightforward to obtain as the formal result on the equivalent pruning power may suggest. Indeed, our first attempt at implementing `ch3` resulted in a slight but noticeable slowdown! On further examination, we realized that this was due to the implementation of the min-domain variable ordering heuristic, which could select many other variables with a singleton domain before the variables associated with the last assignment; as a result, obtaining the same conclusions as AC could be significantly delayed. We solved the problem by keeping a stack of uninstantiated variables with singleton domain, and modifying the min-domain heuristic to pop the most recent variable from that stack whenever it

was not empty. This ensures that FC considers those variables that have just become singletons immediately. The solution has nevertheless an ad-hoc flavor, and suggests that for domains such as QCPs, where propagation often forces a value for variables as opposed to merely pruning part of their domain, a more SAT-like propagation may be more indicated; in other words, it is not always sufficient to rely on the min-domain heuristic to propagate in a timely fashion forced values.

Finally, the following figures display a more detailed picture of how `ch2` and `ch3` compare, showing the time taken to solve all 100 problems in each set, sorted by difficulty, for order 40 and 45 quasigroups at the phase transition. As it can be seen, the `ch3` model is almost always superior, but there are some anomalies that are worth investigating further.





4.3 Introducing SAT to the QCP

This section presents the introduction of SAT techniques to the QCP problem. It also performs a comparison of SAT and CSP methods for solving this problem. First we are going to review the SAT and CSP models for the QCP and present some experimental results for several SAT problems. Then, we are going to theoretically compare the SAT and CSP encodings and to introduce a very effective technique to our CSP solver. Finally, a comparison of all methods considered is provided.

4.3.1 SAT and CSP Encodings

The two SAT encodings of the QCP of order n considered in this research, introduced in [136], use n Boolean variables per cell; each variable represents a color assigned to a cell, and the total number of variables is n^3. The most basic SAT encoding, which is known as 2-dimensional (2-D) encoding, includes clauses that represent the following constraints:

1. at least one color must be assigned to each cell (ALO-1);

2. no color is repeated in the same row (AMO-2); and

3. no color is repeated in the same column (AMO-3).

The other encoding, which is known as 3-dimensional (3-D) encoding, adds to the 2-D encoding redundant clauses that represent the following constraints:

1. each color must appear at least once in each row (ALO-2);

2. each color must appear at least once in each column (ALO-3); and

3. no two colors are assigned to the same cell (AMO-1).

Both encodings have $\mathcal{O}(n^4)$ clauses. The labels associated to each clause set are explained later.

For the sake of brevity and clarity, the only CSP encoding we describe is the "bichannelling model". It consists of:

- A set of *primal variables* $X = \{x_{ij} \mid 1 \leq i \leq n,\ 1 \leq j \leq n\}$; the value of x_{ij} is the color assigned to the cell in the ith row and jth column, and n is the order of the quasigroup, i.e. the number of rows and columns.

- Two sets of *dual variables*: $R = \{r_{ik} \mid 1 \leq i \leq n,\ 1 \leq k \leq n\}$, where the value of r_{ik} is the column j where color k occurs in row i; and $C = \{c_{jk} \mid 1 \leq j \leq n,\ 0 \leq k \leq n\}$ where the value of c_{jk} represents the row i where color k occurs in column j.

The domain of all variables is $\{1, \ldots, n\}$, where these values represent respectively colors, columns, and rows. Variables of different types are linked by channelling constraints:

- *Row channelling constraints* link the primal variables with the row dual variables: $x_{ij} = k \Leftrightarrow r_{ik} = j$.

- *Column channelling constraints* link the primal variables with the column dual variables: $x_{ij} = k \Leftrightarrow c_{jk} = i$.

	% solved				mean				median			
order	Chaff	Berkmin	Satzoo	Satz	Chaff	Berkmin	Satzoo	Satz	Chaff	Berkmin	Satzoo	Satz
35	99	100	100	100	59	24	37	6	3.2	0.5	16	1.2
37	96	99	100	100	232	173	129	42	24	4.7	5	5.8
40	82	86	96	99.5	518	590	861	539	288	112	142	41
43	50.5	62	78.5	84	279	1487	1799	1243	1085	2178	815	358
45	46	46	59.5	68	380	1312	1021	1181	> 12000	> 12000	1857	1184

Table 4.5: Comparison of Chaff, Berkmin, Satzoo and Satz on the 3-D encoding. Time in seconds, mean of solved instances. Cutoff 12000 seconds. 1 GHz.

This model is a complete model of the problem; in particular, the so called primal constraints, which explicitly state that no two colors can be repeated in any one row or column, are redundant, and hinder propagation. CSP "channelling" encodings for permutation problems similar to the one presented here are discussed at length in [118].

4.3.2 Experimental results on random QWH instances

We considered four state-of-the art SAT solvers: Satz [144], Chaff [165], Berkmin [97], and Satzoo [62]. We chose Satz because some authors have claimed that it is the best option to solve QCPs; our experimental results provide evidence of this claim too. We chose Chaff and Satzoo because they were the winners of the two last SAT competitions, and Berkmin because it is often competitive with Chaff. In addition, we tested two CSP solvers, the GAC library described in [224], and the MAC solver by Regin and Bessiere [22]. Note that for binary CSPs they are simply different implementations of the MAC algorithm.

The instances tested in our experiments are of the QWH type (quasigroup with holes [136], generated with `lsencode`), are all satisfiable, and are located near the phase transition.[5] Our samples, with 200 instances each, did not contain "balanced" problems, which are reported to be the hardest; still, we did verify that they are much harder for all solvers than the balanced problems tested and discussed in the previous section, which were not close enough to the phase transition for their class.

[5]Specifically, QWH instances of order n are generated with $\lceil 1.6 \times n^{1.55} \rceil$ holes.

	% solved		mean (solved)		median	
order	Satz	GACvo	Satz	GACvo	Satz	GACvo
35	100	37	6	2970	1.2	> 12000
37	100	11	42	2572	5.8	> 12000
40	99.5	7	539	4546	41	> 12000

Table 4.6: Comparison of Satz on the 3-D encoding and GAC-vo. Time in seconds. Cutoff 12000 seconds. 1 Ghz.

Of all the solutions tried, we can discard the 2D SAT encoding and the primal CSP models, as they give significantly worse results. Of the remaining encodings, the 3D encoding was clearly superior with the four SAT solvers, with Satz scaling somewhat better than Satzoo and both much better than chaff. On the other hand, the CSP approach which uses MAC on the bichannelling model, scaled much worse on the (harder) problems tested in this section. There is therefore a clear dividing line between SAT and CSP encodings in terms of performance. Table 4.5 provides the data for SAT solvers, and Table 4.6 compares our best SAT solver with the CSP approach (labelled GACvo), which seems to be the best one in the literature, using GAC on the bichannelling model with a special value ordering heuristic (named `vdom+` in that paper). Note that the ratio of solved problems for GACvo is much lower than reported in the previous sections for problems of the same order, and that's because our instances are harder.[6]

Discussion We will now explore potential explanations for these observations, and ways to improve these results for the CSP approaches drawn from these explanations. Our first focus will be on comparing representations; later we consider solver-specific issues (most importantly, the extra level of propagation and the heuristics of Satz).

[6]The improvements reported for the trichannelling model do not affect scaling behavior, and are pretty much subsumed by the stronger forms of lookahead discussed later. Hence we did not test this model in this section.

4.3.3 Comparing models

In order to compare our models formally, we need a small detour through *SAT encodings of CSP models*, a third modelling option that we have not considered so far. In this context, the many-valued CSP variables are represented by means of a set of boolean variables, one for each possible assignment. So, for example, a primal variable x_{ij} becomes a set of boolean variables $x_{ij} = 1, \ldots, x_{ij} = n$. The semantics of CSP domains is then captured by including one ALO ("at least one") clause for each variable, specifying that the variable must take at least one of its possible values, and $O(n^2)$ AMO ("at most one") clauses which specify, for every pair of possible values of a variable, that they can not be satisfied simultaneously. In our bichannelling model, we would have variables $x_{ij} = k$, $r_{ik} = j$ and $c_{jk} = i$, for each triple j, k, i, for a total of $3n^3$ variables.

Define the *minimal support encoding* of the bichannelling model as that consisting of AMO-ALO clauses for the three variable types, together with the *channelling clauses* $\neg x_{ij} = k \vee r_{ik} = j$ and $\neg r_{ik} = j \vee x_{ij} = k$, which directly encode the equivalence $x_{i1} = j \Leftrightarrow r_{ij} = k$ which defines the constraint between x_{ij} and r_{ik} (and similarly for column channelling constraints). Clearly, the channelling clauses completely characterize the channelling constraints, hence the minimal support encoding is a complete model.

The *support encoding*, as defined in [89], encodes a constraint between two variables X and Y by adding, for each possible value v of X, the clause $\neg X = v \vee Y = v_1 \vee \ldots \vee Y = v_k$, where $v_1, \ldots, v_k$ is a list of all values w in the domain of Y such that (v, w) satisfies the constraint, i.e. a list of *supports* for the assignment $X = v$. For the bichannelling model, we can observe that the channelling clauses of the minimal support encoding already encode the supports for $x_{ij} = k$ and $r_{ik} = j$. For values $v \neq k$, the supports for $x_{ij} = v$ are given by the clause $\neg x_{ij} = v \vee \bigvee_{h \in \{1,\ldots,n\}, h \neq j} r_{ik} = h$, and for values $v \neq j$, the supports for $r_{ik} = v$ are given by $\neg r_{ik} = v \vee \bigvee_{h \in \{1,\ldots,n\}, h \neq k} x_{ij} = h$.

Proposition 4.3.3.1. Unit resolution obtains the same results on the minimal support encoding as in the support encoding of the bichannelling model.

Proof. Consider e.g. the constraint between x_{i1} and r_{i2} (a similar analysis holds

for column channelling constraints). Since the channelling clauses are preserved in the minimal encoding, it suffices to show that the effect of unit propagation on the additional support clauses is also obtained without them. For $v \neq 2$ we have the support clause $\neg x_{i1} = v \vee \bigvee_{h \in \{1,\ldots,n\}, h \neq 1} r_{i2} = h$. We consider two cases. First, suppose $r_{i2} = 2, \ldots, r_{i2} = n$ are all false; we must show that unit resolution on the remaining clauses imply $\neg x_{i1} = v$. Unit resolution on the ALO for r_{i2} obtains $r_{i2} = 1$, which together with the channelling clauses yield $x_{i1} = 2$, and with the AMO for x_{i1}, $\neg x_{i1} = v$. Second, suppose $x_{i1} = v$ is true and, say, $r_{i2} = 1$ through $r_{i2} = n - 1$ are all false; we need to show that $r_{i2} = n$ follows by unit resolution. Now, $x_{i1} = v$ implies through AMO $\neg x_{i1} = 2$, and thus $\neg r_{i2} = 1$ using the channelling clauses. This together with the hypothesis of the case and the ALO for r_{i2} allows us to obtain $r_{i2} = n$, as desired. □

Our second observation is that the binary theory consisting of the channelling clauses for all constraints can be simplified using a strongly connected components (SCC) algorithm such as in [53]. The SCCs will consist precisely of the triplets of boolean variables of the form $x_{ij} = k$, $r_{ik} = j$ and $c_{jk} = i$. The SCC-based algorithm would then replace each such triplet by a single variable, which we may appropriately call x_{ijk}, as in the 3D SAT encodings, and perform the appropriate replacements in the remaining clauses. The result is the following:

- The ALO and AMO clauses for the CSP variables become clauses of the 3D-encoding. Specifically, the clauses labelled ALO-k and AMO-k ($1 \leq k \leq 3$) in the 3D-encoding are the result of rewriting the ALO and AMO clauses for the primal variables (k=1), row dual variables (k=2) and column dual variables (k=3) in the minimal channelling encoding.

- The channelling clauses become tautologies after variable replacement, so they can be eliminated.

The SCC-simplification formally captures the intuitive idea that the triplet of variables $x_{ij} = k$, $r_{ik} = j$ and $c_{jk} = i$ all "mean the same" –color k is in cell (i, j)–, and hence that each triplet can be "collapsed" into a single boolean variable x_{ijk}, as done in the 3D encoding (and in the "SAT channelling model" of [118]).

	% solved			mean			median		
order	GAC-HLA	MAC-HLA	Satz	GAC-HLA	MAC-HLA	Satz	GAC-HLA	MAC-HLA	Satz
35	98	98.5	100	428	586	6	131	129	1.2
37	86	89.5	100	1360	1913	42	882	822	5.8
40	52	58	99.5	1770	3033	539	5304	8411	41
43	30	39	84	1342	2668	1243	> 12000	> 12000	358
45	24	26	68	2810	3585	1181	> 12000	> 12000	1184

Table 4.7: Comparison of GAC-HLA, MAC-HLA and Satz. Time in seconds, mean of solved instances. Cutoff 12000 seconds. 1 Ghz.

	% solved		mean		median	
order	MAC-LA	MAC-HLA	MAC-LA	MAC-HLA	MAC-LA	MAC-HLA
30	96	100	544	18	482	9
33	91	100	1753	187	1256	52
35	58	98.5	2714	586	4487	129

Table 4.8: Comparison of MAC-LA and MAC-HLA. Time in seconds, mean of solved instances. Cutoff 12000 seconds. 1 Ghz.

Proposition 4.3.3.2. Unit resolution on the 3D model has the same pruning power as MAC on the bichannelling model.

Proof. [89] shows that unit resolution on the support encoding of a CSP problem is equivalent to MAC on the original problem. We have just shown that unit resolution on the minimal support encoding is equivalent to unit resolution on the support encoding of the bichannelling model, and that the 3D encoding is simply the minimal support encoding after SCC simplification, which does not affect the power of unit resolution. □

Thus, the 3D model exactly captures the bichannelling model, without loosing any propagation power, but with 3 times fewer variables (n^3 instead of $3n^3$) and without the $4n^3$ channelling clauses of the minimal channelling model. We did in fact try to solve QCPs using a direct encoding of the bichannelling model, with very bad results due to the size of the resulting theories. The above propositions seem to go a long way toward explaining the success of the 3D model.

For each free variable x **such that** $PROP_z(x)$ is true **do**
(let F' and F'' two copies of the formula F under consideration)

F' := unit-propagation($F' \cup \{x\}$);
F'' := unit-propagation($F'' \cup \{\neg x\}$);
If $\Box \in F'$ **and** $\Box \in F''$ **then return** "F is unsatisfiable"
If $\Box \in F'$ **then** x:=0, $F := F''$
else if $\Box \in F''$ **then** x:=1, $F := F'$
If $\Box \notin F'$ **and** $\Box \notin F''$ **then**
  let $w(x)$ denote the weight of x
  $w(x)$:= number of times that non-binary clauses of F
    have been reduced when deriving F'
  $w(\neg x)$:= number of times that non-binary clauses of F
    have been reduced when deriving F''

For each free variable x **do**
  $H(x) := w(x) * w(\neg x) * 1024 + w(x) + w(\neg x)$;
Branch on the free variable x with greatest $H(x)$

Figure 4.2: The variable selection heuristic of *Satz* for $PROP(x, 4)$

4.3.4 Satz's heuristic in QCPs

We now turn to solver and domain-specific features that may explain the observed performance. Thus our next step was to analyze in depth the behavior on QCP instances of the best solver, Satz, so as to incorporate new propagation techniques and heuristics into the CSP solvers from the insights gained. Before going into details, let us recall the variable selection heuristic that implements Satz, which combines MOMS (Maximum Occurrences in clauses of Minimum Size) and UP (Unit Propagation) heuristics. In both heuristics, the goal is to maximize the power of unit propagation. MOMS picks one variable among those that occur the most often in minimal size clauses, since these are more likely to result in propagation. UP goes a step further by actually measuring the number of propagations from each choice. It examines each variable p occurring in a given CNF formula ϕ by respectively adding the unit clauses p and $\neg p$ to ϕ, and independently making two unit propagations, which are used to derive a score for each variable. As a secondary effect, UP detects so-called *failed literals* in ϕ, which when satisfied falsify ϕ in a single unit propagation.

In order to reduce the time required to propagate all literals, Satz applies UP to a restricted number of variables that occur in binary clauses by applying a unary predicate, called $PROP_z$, which is defined as follows:

Definition 4.1. Let ϕ be a CNF formula; let $PROP(x, i)$ be a binary predicate which is true iff variable x occurs both positively and negatively in binary clauses of ϕ, and there are at least i occurrences of x in binary clauses of ϕ; and let T be an integer. $PROP_z(x)$ is defined to be the first of the three predicates $PROP(x, 4), PROP(x, 3), true$ (in this order) whose denotational semantics contains more than a fixed number T of variables. T is set to 10 in Satz.

After applying unit propagation to a restricted number of variables and detecting failed literals, the heuristic of Satz weights literals with different criteria depending on the predicate applied. For example, when $PROP(x, 4)$ is applied, the heuristic scores each literal $(x, \neg x)$ with the number of times that non-binary clauses have been reduced when propagating the literal. The pseudocode of the variable selection heuristic of Satz for $PROP(x, 4)$ is shown in Figure 4.2. Function $H(x)$ is used to reach a good balance between weights of positive literals and weights of negative literals.

When solving QCP instances using the 3-D encoding with Satz, we observed that Satz almost always uses the predicate $PROP(x, 4)$, which requires x to occur in both positive and negative binary clauses, with at least 4 occurrences in total. A closer look at the 3-D encoding reveals that Boolean variables that fulfill $PROP(x, 4)$ model CSP variables with domain size 2. The reason is that positive literals only occur in the ALO-1, ALO-2 and ALO-3 constraints, hence the only way to have x occur positively in a binary clause is when one of these clauses becomes binary, in which case the corresponding (primal or dual) CSP variable has domain size 2. Further, it is easy to show that the variables in such positive binary clauses have at least three other negative occurrences from AMO clauses, so that $PROP(x, 4)$ holds. This analysis led us to incorporate the technique of failed literals and the heuristic of Satz into CSP solvers as follows:

1. For each free CSP variable of domain size 2, we propagate each value of the

domain in order to see if the domain can be reduced. As a result, the domain can remain as before, can be a singleton or can be empty. In the first case, we weight the variable using the balance function H of Satz's heuristics, where $w(x = i)$ is the number of times that domains have been reduced after propagating the value i. In the second case, we fix the variable to the only value of its domain. In the third case, we have detected an inconsistency and we backtrack.

2. We select the first free CSP variable of domain size 2 with greatest value of function H.

3. If there is no candidate variable in step 2, we apply the default heuristic of the CSP solver (for example, `min-domain`).

The above description corresponds to what we will call simply look-ahead heuristic (LAH). We refer to the version of GAC (MAC) that incorporates LAH as GAC-LAH (MAC-LAH).

4.3.5 New experimental results on random QWH instances

To assess the performance of LAH we performed an empirical investigation. In the first experiment we compared Satz with GAC-LAH and MAC-LAH on sets of 200 instances of order 35, 37, 40 and 45 of the hard region of the phase transition. The results obtained are shown in Table 4.7. We observed that Satz outperforms GAC-LAH and MAC-LAH, but the differences are not so dramatic as with GAC-vo, which was the most competitive CSP option to solve QCPs. MAC-LAH seems to be slightly superior to GAC-LAH.

In the second experiment, we analyzed if the improvements achieved on CSP solvers are due to the use of lookahead to detect potential wipeouts or to the heuristic function. To this end, we compared MAC-LAH with a variant MAC-LA which uses the same lookahead but chooses variables of minimum domain size instead of applying the heuristic function H to a reduced number of variables; we refer to that version as MAC-LA. The results obtained, shown in Table 4.8, clearly indicate that the heuristic function plays a central role.

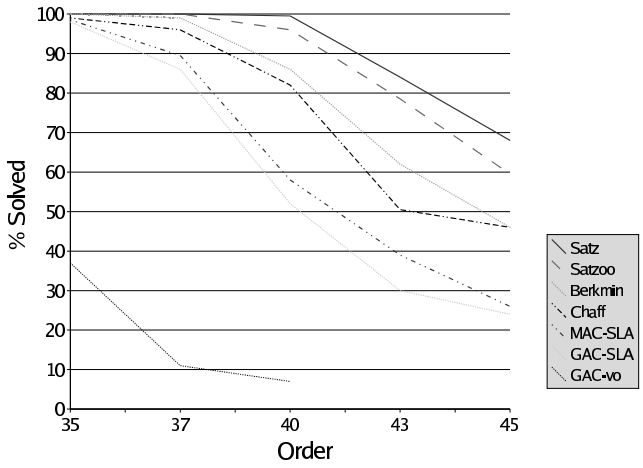


Figure 4.3: Percent solved for the main solvers.

Nevertheless, failed literals do achieve an extra-level of consistency in each search node over that of plain unit propagation, and a natural question to ask is whether stronger forms of consistency could yield better results. We experimented with stronger forms of lookahead without success, but did not try `alldifferent` constraints. Hall's Theorem, as presented in [227], states that:

"the constraint `alldifferent`$(x_1, \ldots, x_n)$ with respective variable domains $D_1, \ldots, D_n$ has a solution if and only if no subset $K \subseteq \{x_1, \ldots, x_n\}$ exists such that $|K| > |\bigcup_{x_i \in K} D_i|$".

However, we observed experimentally that, for the QCP and the solvers considered, the condition of the theorem is only violated by subsets of three CSP variables with domain size two. It is easy to show that the lookahead phase of our heuristic, when applied to a variable of domain size two, finds a contradiction for the two values of the domain and backtracks. So in practice we may be getting the same pruning power as with Hall's theorem.

As a summary of our main results, Figure 4.3 compares the main approaches discussed in this work in terms of scalability, plotting percent of solved instances against the order of quasigroups. It can be seen that SAT encodings still scale better, but that the incorporation of the lookahead heuristic inspired by Satz goes a long

way toward bridging the gap between the best CSP model available to date, GAC-vo, and the SAT approaches.

4.4 Lessons learnt

Constraint Satisfaction and SAT techniques are very powerful techniques for solving optimization problems. They rely on propagation techniques to reduce the search space and on heuristic to drive the search efficiently. Here is the list of useful lessons we have learnt:

- Both techniques seem to be specially suited for satisfaction rather than for optimization.
- Both approaches strongly rely on propagation mechanisms, and their efficiency on a given problem seems to be related to the specific trade-off between search and propagation.
- Heuristics have a huge impact on both techniques, although it is not possible to find the optimal heuristic to apply to any problem, nor even to any instance of the same problem.
- They seem not to be suited for very large search space, due to their complete nature, and their impossibility to generate near-optimal solutions.
- They are however necessary when we need to find the optimal solution or all the solutions of a problem.

Chapter 5

Local Search for the Social Golfer Problem

The social golfer problem has attracted significant interest since it was first posted on `sci.op-research` in May 1998. It consists of scheduling $n = g \times p$ golfers into g groups of p players every week for w weeks so that no two golfers play in the same group more than once. An instance of the social golfer is specified by a triple $g-p-w$, where g is the number of groups, p is the size of a group, and w is the number of weeks in the schedule.

The scheduling of social golfers is a highly combinatorial and symmetric problem and it is not surprising that it has generated significant attention from the constraint programming community (e.g., [72, 209, 178, 200, 199, 13, 184]). Indeed, it raises fundamentally interesting issues in modeling and symmetry breaking, and it has become one of the standard benchmarks for evaluating symmetry-breaking schemes. Recent developments (e.g., [13, 184]) approach the scheduling of social golfers using innovative, elegant, but also complex, symmetry-breaking schemes.

This research approaches the problem from a very different angle. It proposes a local search algorithm for scheduling social golfers, whose local moves swap golfers within the same week and are guided by a tabu-search meta-heuristic. The local search algorithm matches, or improves upon, the best solutions found by constraint programming on all instances but 3. It also found the first solutions to 11 instances

that were previously open for constraint programming.[1] Moreover, the local search algorithm solves almost all instances easily in a few seconds and takes about 1 minute on the remaining (harder) instances. The algorithm also features a constructive heuristic which trivially solves many instances of the form $odd - odd - w$ and provides good starting points for others.

The rest of the chapter is organized as follows. After reviewing some related work it starts by describing the basic local search algorithm, including its underlying modeling, its neighborhood, its meta-heuristic, and its experimental results. It then presents the constructive heuristic and reports the new experimental results when the heuristic replaces the random configurations as starting points of the algorithm. Finally, the chapter concludes by giving a set of lessons learnt.

5.1 Solving the Social Golfer Problem

There is a considerable body of work on scheduling social golfers in the constraint programming community. References [13, 184] describe state-of-the art results using constraint programming and are excellent starting points for more references. See also [199] for interesting theoretical and experimental results on the social golfer problem, as well as the description of SBDD, a general scheme for symmetry breaking. Agren [3] describes a tabu-search algorithm for scheduling social golfers, where the neighborhood consists of swapping the value of a single variable and where all constraints are explicit. The results are also far in quality and performance from those reported here. The neighborhood used in this research, which implicitly maintain the group and week structures, and the randomized tabu-list strategy are fundamental in scheduling hard instances. Another local search approach is introduced in [180], where the symmetry breaking is shown counter-productive for local search and adding symmetries (super-symmetries) is proposed instead. Hybrid local search and constraint programming approaches have been tried on the social golfer problem [177]. In both cases, the results are significantly dominated by those presented in this chapter. The idea of

[1] For the current statuses of the instances, see Warwick Harvey's web page at `http://www.icparc.ic.ac.uk/wh/golf`.

weeks	group 1	group 2	group 3	group 4	group 5
week 1	1 2 3 4 5	6 7 8 9 10	11 12 13 14 15	16 17 18 19 20	21 22 23 24 25
week 2	1 6 11 16 21	2 7 12 17 22	3 8 13 18 23	4 9 14 19 24	5 10 15 20 25
week 3	1 7 13 19 25	2 8 14 20 21	3 9 15 16 22	4 10 11 17 23	5 6 12 18 24
week 4	1 8 15 17 24	2 9 11 18 25	3 10 12 19 21	4 6 13 20 22	5 7 14 16 23
week 5	1 9 12 20 23	2 10 13 16 24	3 6 14 17 25	4 7 15 18 21	5 8 11 19 22
week 6	1 10 14 18 22	2 6 15 19 23	3 7 11 20 24	4 8 12 16 25	5 9 13 17 21

Table 5.1: A solution for the problem $5-5-6$

separating the problem constraints into soft and hard constraints is part of the folklore of local search. It was studied theoretically and experimentally in [74], in which conditions to preserve connectivity are discussed. The connectivity is trivial in the applications considered here since feasible solutions are permutations.

5.2 The Social Golfer

Thi application is the well-known social golfer problem, which has attracted significant interest since its posting on `sci.op-research` in May 1998. It is also problem 10 in the CSPLIB [90]. The social golfer problem consists of scheduling $n = g \times p$ golfers into g groups of p players every week for w weeks so that no two golfers play in the same group more than once. An instance of the social golfer is specified by a triple $g - p - w$, where g is the number of groups, p is the size of a group, and w is the number of weeks in the schedule. Figure 5.1 depicts a solution for the $5-5-6$ social golfer problem.

5.2.1 The Modeling

There are many possible modelings for the social golfer problem, which is one of the reasons it is so interesting. This paper uses a modeling that associates a decision variable $x[w, g, p]$ with every position p of every group g of every week w. We consider every $w_i \in W$, $g_i \in G$ and $p_i \in P$, where $W = 1..w$, $G = 1..g$ and $P = 1..p$. We abuse notation and denote any given week as w, group as g and position as p.

Given a schedule σ, i.e., an assignment of values to the decision variables, the value $\sigma(x[w, g, p])$ denotes the golfer scheduled in position p of group g in week w. There are two kinds of constraints:

1. A golfer plays exactly once a week;

2. Two golfers can play together at most once.

The first type of constraints is implicit in the algorithms presented in this paper: It is satisfied by the initial assignments and is preserved by local moves. Therefore, in this section, we always assume that schedules satisfies the first set of constraints. The second set of constraints is represented explicitly. The model contains a constraint $m[a, b]$ for every distinct pair (a, b) of golfers: Constraint $m[a, b]$ holds for an assignment σ if golfers a and b are not assigned more than once to the same group. More precisely, if $\#_\sigma(a, b)$ denotes the number of times golfers a and b meet in schedule σ, i.e.,

$$\#_\sigma(a, b) = \#\{(w, g) \mid \exists p, p' \in P : \ \sigma(x[w, g, p]) = a \ \& \ \sigma(x[w, g, p']) = b\},$$

constraint $m[a, b]$ holds if

$$\#_\sigma(a, b) \leq 1. \tag{5.1}$$

To guide the algorithm, the model also specifies violations of the constraints. Informally speaking, the violations $\upsilon_\sigma(m[a, b])$ of a constraint $m[a, b]$ is the number of times golfers a and b are scheduled in the same group in schedule σ beyond their allowed meeting. In symbols, and generalizing

$$\upsilon_\sigma(m[a, b]) = \max(0, \#_\sigma(a, b) - 1). \tag{5.2}$$

As a consequence, the social golfer problem can be modeled as the problem of finding a schedule σ minimizing the total number of violations $f(\sigma)$ where

$$f(\sigma) = \sum_{a,b \in \mathcal{G}} \upsilon_\sigma(m[a, b]). \tag{5.3}$$

and $\mathcal{G}$ is the set of $g \times p$ golfers. A schedule σ with $f(\sigma) = 0$ is a solution to the social golfer problem.

5.2.2 The Neighborhood

The neighborhood of the local search consists of swapping two golfers from different groups in the same week. The set of swaps is thus defined as

$$\mathcal{S} = \{(\langle w, g_1, p_1\rangle, \langle w, g_2, p_2\rangle) \mid w \in W, g_1, g_2 \in G, p_1, p_2 \in P, g_1 \neq g_2\}.$$

Note that the neighborhood is connected since a feasible solution, if it exists, can always be obtained by swapping golfers in the same week.

It is more effective however to restrict attention to swaps involving at least one golfer in conflict with another golfer in the same group. This ensures that the algorithm focuses on swaps which may decrease the number of violations. More formally, a triple $\langle g, w, p\rangle$ is said to be in conflict in schedule σ, which is denoted by $\upsilon_\sigma(\langle g, w, p\rangle)$, if

$$\exists p' \in P : \upsilon_\sigma(m[\sigma(x[w, g, p]), \sigma(x[w, g, p'])]) > 1. \tag{5.4}$$

With this restriction, the set of swaps $\mathcal{S}^-(\sigma)$ considered for a schedule σ becomes

$$\mathcal{S}^-(\sigma) = \{(\langle w, g_1, p_1\rangle, \langle w, g_2, p_2\rangle) \in S \;\mid\; \upsilon_\sigma(\langle w, g_1, p_1\rangle)\}.$$

The neighbors of a schedule σ is given by

$$\{\sigma(x[w, g_1, p_1]) \leftrightarrow \sigma(x[w, g_2, p_2]) \mid (\langle w, g_1, p_1\rangle, \langle w, g_2, p_2\rangle) \in \mathcal{S}^-(\sigma)\}.$$

5.2.3 The Tabu Component

The tabu component of the algorithm is based on three main ideas. First, the tabu list is distributed across the various weeks, which is natural since the swaps only consider golfers in the same week. The tabu component thus consists of an array *tabu* where

$tabu[w]$ represents the tabu list associated with week w. Second, for a given week w, the tabu list maintains triplet $\langle a, b, i\rangle$, where a and b are two golfers and i represents the first iteration where golfers a and b can be swapped again in week w. Observe that the tabu lists store golfers, not positions $\langle w, g, p\rangle$. Third, the tabu tenure, i.e., the time a pair of golfers (a, b) stays in the list, is dynamic: It is randomly generated in the interval $[4, 100]$. At iteration k, swapping two golfers a and b is tabu, which is denoted by

$$tabu[w](a, b, k),$$

if the Boolean expression

$$\langle a, b, i\rangle \in tabu[w] \ \&\ i \leq k$$

holds. As a result, for schedule σ and iteration k, the neighborhood consists of the set of schedules obtained by applying moves in

$$\mathcal{S}^t(\sigma, k) = \{(t_1, t_2) \in \mathcal{S}^-(\sigma) \mid \neg tabu[w](\sigma(x[t_1]), \sigma(x[t_2]), k)\}.$$

where we abuse notations and use $x[\langle w, g, p\rangle]$ to denote $x[w, g, p]$.

Aspiration In addition to the non-tabu moves, the neighborhood also considers moves that improve the best solution found so far, i.e.,

$$\mathcal{S}^*(\sigma, \sigma^*) = \{(t_1, t_2) \in \mathcal{S}^-(\sigma) \mid f(\sigma[x[t_1] \leftrightarrow x[t_2]]) < f(\sigma^*)\},$$

where $\sigma[x_1 \leftrightarrow x_2]$ denotes the schedule σ in which the values of variables x_1 and x_2 have been swapped and σ^* denotes the best solution found so far.

5.2.4 The Tabu-Search Algorithm

Figure 5.1 depicts the basic local search algorithm SGLS, which is a tabu search with a restarting component. Lines 2–7 perform the initializations. In particular, the tabu list is initialized in lines 2–3 and the initial schedule is generated randomly in line 4.

Lines 5–7 then initialize the best schedule found so far σ^*, the iteration counter k, and the stability counter s. The initial configuration σ randomly schedules all golfers in the various groups for every week, satisfying the constraint that each golfer plays exactly once a week.

The core of the algorithm are lines 8–23. They iterate local moves for a given number of iterations or until a solution is found. The local move is selected in line 9. The key idea is to select a swap in

$$\mathcal{S}^t(\sigma, k) \ \cup \ \mathcal{S}^*(\sigma, \sigma^*)$$

minimizing

$$f(\sigma[x[t_1] \leftrightarrow x[t_2]]).$$

Observe that the expression $f(\sigma[x[t_1] \leftrightarrow x[t_2]])$ represents the number of violations obtained after swapping t_1 and t_2. The tabu list is updated in line 11, where function *week* is defined as

$$week(< w, g, p >) = w.$$

The new schedule is computed in line 12. Lines 13–15 update the best schedule, while lines 16–20 specify the restarting component.

The restarting component simply reinitializes the search from a random configuration whenever the best schedule found so far has not been improved upon for *maxStable* iterations. Note that the stability counter s is incremented in line 22 and reset to zero in line 15 (when a new best schedule is found) and in line 18 (when the search is restarted).

5.3 Experimental Results

This section reports the experimental results for the SGLS algorithm. The algorithm was implemented in C and the experiments were carried out on a 3.06GHz PC with 512MB of RAM. Algorithm SGLS was run 100 times on each instance and the results report average values for successful runs, as well as the percentage of unsuccessful

```
1.  SGLS(W, G, P)
2.      forall w ∈ W
3.          tabu[w] ← {};
4.      σ ← random configuration;
5.      σ* ← σ;
6.      k ← 0;
7.      s ← 0;
8.      while k ≤ maxIt  &  f(σ) > 0 do
9.          select (t1, t2) ∈ S^t(σ, k)  ∪  S*(σ, σ*)
                minimizing f(σ[x[t1] ↔ x[t2]]);
10.         τ ← RANDOM([4,100]);
11.         tabu[week(t1)] ←
                tabu[week(t1)] ∪ {⟨σ(x[t1]), σ(x[t2]), k + τ⟩};
12.         σ ← σ[x[t1] ↔ x[t2]];
13.         if f(σ) < f(σ*) then
14.             σ* ← σ;
15.             s ← 0;
16.         else if s > maxStable then
17.             σ ←random configuration;
18.             s ← 0;
19.             forall w ∈ W do
20.                 tabu[w] = {};
21.         else
22.             s++;
23.         k++;
```

Figure 5.1: Algorithm SGLS for Scheduling Social Golfers

runs (if any).

Tables 5.2 and 5.3 report the experimental results for SGLS when trying to match the constraint-programming results. Note that no explicty comparison is given for constraint-programming approaches since all the methods in the literature merely report single instances usually solved for a lower number of weeks. Given a number of groups g and a group size p, the tables only give the results for those instances $g-p-w$ maximizing w since they also provide solutions for $w' < w$. Table 5.2 reports the number of iterations (moves), while Table 5.3 reports the execution times. Bold entries indicate that SGLS matches the best known number of weeks for a given

	size 3		size 4		size 5		size 6		size 7		size 8		size 9		size 10	
g	w	I	w	I	w	I	w	I	w	I	w	I	w	I	w	I
6	**8**	**282254.0**	6	161530.3	**6**	**16761.5**	**3**	**15.8**	-	-	-	-	-	-	-	-
7	**9**	**12507.6**	**7**	**274606.0**	**5**	**102.9**	**4**	**100.4**	3	23.4	-	-	-	-	-	-
8	**10**	**653.9**	8	323141.5	**6**	**423.7**	**5**	**1044.9**	**4**	**237.5**	4	153301.6	-	-	-	-
9	**11**	**128.3**	**8**	**84.4**	**6**	**52.7**	**5**	**55.5**	**4**	**44.8**	**3**	**27.7**	**3**	**43.9**	-	-
10	**13**	**45849.1**	**9**	**100.2**	**7**	**80.8**	**6**	**110.7**	**5**	**94.6**	**4**	**61.8**	**3**	**36.1**	**3**	**53.3**

Table 5.2: Number of Iterations for SGLS with Maximal Number of Weeks. Bold Entries Indicate a Match with the Best Known Number of Weeks.

	size 3			size 4			size 5		size 6		size 7		size 8		size 9		size 10	
g	w	T	$\%F$	w	T	$\%F$	w	T	w	T	w	T	w	T	w	T	w	T
6	**8**	**48.93**	6	6	47.75		**6**	**107.18**	**3**	**0.01**	-	-	-	-	-	-	-	-
7	**9**	**3.06**		**7**	**107.62**	8	**5**	**0.07**	**4**	**0.09**	3	0.03	-	-	-	-	-	-
8	**10**	**0.23**		8	207.77	9	**6**	**0.37**	**5**	**1.21**	**4**	**0.39**	4	360.00	-	-	-	-
9	**11**	**0.08**		**8**	**0.09**		**6**	**0.09**	**5**	**0.13**	**4**	**0.14**	**3**	**0.09**	**3**	**0.19**	-	-
10	**13**	**30.82**		**9**	**0.16**		**7**	**0.19**	**6**	**0.34**	**5**	**0.41**	**4**	**0.33**	**3**	**0.20**	**3**	**0.39**

Table 5.3: CPU Time in Seconds for SGLS with Maximal Number of Weeks. Bold Entries Indicate a Match with the Best Known Number of Weeks.

number of groups and a given group size. The percentage of unsuccessful runs is shown between parentheses in Table 5.3.

As can be seen from the tables, Algorithm SGLS finds solutions to all the instances solved by constraint programming except 4. Moreover, almost all entries are solved in less than a second. Only a few instances are hard for the algorithm and require around 1 minute of CPU time. Interestingly, algorithm SGLS also solves 7 new instances (with format $\langle g-s-w \rangle$: $9-4-9$, $9-5-7$, $9-6-6$, $9-7-5$, $9-8-4$, $10-5-8$ and $10-9-4$. Those are not shown in the tables but more detail on these are given below.

It is interesting to observe that algorithm SGLS does not break symmetries and does not exploit specific properties of the solutions. This contrasts with constraint-programming solutions that are often quite sophisticated and involved. See, for instance, the recent papers [13, 184] which report the use of very interesting symmetry-breaking schemes to schedule social golfers.

weeks	group 1	group 2	group 3	group 4
week 1	1 2 3	4 5 6	7 8 9	10 11 12
week 2	1 4 7	10 2 5	8 11 3	6 9 12
week 3	1 5 9	10 2 6	7 11 3	4 8 12

Table 5.4: The initial configuration for the problem $4-3-3$

weeks	group 1	group 2	group 3	group 4	group 5
week 1	1 2 3 4 5	6 7 8 9 10	11 12 13 14 15	16 17 18 19 20	21 22 23 24 25
week 2	1 6 11 16 21	2 7 12 17 22	3 8 13 18 23	4 9 14 19 24	5 10 15 20 25
week 3	1 7 13 19 25	2 8 14 20 21	3 9 15 16 22	4 10 11 17 23	5 6 12 18 24
week 4	1 8 15 17 24	2 9 11 18 25	3 10 12 19 21	4 6 13 20 22	5 7 14 16 23
week 5	1 9 12 20 23	2 10 13 16 24	3 6 14 17 25	4 7 15 18 21	5 8 11 19 22
week 6	1 10 14 18 22	2 6 15 19 23	3 7 11 20 24	4 8 12 16 25	5 9 13 17 21

Table 5.5: The initial configuration for the problem $5-5-6$

5.4 A Constructive Heuristic

The quality of SGLS can be further improved by using a constructive heuristic to find a good starting, and restarting, configuration. The heuristic [39] trivially solves $p-p-(p+1)$ instances when p is prime and provides good starting points (or solutions) for other instances as well. Examples of such initial configurations are given in Tables 5.4 and 5.5, which will be used to explain the intuition underlying the constructive heuristic. The heuristic simply aims at exploiting the fact that all golfers in a group for a given week must be assigned a different group in subsequent weeks. As a consequence, the heuristic attempts to distribute these golfers in different groups in subsequent weeks.

Table 5.5 is a simple illustration of the heuristic with 5 groups of size 5 (i.e., 25 golfers) and 6 weeks. The first week is simply the sequence 1..25. In the second week, group i consists of all golfers in position i in week 1. In particular, group 1 consists of golfers $1, 6, 11, 16, 21$, group 2 is composed of golfers $2, 7, 12, 17, 22$ and so on. In other words, the groups consist of golfers in the same group position in week 1. The third week is most interesting, since it gives the intuition behind the heuristic. The key idea is to try to select golfers whose positions are j,j+1,j+2,j+3,j+4 in the first week, the

```
1.  heuristicSchedule(w, g, p)
2.      n ← g × p;
3.      P_0 ← ⟨1, ..., n⟩;
4.      forall we ∈ 1..w − 1
5.          P_we ← scheduleWeek(we, g, p, n);

6.  scheduleWeek(we, g, p, n)
7.      P_we ← ⟨1⟩;
8.      po ← 0;
9.      gr ← 1;
10.     Δ ← we − 1;
11.     forall go ∈ 1..n − 1
12.         s ← select(gr, (po + Δ)%p);
13.         po ← position(s);
14.         gr ← (gr + 1)%g;
15.         P_we ← P_we :: ⟨s⟩;
16.     return P_we;
```

Figure 5.2: The Constructive Heuristic for Scheduling Social Golfers

addition being modulo the group size. In particular, group 1 is obtained by selecting the golfers in position i from group i in week 1, i.e., golfers $1, 7, 13, 19, 25$. Subsequent weeks are obtained in similar fashion by simply incrementing the offset. In particular, the fourth week considers sequences of positions of the form j,j+2,j+4,j+6,j+8 and its first group is $1, 8, 15, 17, 24$. Table 5.4 illustrates the heuristic on the 4-3-3 instance. Note that the first group in week 2 has golfers in the first position in groups 1, 2, and 3 in week 1. However, the first golfer in week 4 must still be scheduled. Hence the second group must select golfer 10, as well as golfers 2 and 5.

Figure 5.2 depicts the code of the constructive heuristic. The code takes the convention that the weeks are numbered from 0 to $w-1$, the groups from 0 to $g-1$, and the positions from 0 to $p-1$, since this simplifies the algorithm. The key intuition to understand the code is to recognize that a week can be seen as a permutation of the golfers on which the group structure is superimposed. Indeed, it suffices to assign the first p positions to the first group, the second set of p positions to the second group and so on. As a consequence, the constructive heuristic only focuses on the

problem of generating w permutations $P_0, \ldots, P_{w-1}$.

The top-level function is HEURISTICSCHEDULE which specifies the first week and calls function SCHEDULEWEEEK for the remaining weeks. Scheduling a week is the core of the heuristic. All weeks start with golfer 1 (line 7) and initialize the position po to 0 (line 8), the group number gr to 1 (line 9), and the offset Δ to $we - 1$. The remaining golfers are scheduled in lines 11-15.

The key operation is line 12, which selects the first *unscheduled* golfer s from group gr of week 0 (specified by P_0) starting at position $(po + \Delta)\%p$ and proceeding by viewing the group as a circular list. The next three instructions update the position po to the position of s in group gr of week 0 (line 13), increment the group to select a golfer from the next group, and extend the permutation by concatenating s to P_{we}. By specification of SELECT, which only selects unscheduled golfers and the fact that the heuristic selects the golfers from the groups in a round-robin fashion, the algorithm is guaranteed to generate a permutation.

5.5 Experimental Results using the Constructive Heuristic

This section discusses the performance of algorithm SGLS-CH that enhances SGLS with the constructive heuristic to generate starting/restarting points. Although the starting point is deterministic, the algorithm still uses restarting, since the search itself is randomized, i.e., ties are broken randomly.

5.5.1 The $odd - odd - w$ Instances

It is known that the constructive heuristic finds solutions for $p - p - (p + 1)$ instances when p is prime. Moreover, it also provides solutions to many instances of the form $odd - odd - w$ as we now show experimentally. The results were performed up to $odd = 49$. For all (odd) prime numbers p lower than 49, the heuristic solves the instances $p - p - w$, where w is the maximal number of weeks for p groups and periods. When odd is divisible by 3, the heuristic solves instances of the form $odd - odd - 4$,

when *odd* is divisible by 5, it solves instances of the form $odd - odd - 6$, and when *odd* is divisible by 7, it solves instances of the form $odd - odd - 8$. For instance, the constructive heuristic solves instance 49-49-8.

It is interesting to relate these results to mutually orthogonal latin squares[2]. Indeed, it is known that finding a solution for instances of the form $g-g-4$ is equivalent to the problem of finding two orthogonal latin squares of size g. Moreover, instances of the form $g-g-n$ are equivalent to the problem of finding $n-2$ mutually orthogonal latin squares of size g [39, 199]. Instances of the form $g-g-4$ can be solved in polynomial time when g is odd. This provides some insight into the structure of these instances and some rationale why the constructive heuristic is able to solve many of the $odd - odd - w$ instances. Table 5.6 summarizes the results on the $odd - odd - w$ instances. The columns respectively specify the instances, the largest w found by the constructive heuristic, and the number of weeks w for the social golfers that corresponds to the best lower bound on the latin square as given in [40]. Rows in bold faces indicate closed instances. This constructive heuristic has been extended to deal with other types of instance in [113].

It is interesting to observe that the lower bounds on the mutually orthogonal latin squares vary significantly. Indeed, the lower bound for size 17 is 16, while it is 4 for size 15. These lower bounds give some additional insights on the inherent difficulty of these instances and on the behavior of the constructive heuristic.

5.5.2 Hard Instances

Table 5.7 compares the tabu-search algorithm with and without the constructive heuristic on the hard instances from Table 5.3. Note that $7-7-7$ and $7-7-8$ are now trivially solved, as well as $9-9-4$ which was also open. SGLS-CH does not strictly dominates SGLS, as there are instances where it is slightly slower. However, on some instances, it is clearly superior (including on $8-8-5$ which can now be solved). Algorithm SGLS-CH also closes two additional open problems: $7-5-6$ and

[2]A Latin Square corresponds to a Quasigroup, explained in chapter 4. Two Latin Squares of order n are said to be orhtogonal if one can be superimposed on the other, and each of the n^2 combinations of the symbols occurs exactly one in the n^2 cells of the array

instances	$CH : w$	Gol:LB
3-3-w	4	4
5-5-w	6	6
7-7-w	8	8
9-9-w	4	10
11-11-w	12	12
13-13-w	14	14
15-15-w	4	6
17-17-w	18	18
19-19-w	20	20
21-21-w	4	7
23-23-w	24	24
25-25-w	6	26
27-27-w	4	28
29-29-w	30	30
31-31-w	32	32
33-33-w	4	7
35-35-w	6	7
37-37-w	38	38
39-39-w	4	6
41-41-w	42	42
43-43-w	44	44
45-45-w	4	8
47-47-w	48	48
49-49-w	8	50

Table 5.6: Results on the $odd - odd - w$ Instances

$10 - 4 - 10$. Table 5.8 depicts the performance of algorithm SGLS-CH on the new solved instances.

5.5.3 Summary of the Results

Table 5.9 summarizes the results of this work. It depicts the status of maximal instances for SGLS-CH and whether the instances are hard (more than 10 seconds) or easy (less than 10 seconds). The results indicate that SGLS-CH matches or improves the best results for all but 3 instances. In addition, it produces 11 new solutions

	random			new		
instances	I	T	$\%F$	I	T	$\%F$
6-3-8	282254.07	48.93	6	250572	43.84	4
6-4-6	161530.35	47.75		168000	49.66	
7-4-7	274606.00	107.18		200087	124.15	
8-4-8	323141.52	107.62	8	316639	141.91	3
8-8-4	153301.61	360.00		8380.45	19.54	
8-8-5	–	–	100	108654.00	496.82	
10-3-13	45849.00	30.82		51015.00	34.28	

Table 5.7: Comparison between SGLS and SGLS-CH.

instance	I	T	**%solved**
7-5-6	487025.0	370.50	10
9-4-9	469156.4	402.55	100
9-5-7	4615.0	5.39	100
9-6-6	118196.7	196.52	100
9-7-5	64283.9	155.16	100
9-8-4	1061.3	2.92	100
10-4-10	548071.6	635.20	100
10-5-8	45895.4	76.80	100
10-9-4	5497.9	24.42	100

Table 5.8: Experimental Results of SGLS-CH on the New Solved Instances.

with respect to earlier results. These results are quite remarkable given the simplicity of the approach. Indeed, constraint-programming approaches to the social golfer problem are typically very involved and use elegant, but complex, symmetry-breaking techniques. Algorithm SGLS-CH, in contrast, does not include any such symmetry breaking.

It is interesting to observe the highly constrained nature of the instances for which SGLS-CH does not match the best-known results. Hence it is not surprising that constraint programming outperforms local search on these instances. Note also that Brisset and Barnier [13] proposed a very simple constraint-programming model to solve $8 - 4 - 9$ in a few seconds. So, once again, there seems to be a nice complementarity between constraint programming and local search on the social golfer

	size 3		size 4		size 5		size 6		size 7		size 8		size 9		size 10	
#groups	w	status	w	status	w	status	w	status	w	status	w	status	w	status	w	status
6	**8**	**Hard**	6	Hard	**6**	**Hard**	**3**	**Easy**	-	-	-	-	-	-	-	-
7	**9**	**Easy**	**7**	**Hard**	**6**	**New**	**4**	**Easy**	**8**	**New**	-	-	-	-	-	-
8	**10**	**Easy**	8	Hard	**6**	**Easy**	**5**	**Easy**	**4**	**Easy**	5	Hard	-	-	-	-
9	**11**	**Easy**	**9**	**New**	**7**	**New**	**6**	**New**	**5**	**New**	**4**	**New**	**4**	**New**	-	-
10	**13**	**Hard**	**10**	**New**	**8**	**New**	**6**	**Easy**	**5**	**Easy**	**4**	**Easy**	**4**	**New**	**3**	**Easy**

Table 5.9: Summary of the Results for SGLS-CH with Maximal Number of Weeks.
Bold entries represent a match or an improvement over existing solutions.
The status is *new* (for improvement), hard ($>$ 10 seconds), and easy ($\leq$ 10 seconds).

problem.

5.6 Lessons learnt

Local Search is a heuristic algorithm that relies on a fitness function and a neighborhood structure to drive the search towards high quality solutions in the search space. Here is the list of lessons we have learnt:

- LS is better suited for optimization, although it is also effective for satisfaction. However, in the latter case it is not possible for the LS algorithm to find all the solutions.
- LS algorithms tend to quickly converge to a local optima, however, it is sometimes very difficult to escape from it and direct the search towards global optima.
- LS can be easily fed with constructive heuristics to generate initial candidate. This has a great impact on the performance of the algorithm.
- Tabu search is a very powerful LS technique since it allows degrading moves to help escape local optima while not excessively degrading the solution quality, and it also maintains abstractions of visited solutions in order to avoid revisiting them during search.
- LS algorithms are not very difficult to implement and the most time consuming part is usually devoted to come up with the right modeling and data structures.

Chapter 6

A Memetic Algorithm for the Golomb Ruler Problem

Finding Golomb rulers is an extremely challenging combinatorial problem which has received considerable attention over the last decades. An n-mark Golomb ruler is an ordered sequence of n distinct nonnegative integers $\langle m_1, \ldots, m_n \rangle$ $(m_i < m_{i+1})$ such that all distances

$$m_j - m_i \quad (1 \leq i < j \leq n) \tag{6.1}$$

are distinct. Each integer m_i corresponds to a mark on the ruler and the *length* of the ruler is the difference $m_n - m_1$. By convention, the first mark m_1 can be placed in position 0, in which case the length is given by m_n. An n-mark Golomb ruler is *optimal* if there exists no n-mark Golomb ruler of smaller length.

Golomb rulers have applications in a wide variety of fields including radio communications ([27, 114]), x-ray crystallography ([26]), coding theory ([56, 139]), and radio astronomy. Moreover, because of their highly combinatorial nature,[1] they have become a standard benchmark to evaluate and compare a variety of search techniques. In particular, genetic algorithms, constraint programming, local search, and their hybridizations have all been applied to the problem of finding Golomb rulers (e.g., [43, 76, 173, 176, 210, 213]).

[1] The search for a 19-mark Golomb ruler took approximately 36,200 CPU hours on a Sun Sparc workstation using a very specialized algorithm [56].

This research proposes a novel hybrid evolutionary algorithm for finding near-optimal Golomb rulers in reasonable time. The algorithm embeds a local search into a genetic algorithm and outperforms earlier genetic algorithms, as well as constraint programming algorithms and their hybridizations with local search. In particular, the algorithm quickly finds optimal rulers for up to 13 marks and was able to find optimal rulers for 14 and 15 marks, which is clearly out of reach for the above mentioned algorithms. The algorithm also finds near-optimal rulers in reasonable time, clearly indicating the effectiveness of hybrid evolutionary algorithms on this highly combinatorial application. Of particular interest is the conceptual simplicity and elegance of the algorithm.

Even though there are solutions for higher number of marks for other complete search approaches, evolutionary algorithms have the advantage of providing good quality solutions in a short period of time. This is a main contribution of this research as well, providing high quality solutions (improving all previous evolutionary approaches) in a few seconds or minutes.

The main technical contribution of the novel hybrid evolutionary algorithm is its focus on feasibility. Indeed, the main step of the evolutionary algorithm is to find a Golomb ruler of a specified length (or smaller), using constraint violations to guide the search. Near-optimal rulers are obtained indirectly by solving a sequence of feasibility problems.

The rest of this chapter starts by a brief overview of related work. It then presents presents the local search and the hybrid evolutionary algorithms for finding Golomb rulers of a specified length, before generalizing the algorithm to find near-optimal rulers and concluding with the lessons learnt.

6.1 Finding Golomb Rulers

Two main approaches can be essentially considered for tackling the Optimal Golomb Ruler (OGR) problem with EAs. The first one is the *direct* approach, in which the EA conducts the search in the space $\mathcal{S}_G$ of all possible Golomb rulers. The second one is the *indirect* approach, in which an auxiliary $\mathcal{S}_{aux}$ space is used by the EA. In

this latter case, a decoder [140] must be utilized in order to perform the $\mathcal{S}_{aux} \longrightarrow \mathcal{S}_G$ mapping. Examples of the former (direct) approach are the works of Soliday *et al.* [213], and Feeney [76]. As to the latter (indirect) approach, we can cite the work by Pereira *et al.* [173] (based on the notion of random-keys [18]), and Cotta and Fernández [43] (based on ideas from GRASP [190]). This latter paper is specifically interesting since generalizations of the core idea presented there have been used in this work. To be precise, the key idea was using a problem-aware procedure (inspired in GRASP) to perform the genotype-to-phenotype mapping. This method ensured the generation of feasible solutions, and was shown to outperform other previous approaches.

In 1995, Soliday, Homaifar and Lebby [213] used a genetic algorithm on different instances of the Golomb ruler problem. They chose a direct approach where each chromosome is composed by a permutation of $n-1$ integers that represents the sequence of the $n-1$ lengths of its segments. Two evaluation criteria were followed: the overall length of the ruler, and the number of repeated measurements. This latter quantity was used in order to penalize infeasible solutions. The mutation operator consisted of either a permutation in the segment order, or a change in the segment lengths. As to crossover, it was designed to guarantee that descendants are valid permutations.

Later, Feeney studied the effect of hybridizing genetic algorithms with local improvement techniques to solve Golomb rulers [76]. The direct representation used consisted of an array of integers corresponding to the marks of the ruler. The crossover operator was similar to that used in Soliday *et al.*'s approach although a sort procedure was added at the end. The mutation operator consisted in adding a random amount in the range $[-x, x]$ -where x is the maximum difference between any pair of marks in any ruler of the initial population– to the segment mark selected for mutation. As it will be shown later, we can use a similar concept in order to define a distance measure on the fitness landscape. Pereira *et al.* presented in [173] an indirect approach based EA using the notion of random keys [18] o codify the information contained in each chromosome. The basic idea consists of generating n random numbers (i.e., the keys) sampled from the interval $[0, 1]$ and ordered by its

position in the sequence $1, \ldots, n$; then the keys are sorted in decreasing order. The indices of the keys thus result in a feasible permutation of $\{1, \cdots, n\}$. A similar evaluation criteria as described in [213] was followed. They also presented an alternative algorithm that adds a heuristic, favoring the insertion of small segments. A related approach has been presented in [43]. This proposal incorporates ideas from greedy randomized adaptive search procedures (GRASP) [190] in order to perform the genotype-to-phenotype mapping. More precisely, the mapping procedure proceeds by placing each of the $n-1$ marks (the first mark is assumed to be $a_1 = 0$) one at a time; the $(i+1)^{\text{th}}$ mark can be obtained as $a_{i+1} = a_i + l_i$, where $l_i \geqslant 1$ is the $i-$th segment length. Feasible segment lengths (i.e., those not leading to duplicate measurements) can be sorted in increasing order. Now, the EA needs only specifying at each step the index of a certain segment within this list (obviously, the contents of the list are different in each of these steps). This implies that each individual would be a sequence $\langle r_1, \cdots, r_{n-1} \rangle$, where r_i would be the index of the segment used in the $i-$th iteration of the construction algorithm. Notice that in this last placement step it does not make sense to pick any other segment length than the smallest one. For this reason, $r_{n-1} = 1$; hence, solutions need only specify the sequence $\langle r_1, \cdots, r_{n-2} \rangle$. This representation of solutions is orthogonal [186], i.e., any sequence represents a feasible solution, and hence, standard operators for crossover and mutation can be used to manipulate them. This GRASP-based approach was reported to perform better than the previous (indirect and direct) approached mentioned.

6.2 Golomb Rulers of Fixed Lengths

This section describes hybrid evolutionary algorithm for finding Golomb rulers of specified lengths. It starts with the problem modeling, then describes the local search and the hybrid evolutionary algorithms, and concludes with the experimental results.

6.2.1 Modeling

The problem modeling in the hybrid evolutionary algorithm is natural and associates a decision variable m_x with every mark x. Given a ruler σ, i.e., an assignment of values to the decision variables, the value $\sigma(m_x)$ denotes the position of mark x within the ruler. Since the length l of the ruler is known in this section, the values $\sigma(m_1)$ and $\sigma(m_n)$ are fixed to 0 and l respectively. There are three kinds of constraints in the Golomb ruler:

1. The marks have different positions in the ruler.
2. The marks are ordered, i.e., $\sigma(m_i) < \sigma(m_{i+1})$.
3. The distances $d_{ij} = m_j - m_i$ $(j > i)$ are all different.

The first two types of constraints are implicit in the algorithms presented in this work: They are satisfied by the initial assignments and are preserved by local moves and genetic operators. The goal of the algorithms is thus to satisfy the third set of constraints.

To guide the search, the algorithms use a notion of constraint violations on the distances. The violation $\upsilon_\sigma(d)$ of a distance d in a n-mark ruler σ is the number of times distance d appears between two marks in the ruler σ beyond its allowed occurrences, i.e.,

$$\upsilon_\sigma(d) = \max(0, \#\{d_{ij} = d \mid 1 \leq i < j \leq n\} - 1) \tag{6.2}$$

where $d_{ij} = \sigma(m_j) - \sigma(m_i)$. The violations $\upsilon(\sigma)$ of a n-mark ruler σ is simply the sum of the violations of its distances d, i.e.,

$$\upsilon(\sigma) = \sum_{d \in D} \upsilon_\sigma(d) \tag{6.3}$$

where $D = \{d_{i,j} \mid 1 \leq i < j \leq n\}$. Obviously, a ruler σ with $\upsilon(\sigma) = 0$ is a solution to the Golomb ruler problem.

6.2.2 The Tabu Search

We now turn to the tabu search algorithm for finding Golomb rulers of specified lengths.

The Neighborhood The moves in the local search consists of changing the value of a single mark. Since the marks are ordered, a mark x can only take a value in the interval

$$I_\sigma(x) = [\sigma(m_{x-1}) + 1, \sigma(m_{x+1}) - 1].$$

As a consequence, the sets of possible moves is

$$\mathcal{M}(\sigma) = \{(x, p) \mid 0 < x < n \ \& \ p \in I_\sigma(x)\}.$$

Observe that $\sigma(m_1)$ and $\sigma(m_n)$ are fixed to 0 and l.

The Tabu Component The tabu component of the local search prevents a mark from being reassigned the same value for a number of iterations. The tabu list thus consists of a triplet $\langle x, p, i\rangle$, where x is a mark and p is a possible position for mark x and i represents the first iteration where mark x can be assigned to p again. The tabu tenure, i.e., the number of iteration (x, p) stays in the list, is dynamic and is randomly generated in the interval $[4, 100]$. For a ruler σ and an iteration k, the set of legal moves is thus defined as

$$\mathcal{M}^+(\sigma, k) = \{(x, p) \in \mathcal{M}(\sigma) \mid \neg tabu(x, p, k)\}.$$

where $tabu(x, p, k)$ holds if the assignment $m_x \leftarrow p$ is tabu at iteration k. The tabu status can be overridden whenever an assignment would reduce the smallest number of violations found so far. In other words, if σ^* is the ruler with the smallest number of violations found so far, the neighborhood also includes the moves

$$\mathcal{M}^*(\sigma, \sigma^*) = \{(x, p) \in \mathcal{M}(\sigma) \mid \upsilon(\sigma[m_x \leftarrow p]) < \upsilon(\sigma^*)\}$$

where $\sigma[m_x \leftarrow p]$ denotes the ruler σ where variable m_x is assigned to p.

The Tabu-Search Algorithm We are now ready to present the basic local search algorithm GRLS. The algorithm, depicted in Figure 6.1, a tabu search with an intensification component[2]. Lines 2-6 perform the initializations. In particular, the tabu list is initialized in line 2, the initial ruler is generated randomly in line 3, while lines 5 and 6 initialize the iteration counter k, and the stability counter s. The initial configuration σ randomly assigns values for all marks, satisfying the constraints that each mark is assigned to a different value and are ordered. Moreover, the position of the first mark is 0 and the position of the last mark is the length l of the ruler. The best ruler found so far σ^* is initialized to σ. The core of the algorithm are lines 7-21 which perform local moves for a number of iterations or until a solution is found. The local move is selected in line 8. The key idea is to select the best assignment in the neighborhood

$$\mathcal{M}^+(\sigma, k) \ \cup \ \mathcal{M}^*(\sigma, \sigma^*),$$

i.e., the non-tabu moves and those which improve the best ruler. Observe that the expression $\upsilon(\sigma[m_x \leftarrow v])$ represents the number of violations obtained after assigning p to mark x. The tabu list is updated in line 10, and the new ruler is computed in line 11. Lines 12-14 update the best ruler, while lines 15-18 specify the intensification component. The intensification component simply reinitializes the search from the best available ruler whenever no improvement in the number of violations took place for *maxStable* iterations. Note that the stability counter s is incremented in line 20 and reset to zero in line 14 (when a new best ruler is found) and in line 17 (when the search is restarted).

6.2.3 The Hybrid Evolutionary Algorithm

We now turn to the hybrid evolutionary (HE) algorithm for finding Golomb rulers of specified lengths. The algorithm maintains a population of rulers and performs

[2]Remember that intensification consists of maintaining a list of good solutions that the algorithm will revisit at some point during the search

```
1.  GRLS(n,l)
2.      tabu ← {};
3.      σ ← RANDOMCONFIGURATION(n,l);
4.      σ* ← σ;
5.      k ← 0;
6.      s ← 0;
7.      while k ≤ maxIt  &  υ(σ) > 0 do
8.          select (x,p) ∈ M+(σ,k) ∪ M*(σ,σ*)
                minimizing υ(σ[m_x ← p]);
9.          τ ← RANDOM([4,100]);
10.         tabu ← tabu ∪ {⟨x,p,k+τ⟩};
11.         σ ← σ[m_x ← p];
12.         if υ(σ) < υ(σ*) then
13.             σ* ← σ;
14.             s ← 0;
15.         else if s > maxStable then
16.             σ ← σ*;
17.             s ← 0;
18.             tabu ← {};
19.         else
20.             s++;
21.         k++;
```

Figure 6.1: Algorithm GRLS for Finding Golomb Rulers

a number of iterations until a solution is found. Each iteration selects two rulers in the population and, with some probabilities, crosses and/or mutates them. The two rulers so obtained replace their parents in the population. Each of these steps is now reviewed in more detail.

Selection Each iteration selects two rulers in the population (the parents). Two strategies were studied for selecting the parents: a random strategy which randomly selects two rulers from the population and a "roulette wheel" strategy that biases the search toward rulers with fewer violations.

Crossover The HE algorithm uses a one-point crossover for crossing two rulers σ_1 and σ_2. It selects a random number k in $1..n$. The first child is obtained by selecting the first k marks from σ_1 and the remaining $n-k$ marks from σ_2. The second child is obtained in a similar fashion by swapping the role of the parents. There is a minor difficulty to address when crossing two rulers: the two rulers may include the same markers. Consider the two parents

$$\sigma_1 = \langle\ 0\ 1\ 5\ 12\ 23\ 34\ 37\ 41\ 44\ \rangle$$
$$\sigma_2 = \langle\ 0\ 3\ 6\ 10\ 16\ 23\ 39\ 42\ 44\ \rangle$$

and $k = 5$. Without extra care, the first child would be

$$\langle\ 0\ 1\ 5\ 12\ 23\ /\ 23\ 39\ 42\ 44\ \rangle$$

repeating position 23. Instead, the crossover selects the last $n-k$ elements in σ_2 which are not found in σ_1, giving

$$\langle\ 0\ 1\ 5\ 12\ 23\ /\ 16\ 39\ 42\ 44\ \rangle.$$

The ruler is then ordered to obtain the first child

$$\langle\ 0\ 1\ 5\ 12\ 16\ 23\ 39\ 42\ 44\ \rangle.$$

The second child is obtained in a symmetric way.

Mutation Mutations in the HE algorithm are performed by the local search GRLS. The best solution obtained by GRLS is the result of the mutation, unless this solution is already in the population. In this last case, the mutation is simply the ruler when the local search terminates. This design choice is motivated by the desire to preserve diversity during the search.

Restarting Policy The algorithm is restarted from scratch when the diversity of the population is too low. The restarting policy is based on the empirical observation that the population is not diverse enough when too many rulers have few violations. As a consequence, the HE algorithm restarts when more than half of the population

```
1.  GRHEA(n, l)
2.      forall i ∈ 1..PopulationSize
3.          Σ ← Σ ∪ {RANDOMCONFIGURATION(n, l)};
4.      g ← 0;
5.      while g ≤ maxGen & υ(Σ) > 0 do
6.          i ← 0;
7.          Σ⁺ ← ∅;
8.          while i ≤ populationSize do
9.              select (σ1, σ2) ∈ Σ;
10.             with probability Pc
11.                 (σ1, σ2) ← crossover(σ1, σ2);
12.             with probability Pm
13.                 σ1 ← GRLS(σ1);
14.                 σ2 ← GRLS(σ2);
15.             Σ⁺ ← Σ⁺ ∪ {σ1, σ2};
16.             i ← i + 2;
17.         Σ ← Σ⁺;
18.         g ← g + 1;
19.         if diversity(Σ) < ϒ
20.             forall i ∈ 1..PopulationSize
21.                 Σ ← Σ ∪ {RANDOMCONFIGURATION(n, l)};
```

Figure 6.2: Algorithm GRHEA for Finding Golomb Rulers

has fewer violations than a specified threshold Υ. This strategy is only applied when the parents are selected using the "roulette wheel" strategy which has a tendency to decrease the diversity of the population significantly over time. In the following, we use $diversity(\Sigma)$ to denote the median violation in Σ and $\upsilon(\Sigma)$ to denote the smallest violation in Σ.

The Hybrid Algorithm We are now ready to present the HE algorithm GRHEA which is depicted in Figure 6.2. Lines 2-4 perform the initializations. In particular, the population is randomly generated in lines 2-3 and the generation counter g is initialized in line 4.

The core of the algorithm is in lines 5-21. They generate new generations of

	CPU Time(secs)		Local Moves		Failures			CLS	
# marks	avg	mdn	avg	mdn	%F	MaxGen	time Uns.	Backtracks	CPU Time
5	0.0	0.0	3.46	1	0	10	-	15	0.0
6	0.0	0.0	8.78	5	0	10	-	24	0.0
7	0.0	0	42.44	21	0	10	-	145	0.0
8	0.03	0.02	1125.54	564	0	10	-	5114	0.08
9	0.24	0.19	5711.32	4339.5	0	10	-	23118	0.47
10	3.49	2.29	5674.5	37479.5	0	10	-	74860	1.87
11	8.15	5.86	84606.2	60836.5	0	10	-	269905	8.16
12	199.45	166.75	1531640.67	1288230.5	1	20	2411.1	2005597	72.2
13	1071.74	959.55	5655670.67	4969063	1	50	990.36	20360198	860
14	1013.2	3861.69	3939817.5	14965000	98	50	3860.93		

Table 6.1: Experimental Results of GRHEA for Rulers from 5 to 14 Marks.

rulers for a number of iterations or until a solution is found. The new generation is initialized in line 7, while lines 8-16 create the new generation. The new rulers are generated by selecting the parents in line 9, applying a crossover with probability P_c (lines 10-11), and applying a mutation with probability P_m (lines 12-14). Note that the function GRHEA(σ) denotes the execution of GRLS starting from ruler σ. The new rulers are added to the new population in line 15. The new population becomes the current population in line 17. If the new population is not diverse enough (line 19), it is reinitialized from scratch (lines 20-21).

Experimental Results Table 6.1 reports the experimental results for algorithm GRHEA. Algorithm GRHEA was run 50 times for each ruler with a population size of 50 and with a maximum of 10,000 iterations for the local search. The crossover and mutation probabilities were both set to 0.6 and the diversity parameter Υ is set to 5. These parameters were determined from a limited number of experiments and can certainly be tuned for specific instances. Only results with roulette selection are reported. The results of random selection are relatively close, but near-optimal results only use roulette selection.

The results are compared to those of [176], where a hybrid Complete and Local Search algorithm named Constrained Local Search (CLS) is introduced. Note that CLS performs better for higher number of marks but it is not able to solve rulers of

14 marks while our algorithm is.

6.3 Near Optimal Golomb Rulers

The algorithms described so far compute Golomb rulers of specified lengths. This section discusses how to generalize them to find near-optimal Golomb rulers.

6.3.1 The Difficulty

Consider first the problem of generalizing the tabu-search algorithm for finding near-optimal Golomb rulers. A natural approach is to solve a sequence of feasibility problems. Starting from an upper bound l on the optimal length of the ruler, the algorithm then searches for rulers of length l, $l-1$, ... until no solution can be found. This approach, although conceptually simple, performs poorly. Indeed, it essentially solves a sequence of mostly unrelated problems, since no information is reused across the searches and, in addition, the search for a ruler of length l is not necessarily simpler than the search for a ruler of smaller length.

A second approach consists of integrating the ruler length as part of the objective function and to consider the last mark m_n as a decision variable. The objective function now combines constraint violations and the ruler length in order to guide the search toward optimal rulers. The violations and the length can be combined in different fashions. However, preliminary experimental results with this approach were not encouraging, although there may exist effective ways to combine these two conflicting objectives effectively for tabu-search or other meta-heuristics.

6.3.2 Generalizing the Hybrid Evolutionary Algorithm

Interestingly, the HE algorithm can be generalized to produce an indirect, but effective, approach for finding near-optimal Golomb rulers in reasonable time. The approach consists again of solving a sequence of feasibility problems, starting from an upper bound l and producing a sequence of rulers of length $l_1 > l_2 > \ldots > l_i > \ldots$. The key idea however is not to fix the length of the ruler in the HE algorithm. More

```
1.  GROHEA(n, u)
2.      σ ← GRGHEA(n, u);
3.      while υ(σ) = 0 do
4.          σ* ← σ;
5.          σ ← GRGHEA(n,LENGTH(σ*)-1);
6.      return σ*;
```

Figure 6.3: Algorithm GROHEA for Near-Optimal Rulers

precisely, the new HE (GRGHEA) algorithm considers the last mark m_n as a decision variable whose value is at most l, where l is the best available upper bound. The initial population consists of random rulers whose lengths are at most l, but are likely to be shorter. Crossover operations proceed as before. Mutations are again performed by the local search algorithm which still minimizes the number of violations but now considers the last mark as a decision variable. This algorithm differs from the previous one only in lines 13 and 14 (figure 6.2), where instead of using the GRLS, it would make use of a slightly modified procedure which will take into account the last mark of the ruler; this translates to the fact that $\sigma(m_n)$ is now not fixed (see remark in equation 5). Note that the length of the ruler is not incorporated in the objective function which focuses exclusively on feasibility.

The generalized HE algorithm GROHEA for finding near-optimal rulers is depicted in Figure 6.3. Given an upper bound u on the length of an n-mark ruler, the algorithm first searches for a ruler of length at most u (line 2). It then performs a number of iterations, each of which producing rulers of smaller length (lines 3-5), until no feasible solution can be found for a specified length. The main step is in line 5: It uses the HE algorithm GRGHEA for finding a ruler of length smaller than LENGTH(σ^*), where σ^* is the smallest ruler found so far and LENGTH(σ^*) is simply the value $\sigma^*(m_n)$ of the last mark. Note also that algorithm GRGHEA is the HE algorithm GRHEA(n, l) presented earlier, except that the last mark is now a decision variable and the initial population are rulers whose length is at most l but may be shorter.

Algorithm GROHEA is best viewed as solving a sequence of feasibility problems to find rulers of decreasing lengths. However, algorithm GROHEA does not artificially

		HGRASP			GROHEA				
#marks	Opt	Best	Median	Time	Best	Median	Time	Last(time)	Opt(time)
11	72	74(2.8)	74(2.8)	1.5	72	72	0.3	0.3	0.1
12	85	94(10.6)	95(11.8)	2.4	85	91(7.1)	2.3	1	1.8
13	106	111(4.7)	114(7.5)	3.6	106	112(5.6)	3.9	2	1.7
14	127	135(6.3)	139(9.4)	5.3	131(3.1)	136(7.1)	6	3.2	40.7
15	151	162(7.3)	169(11.9)	7.6	158(4.6)	164(8.6)	8.7	4.7	-
16	177	189(6.8)	197(11.3)	11.3	187(5.6)	195(10.2)	13.4	5.9	-

Table 6.2: Experimental Results for the GROHEA Algorithm. Time in minutes.

constrain the ruler length. Instead, the search is directed by constraint violations and the length of the ruler, i.e., the value of the last mark, is modified appropriate to minimize violations.

6.3.3 Experimental Results

Table 6.2 reports the experimental results for algorithm GROHEA and compare them with the HGRASP algorithm of [43]. All experiments use a roulette wheel selection and are based on the following settings. The maximum number of iterations for the tabu search is $10,000$, the size of the population is 50, the probabilities P_c and P_m are both 0.6, and Υ is 5. For a n-mark ruler, the algorithm uses the optimal length of an $n+1$-mark ruler as initial upper bound and is iterated until no improved ruler is found for two successive generations, except for $n = 16$ where we use three generations. The GROHEA is run 30 times for each ruler (like the HGRASP in [43]). Finally, we also let algorithm GROHEA without time/generation limits to determine whether it can find optimal rulers (these results are for a small number of runs). Both algorithms were run on similar machines.

The table reports the best and median lengths for rulers with 11 to 16 marks found by algorithms HGRASP and GROHEA within their time limits (algorithm GROHEA easily finds optimal rulers for smaller lengths). It also reports the average times of both algorithms in minutes. In addition, for algorithm GROHEA, the table also gives the time to find the last solution (if it is not the optimal solution the algorithm will keep on trying to find it, but it might not be able to find any other ruler, in that

case, we report time to find the last valid ruler). The last column reports the time of GROHEA to find optimal rulers.

The results are particularly impressive. First observe that GROHEA systematically finds optimal rulers up to 11 marks very quickly. Algorithm HGRASP does not find optimal rulers systematically even for 10 marks and never finds optimal rulers for 11 marks. Algorithm GROHEA also finds optimal rulers for 12 and 13 marks in less than two minutes and for 14 marks in about 40 minutes. Algorithm GROHEA also improves the near-optimal solutions significantly. For 14 marks, the best solutions of GROHEA are with 3.1% of the optimal rulers (instead of 6.3% for HGRASP) in about 6 minutes. They are with 4.6% and 5.6% for 15 and 16 marks in about 9 and 13 minutes. These represent improvements ranging from 1.4% to 3.2% compared to HGRASP. Similar results are obtained for median values as well.

A fundamental benefit of GROHEA is its ability to improve its solutions over time, which does not seem to be the case of prior generic and/or hybrid evolutionary algorithms. Contrary to GROHEA, earlier algorithms were not able to find optimal solutions for 13 and 14 marks. Algorithm GROHEA also finds a solution of length 153 in about an hour on 15 marks (151 is the optimal length), showing that better solutions can be found when the algorithm is given more time. This is particularly interesting given the natural modeling and conceptual simplicity of the algorithm.

It is also important to stress that these results were obtained without tuning of the parameters. In particular, larger instances are likely to benefit from longer tabu searches and, possibly, more sophisticated crossovers. But the results clearly indicate the potential of hybrid evolutionary algorithms for finding near-optimal rulers.

6.4 Lessons learnt

Genetic Algorithms are population-based algorithms that are easily hybridized with LS techniques. Contrary to the opinion of many researchers within the combinatorial optimization field, they can be very efficient when solving hard problems, and especially when generating fast near-optimal solutions. Here is the list of lessons we have learnt:

- GAs are very useful to provide a framework in which to maintain a set of diverse and high quality solutions.
- Recombination operators can sometimes yield valid, optimal or near-optimal solutions.
- When solving hard combinatorial problems they greatly benefit from the incorporation of LS techniques that allow a faster convergence.
- A fast convergence of the population is also problematic. Restarts and other mechanism are needed in order to regenerate the population and drive the search towards different regions in the search space. However, it is not always straightforward to implement the right restarting condition.
- The Local Search is greatly enriched by having a population of diverse solutions. LS typically improves a solution until it gets stuck on a local optima, when the algorithm commonly restarts and attempts to improve a different solution. In this case, we can see it as if the LS had a set of good solutions available at any time to be optimized in turns.
- GAs can not only incorporate LS procedures to improve the efficiency of their recombination operators, but also use information yielded by those processes to dynamically adapt themselves.

Part III

The Last Hybrid

Chapter 7

Adding CP and Clustering to Solve the Golomb Ruler Problem

In this section a new hybrid algorithm is presented in two steps: first a very sophisticated memetic algorithm; and second, the introduction of CP and clustering techniques to boost performance. As in the previous chapter, the problem we are going to be dealing with is that of the Golomb Ruler. Remember that Golomb Rulers [9, 26] are a class of undirected graphs that, unlike usual rulers, measure more discrete lengths than the number of marks they carry. More formally, a n-mark Golomb ruler is an ordered sequence of n distinct nonnegative integers $\langle m_1, \ldots, m_n \rangle$ $(m_i < m_{i+1})$ such that all distances $m_j - m_i \quad (1 \leqslant i < j \leqslant n)$ are distinct. Each integer m_i corresponds to a mark on the ruler and the *length* of the ruler is the difference $m_n - m_1$. By convention, the first mark m_1 can be placed in position 0, in which case the length is given by m_n.

The particularity of Golomb Rulers that on any given ruler, all differences between pairs of marks are unique makes them really interesting in many practical applications (cf. [76, 187]). It turns out that finding optimal or near-optimal Golomb rulers (a n-mark Golomb ruler is optimal if there exists no n-mark Golomb ruler of smaller length) is an extremely challenging combinatorial problem. To date, the highest number of marks for which the optimal Golomb ruler (OGR) is known is 23 marks[1] [205, 198].

[1]The search for an optimal 19-marks Golomb ruler took approximately 36,200 CPU hours on

Finding optimal Golomb rulers has thus become a standard benchmark to evaluate and compare a variety of search techniques. In particular, evolutionary algorithms (EAs), constraint programming (CP), local search (LS), and their hybridizations have all been applied to this problem (e.g., [76, 43, 173, 176, 210, 213]).

In these next sections, we present a hybrid EA designed to find optimal or near-optimal Golomb Rulers. This algorithm makes use of both an indirect approach and a direct approach in different stages of the search. More specifically, the indirect approach is used in the phases of initialization and restarting of the population and takes ideas borrowed from the GRASP-based evolutionary approach published in [43]. The direct approach is considered in the stages of recombination and local improvement; particularly, the local improvement method is based on the tabu search (TS) algorithm described in the previous chapter. Experimental results show that this algorithm succeeds where another evolutionary algorithms did not. OGRs up to 15 marks (included) can now be found. Moreover, the algorithm produces Golomb rulers for 16 marks that are very close to the optimal value (i.e., 1.1% far), thus improving significantly the results previously reported in the EA literature. Finally, we show the last improvements which rely on clustering to achieve diversity in the reference set and complete search to attempt to find optimal rulers at the recombination step. These enhancements produce superior results, and the new hybrid is now capable of solving rulers up to 16 marks. The chapter concludes with a brief summary and a review of all the lessons learnt throughout the thesis and how they are reflected in this last hybrid.

7.1 Scatter Search for the Golomb Ruler Problem

Scatter search (SS) is a metaheuristic based on population-based search whose origin can be traced back to the 1970s in the context of combining decision rules and problem constraints [142]. Figure 7.1 depicts the SS template. Among the salient features

a Sun Sparc workstation using a very specialized algorithm [56]. Optimal solutions for 20 up to 23 marks were obtained by massive parallelism projects, taking several months for each of those instances [187, 85].

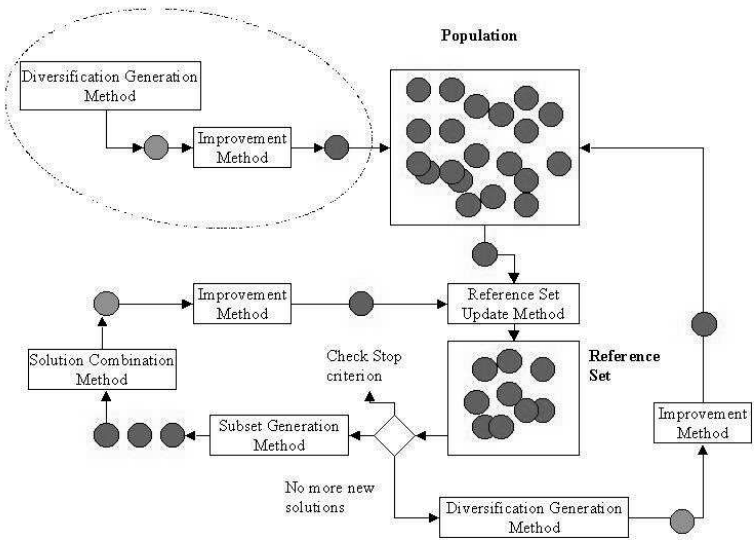


Figure 7.1: A generic SS algorithm diagram

of SS we can cite the absence of biological motivation, and the emphasis put in the use of problem-aware mechanisms, such as specialized recombination procedures, and LS techniques. In a striking example of convergent evolution, these are also distinctive features of memetic algorithms (MAs) [164]. Indeed, although SS evolved independently from MAs, SS can be regarded with hindsight as a particular case of MA (or, at least, as an alternative formulation of a common underlying paradigm). There is just one remarkable methodological difference between mainstream versions of SS and MAs: unlike other population-based approaches, SS relies more on deterministic strategies rather than on randomization. At any rate, this general methodological principle is flexible. This is particularly the case in our approach, in which we use a non-deterministic component within our algorithm. For this reason, we will use the terms MA and SS interchangeably in the context of this work. In the following we will describe each of the components of our algorithm.

7.1.1 Diversification Generation Method

The diversification generation method serves two purposes in the SS algorithm considered: it is used for generating the initial population from which the reference set will be initially extracted, and it is utilized for refreshing the reference set whenever a restart is needed.

The generation of new solutions is performed by using a randomized procedure that tries to generate diverse solutions. The basic method utilizes the GRASP-decoding techniques introduced in [43]. Solutions are incrementally constructed as follows: in the initial step, only mark $m_1 = 0$ is placed; subsequently, at each step i an ordered list is built using the n first integers $l_1, \cdots, l_n$ such that placing a new mark $m_i = m_{i-1} + l_j$, $1 \leqslant j \leqslant n$, would result in a feasible Golomb ruler. A random element is drawn from this list, and used to place mark m_i. The process is iterated until all marks have been placed. Notice that this results in a feasible solution.

A variant of this process is used in subsequent invocations to this method for refreshing the population. This variant is related to an additional dynamic constraint that is imposed in the algorithm: in any solution, it must hold that $m_n < L$, where L is the length of the best feasible Golomb ruler found so far. To fulfill this constraint, new solutions are constructed by generating two feasible rules following the procedure described before, and submitting them to the combination method (see Sect. 7.1.3), which guarantees compliance with the mentioned constraint.

7.1.2 Local Improvement Method

The improvement method is responsible for enhancing raw solutions produced by the diversification generation method, or by the solution combination method. In this case, improvement is achieved via the use of a tabu-search algorithm. This TS algorithm works on tentative solutions that may be infeasible, i.e., there may exist some repeated distances between marks. The goal of the algorithm is precisely to turn infeasible rulers into feasible ones, respecting the dynamic constraint $m_n < L$. Whenever this is achieved, a new incumbent solution is obviously found.

To guide the search, the algorithm uses a notion of constraint violations on the

distances. The violation $\upsilon_\sigma(d)$ of a distance d in a n-mark ruler σ is the number of times distance d appears between two marks in the ruler σ beyond its allowed occurrences, i.e.,

$$\upsilon_\sigma(d) = \max(0, \#\{d_{ij} = d \mid 1 \leqslant i < j \leqslant n\} - 1) \tag{7.1}$$

where $d_{ij} = m_j - m_i$. The overall violation $\upsilon(\sigma)$ of a n-mark ruler σ is simply the sum of the violations of its distances d, i.e., $\upsilon(\sigma) = \sum_{d \in D} \upsilon_\sigma(d)$, where $D = \{d_{ij} \mid 1 \leqslant i < j \leqslant n\}$.

The moves in the local search consists of changing the value of a single mark. Since marks are ordered, a mark m_x can only take a value in the interval $I_\sigma(x) = [m_{x-1}+1, m_{x+1}-1]$. As a consequence, the set of possible moves is $\mathcal{M}(\sigma) = \{(x,p) \mid (1 < x < n) \wedge (p \in I_\sigma(x))\}$. Observe that m_1 is fixed to 0, and m_n is not allowed to grow. To prevent cycling, a tabu list of movements is kept. The list stores triplets $\langle x, p, i\rangle$, where x is a mark, p is a possible position for mark x, and i represents the first iteration where mark x can be assigned to p again. The tabu tenure, i.e., the number of iterations (x,p) stays in the list, is dynamic and randomly generated in the interval $[4, 100]$. For a ruler σ and an iteration k, the set of legal moves is thus defined as

$$\mathcal{M}^+(\sigma, k) = \{(x,p) \in \mathcal{M}(\sigma) \mid \neg tabu(x,p,k)\}.$$

where $tabu(x,p,k)$ holds if the assignment $m_x \leftarrow p$ is tabu at iteration k. The tabu status can be overridden whenever an assignment reduces the smallest number of violations found so far. Thus, if σ^* is the ruler with the smallest number of violations found so far, the neighborhood also includes the moves

$$\mathcal{M}^*(\sigma, \sigma^*) = \{(x,p) \in \mathcal{M}(\sigma) \mid \upsilon(\sigma[m_x \leftarrow p]) < \upsilon(\sigma^*)\}$$

where $\sigma[m_x \leftarrow p]$ denotes the ruler σ where variable m_x is assigned to p. To intensify the search, the current solution is reinitialized to the initial ruler σ_0 (in the actual TS run) whenever no improvement in the number of violations took place for *maxStable* iterations. The algorithm returns the best solution σ^* found. Fig. 7.2 shows the

complete pseudocode of the TS algorithm.

```
1.  TS(σ_0)
2.      tabu ← {};
4.      σ* ← σ_0;
5.      k ← 0;
6.      s ← 0;
7.      while k ⩽ maxIt  &  υ(σ) > 0 do
8.          select (x, p) ∈ M+(σ, k)  ∪  M*(σ, σ*)
                minimizing υ(σ[m_x ← p]);
9.          τ ← RANDOM([4,100]);
10.         tabu ← tabu ∪ {⟨x, p, k + τ⟩};
11.         σ ← σ[m_x ← p];
12.         if υ(σ) < υ(σ*) then
13.             σ* ← σ;
14.             s ← 0;
15.         else if s > maxStable then
16.             σ ← σ_0;
17.             s ← 0;
18.             tabu ← {};
19.         else
20.             s++;
21.         k++;
22.     return σ*;
```

Figure 7.2: Pseudocode of the TS algorithm

7.1.3 Solution Combination Method

The combination of solutions is performed using a procedure that bears some resemblance with the GRASP-decoding mentioned in Sect. 7.1.1. There are some important differences though: firstly, the procedure is fully deterministic; secondly, the solution produced by the method is entirely composed of marks taken from either of the parents; finally, the method ensures that the $m_n < L$ constraint is fulfilled.

The combination method begins by building a list $\mathcal{L}$ of all marks x present in

either of the parents, such that $x < L$ [2]. Then, starting from $m_1 = 0$, a new mark x is chosen at each step i such that (i) $m_{i-1} < x$, (ii) there exist $n - i$ marks greater than x in $\mathcal{L}$, and (iii) a local optimization criterion is optimized. This latter criterion is minimizing $\sum_{j=1}^{i-1} \upsilon_\sigma (x - m_j)^2 + (x - m_{i-1})$, where σ is the partial ruler. This expression involves minimizing the number of constraints violated when placing the new mark, as well as the subsequent increase in length of the ruler. The first term is squared to raise its priority in the decision-making.

7.1.4 Subset Generation and Reference Set Update

This subset generation method creates the groups of solutions that will undergo combination. The combination method used is in principle generalizable to an arbitrary number of parents, but we have considered the standard two-parent recombination. Hence the subset generation method has to form pairs of solutions. This is done exhaustively, producing all possible pairs. It must be noted that since the combination method utilized is deterministic, it does not make sense to combine again pairs of solutions that were already coupled before. The algorithm keeps track of this fact to avoid repeating computations.

As to the reference set update method, it must produce the reference set for the next step by using the current reference set and the newly produced offspring (or by using the initial population generated by diversification at the beginning of the run or after a restart). Several strategies are possible here. Quality is an obvious criterion to determine whether a solution can gain membership to the reference set: if a new solution is better than the worst existing solution, the latter is replaced by the former. In the OGR, we consider that a solution x is better than a solution y if the former violates less constraints, or violates the same number of constraints but has a lower length. It is also possible to gain membership of the reference set via diversity. To do so, a subset of *diverse* solutions (i.e., *distant* solutions to the remaining high-quality solutions in the set – an appropriate definition of a distance measure is needed for this purpose) is kept in the reference set, and updated whenever a new solution improves

[2] It might happen that the number of such marks were not enough to build a new ruler. In that case, a plain solution with length ∞ (that is, the worst possible value) is returned.

the diversity criterion.

If at a certain iteration of the algorithm no update of the reference set takes place, the current population is considered stagnated, and the restart method is invoked[3]. This method works as follows: let μ be the size of the reference set; the best solution in the reference set is preserved, $\lambda = \mu(\mu - 1)/2$ solutions are generated using the diversification generation method and the improvement method, and the best $\mu - 1$ out of these λ solutions are picked and inserted in the reference set.

7.2 Experimental Results

To evaluate our memetic approach, a set of experiments for problem sizes ranging from 10 marks up to 16 marks has been realized. In all the experiments, the maximum number of iterations for the tabu search was set to $10,000$, the size of the population and reference set was 190 and 20 respectively, and the arity of the combination method was 2. The reference set is only updated on the basis of the quality criterion. One of the key points in the experimentation has been analyzing the influence of the local search strategy with respect to the population-based component. To this end, we have experimented with partial Lamarckism [125], that is, applying the local improvement method just on a fraction of the members of the population. To be precise, we have considered a probability p_{ts} for applying LS to each solution. The values $p_{ts} \in \{0.1, 0.2, 0.4, 0.6, 0.8, 1.0\}$ have been considered. All algorithms were run 20 times until an optimal solution was found, or a limit in the whole number of evaluations was exceeded. This number of evaluations was set so as to allow a fixed average number e of LS invocations ($e = 10,000$ TS runs). Thus, the number of evaluations was limited in each of the instances to e/p_{ts}. This is a fair measure since the computational cost is dominated by the number of TS invocations.

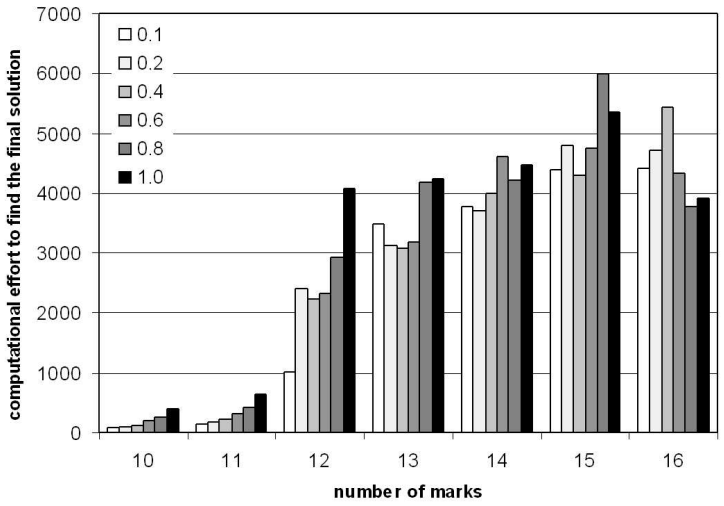
Table 7.1 reports the experimental results for the different instances considered. Row MAxx corresponds to the execution of the MA with a local improvement rate

[3]Notice that the TS method used for local improvement is not deterministic. Thus, it might be possible that further applications of TS on the stagnated population resulted in an improvement. However, due to the computational cost of this process, it is advisable to simply restart.

		10	11	12	13	14	15	16
HGRASP	Best	N/A	2.8	10.6	4.7	6.3	7.3	6.8
	Median	N/A	2.8	11.8	7.5	9.4	11.9	11.3
GROHEA	Best	**0**	**0**	**0**	**0**	3.1	4.6	5.6
	Median	0	0	7.1	5.6	7.1	8.6	10.2
MA1.0	Best	**0**	**0**	**0**	**0**	1.6	**0**	4.0
	Median	0	0	0	0	2.4	4.0	6.2
MA0.8	Best	**0**	**0**	**0**	**0**	0.8	1.3	2.3
	Median	0	0	0	0	1.6	3.3	5.6
MA0.6	Best	**0**	**0**	**0**	**0**	0.8	**0**	2.8
	Median	0	0	0	0	1.6	4.0	6.2
MA0.4	Best	**0**	**0**	**0**	**0**	**0**	1.3	**1.1**
	Median	0	0	0	0	1.6	4.0	5.6
MA0.2	Best	**0**	**0**	**0**	**0**	**0**	0.7	3.4
	Median	0	0	0	0	1.6	4.0	6.2
MA0.1	Best	**0**	**0**	**0**	**0**	**0**	0.7	3.4
	Median	0	0	0	0	1.6	3.3	5.6

Table 7.1: Relative distances to optimum for different probabilities of the MA and the algorithms GROHEAand HGRASP. Globally best results (resp. globally best median results) for each instance size are shown in boldface (resp. underlined). Results of HGRASP are not available for 10 marks.

of $p_{ts} = xx$. The table reports the relative distance (percentage) to the known optimum for the best and median solutions obtained. The table also shows the results obtained by the algorithms described in [43] (i.e., HGRASP) and in the previous chapter (GROHEA). Algorithm HGRASP is grounded on the evolutionary use of the GRASP-based solution generation method used in the basic diversification method of our algorithm. As to algorithm GROHEA, it provides the best results reported in the literature for this problem via a population-based approach, and therefore it is the benchmark reference for our algorithm. Specifically for this latter algorithm, as reported in the previous chapter, the maximum number of iterations for the tabu search was also $10,000$, the size of the population was 50, and the probabilities p_m and p_X were both set to 0.6. Both algorithms (GROHEA and HGRASP) were run 30 times for each ruler.



	0.1	0.2	0.4	0.6	0.8	1.0
0.1	•	−+−−−−	+++−−−−	+++−−−−	+++−−−−	+++−−−−
0.2	−+−−−−	•	−−−−−−	++−−−−	++−−−−	+++−−−−
0.4	++−−−−	−−−−−−	•	++−−−−	+−−−−+	++−−−−
0.6	++−−−−	++−−−−	+−−−−−	•	++−−−−	++−−−−
0.8	++−−−−	++−−−−	+−−−−+	++−−−−	•	++−−−−
1.0	++−−−−	+++−−−	++−−−−	++−−−−	++−−−−	•

Figure 7.3: (Top) Computational effort (measured in number of TS invocations) to find the best solution. (Bottom) Statistical comparison of the computation effort. In each cell, the results ('+'=significant, '−'=non-significant) correspond from left to right to instance sizes from 10 up to 16.

The results are particularly impressive. Firstly, observe that our memetic algorithm systematically find optimal rulers for up to 13 marks. GROHEA is also capable of eventually finding some optimal solutions for these instance sizes, but notice that the median values are drastically improved in the MA. In fact, the median values obtained by the MA for these instances correspond exactly to their optimal solutions. Comparatively, the results are even better in larger OGR instances: our MA can find optimal ORGs even for 14 and 15 marks, and computes high-quality near-optimal solutions for 16 (i.e., 1.1% from the optimum). These results clearly outperform GROHEA; indeed, the latter cannot provide optimal values for instance sizes larger than 14 marks. Moreover, all MAxx significantly improve the median values obtained by GROHEAon the larger instances of the problem. These results clearly indicate the potential of hybrid EAs for finding optimal and near-optimal rulers.

We have also conducted statistical tests to ascertain whether there are significant performance differences between the different LS application rates. This has been done using a non-parametric Wilcoxon ranksum test (results are not normally distributed). Except in three head-to-head comparisons for 14 marks ($p_{ts} = 1.0$ vs $p_{ts} = 0.8$ and $p_{ts} = 0.1$, and $p_{ts} = 0.4$ vs $p_{ts} = 0.1$), there is no statistically significant difference (at the standard 0.05 level) in any instance size for the different values of p_{ts}. While this is consistent with the fact that the average number of TS invocations is constant, it raises the issue of whether the associated computational cost is the same or not. The answer to this question can be seen in Fig. 7.3. As expected, the computational cost increases with the size of the problem. Quite interestingly, the average cost decreases for 16 marks. This behavior owes to the higher difficulty of the problem for this latter size: the algorithm quickly reaches a near-optimal value (a remarkable result), and then stagnates (longer runs would be required to improve the solutions from that point on). The table at the bottom of Fig. 7.3 shows the outcome of the statistical comparison between the computational cost of the MAxx for a given instance size. As it can be seen, the differences are almost always significant for the lower range of sizes, and progressively become non-significant as the size increases. For 16 marks, there is just one case of statistically significant difference of computational cost ($p_{ts} = 0.4$ vs $p_{ts} = 0.8$). Since the small values of p_{ts} imply a lower computational cost for instance sizes in the low range, and there is no significant difference in either quality or computational cost with respect to higher values of p_{ts} in the larger instances, it seems that values $p_{ts} \in \{0.1, 0.2\}$ are advisable.

7.3 New Improvements

The algorithm presented this far yields very impressive results, however, we want to pursue it further. There are two aspects (among others) that we can improve very straightforwardly. First, we realized that Constraint Programming can be of help at some point. Second, we believe that diversity in the population is almost as important as the quality of it. Let us then introduce the new features incorporated into our algorithm:

7.3.1 Solution Combination by Complete Search

Recombination methods are usually introduced in order to generate new high quality and diverse individuals. Our current recombination mechanism achieves these goals, however what we pursue here is something different. We are trying to generate optimal solutions with this operator.

We have been dealing with values of marks through all this research. Now we turn to look into the distances between marks. We realized that a complete search procedure that incorporates propagation techniques would be perfectly suited to search for a solution when fed with the appropriate distances. Complete Search procedures tend to be very inefficient with very large search spaces, however we can limit that in this case by only taking into account the distances between marks of the two individuals to be combined. For example, imagine we have the two rulers of 9 marks to be combined:

$$\sigma_1 = \langle\ 0\ 1\ 5\ 13\ 23\ 34\ 47\ 50\ 55\ \rangle$$
$$\sigma_2 = \langle\ 0\ 2\ 7\ 11\ 12\ 24\ 30\ 40\ 47\ \rangle$$

The distances between marks of both rulers are

[1, 2, 3, 4, 5, 6, 7, 8, 10, 11, 12, 13]

Note that we only consider distances between two consecutive marks i, j where $i + 1 = j$. To fully characterize the problem we need to take all the distances into account, however these are the distances that we are going to restrict.

Thus, we use those distances to feed a complete search procedure whose goal is to quickly attempt to generate valid rulers (hopefully optimal). In order to do that we need to formulate the problem as a CSP. Now, the variables are distances D_{ij} between marks (where $i < j$). The domain of the variables D_{ij} where $i + 1 = j$ is reduced to the values previously shown. The rest of the variables can take any value

within $1..m$ where m is the length of the ruler[4]. The set of constraints is as follows:

$$D_{ij} \neq D_{kl} \ \ \forall \ \ i \neq k \ and \ j \neq l$$

Since we are going to execute this procedure within the MA cycle, we can take advantage of dynamic information, such as the length λ of the shortest valid ruler in the population. This is explicitly indicated in the procedure by introducing a constraint:

$$min(l_k) < \lambda$$

where $min(l_k)$ is the minimum length possible for a partial ruler k.

Empirical Observations

We have now fully characterized the problem our complete search procedure is going to be dealing with. However we found two options at this point:

- Use a Constraint Programming solver,
- or take advantage of the data structures already implemented in our algorithm.

The first option implies we can plug a black-box to our MA to which we pass a set of distances and then expect a solution or a confirmation that no valid solution can be found. We can take advantage of efficient propagation techniques and sophisticated heuristics.

On the other hand, taking advantage of the structures already implemented, we can focus on instantiating only variables D_{ij} corresponding to distances between consecutive marks; if we instantiate the variables in the same order as they would physically appear in the ruler, we can easily calculate the rest of the distances and thus, check the validity of the partial solution very quickly. This can be viewed as limiting the search variables to the ones representing distances between consecutive marks and using a lexicographic variable ordering heuristic. Note that in this case

[4]Note that the value of m is not important as we will soon clarify

we do not need to worry about the value of m, upper bound in the value of the non-consecutive distances, since we are not focusing the search on them, but only on the consecutive ones.

Both approaches were tested and we found that the latter was consistently faster than the former; as it allows us to ignore non-consecutive distance variables. Still, the reduction of the search space was not enough to yield a very fast mechanism. Remember that we implement this procedure as a combination operator, and thus, we cannot devote more than a few seconds to it.

In our experimental tests we discovered that, when reducing the search space to consider only the consecutive distances of the optimal ruler, the procedure was able to find a solution in less than a second for up to 14 marks, and less than 5 seconds for 15 and 16 marks. However, introducing more distances slowed down the process exponentially, and if within those distances a valid solution was not possibly found, the time cost grew inmensely.

The final procedure

After a few more experiments we designed the next mechanism:

1. Select the two rulers to be combined.
2. Calculate the consecutive distances[5]
3. Randomly select $n+3$ distances from the previous step, being n the number of marks in the ruler (which is 4 distances more than needed).
4. Run the complete search procedure with those distances, with a time limit of 4 seconds.
5. If a valid solution was found, return it, if not call the old recombination mechanism.

[5]Note that some distances might be repeated; for example, in two 15 mark rulers (14 consecutive distances) we typically find around 20 different distances.

Note that this procedure can also find near optimal rulers if the chosen distances permit it. Obviously, we can be missing some potential optimal rulers by randomly selecting $n + 3$ distances, but we found it to be the best trade-off between time and efficiency. That is, if there was a valid solution for the given distances, the complete search procedure would almost always find it within the given time limit.

7.3.2 Diversity in the Population: Clustering

We also realized that the population got stuck very frequently. The solutions provided by the LS mechanism were of high quality, and thus converged very quickly to the same region of the search space. Restarts were required to drive the search towards different regions. Since the population was selected in an elitist fashion, many times, the algorithm was unable to generate better individuals that could be included in the reference set.

Diversity is thus a key aspect of a population in order to provide the algorithm with individuals different enough as to generate new solutions of relatively high quality.

In this sense we directed our efforts towards implementing a clustering algorithm. Clustering deals with finding a structure in a collection of unlabeled data, and it can be considered the most important unsupervised learning mechanism; a loose definition of clustering could be "the process of organizing objects into groups whose members are similar in some way". A cluster is therefore a collection of objects which are "similar" among them and are "dissimilar" to the objects belonging to other clusters.

In our population we have individuals that are vectors of marks, however, we are going to transform them into distances between marks as in the previous subsection. Our goal is thus to group individuals with similar sets of distances in the same cluster. The algorithm for clustering is very simple; imagine we consider τ clusters:

1. Transform the vectors of marks into vectors of distances. Actually, in binary vectors that indicate whether a distance is included in the individual or not. For example, the individual representing a 9 marks ruler

   $$\sigma_1 = \langle\ 0\ 1\ 5\ 13\ 23\ 34\ 47\ 50\ 55\ \rangle$$

will be transformed into

$$\mathrm{x}(\sigma_1) = [\ 1\ 0\ 1\ 1\ 1\ 0\ 0\ 1\ 0\ 1\ 1\ 0\ 1\ 0\ 0\ 0\ \ldots\ ]$$

where a 1 in $\mathrm{x}(\sigma_1)[i]$ indicates that the distance i is included in the individual σ_1, where i rangs from 1 to three times the number of marks[6].

2. Calculate τ random centroids. The centroids are the vectors that represent the clusters, their central points. Thus, the centroids are vectors of the same length as the individuals that characterize a cluster. If we already had the vectors separated in clusters, the centroid of a cluster k_i would be a vector:

$$centroid(k_i) = [\frac{a_1}{\mid k_i \mid} \frac{a_2}{\mid k_i \mid} \ldots \frac{a_l}{\mid k_i \mid}] \tag{7.2}$$

where $\mid k_i \mid$ is the number of vectors in cluster k_i and a_j is the number of vectors in cluster k_i in which thet j-th bit is set to 1. Since we have no clusters yet we calculate the centroids randomly.

3. Assign every vector to its nearest centroid, creating thus the clusters. The distance measure we use is that of the cosine of the angles formed by the vector and the centroid, and it is explained in the Clustering section of the appendix.

4. Recalculate the centroids with the now real information of the vectors in the clusters.

5. Repeat steps 3 and 4 until no centroid is changed in step 4 or until a maximum number of iterations is reached, in our case 10.

Our population is now divided into clusters. This fact itself does not ensure diversity in the Reference Set. To maintain a high degree of diversity without harnessing its quality we rank the vectors in every cluster and then select the best ω individuals from each cluster, and we include them in the Reference Set.

[6]This limit l was imposed after the observation that optimal rulers try to incorporate the lowest different distances between consecutive marks so that the ruler's length is minimized

		14	15	16
MA0.1	Best	**0**	0.7	3.4
	Median	1.6	3.3	5.6
MA+5-4	Best	**0**	**0**	**0**
	Median	<u>0</u>	<u>0.7</u>	<u>2.8</u>
MA+10-2	Best	**0**	0.7	2.3
	Median	<u>0</u>	0.9	3.7
MA+20-1	Best	**0**	0.7	3.4
	Median	<u>0</u>	0.9	3.4

Table 7.2: Relative distances to optimum for different probabilities of the MA0.1 and the improved algorithm MA+. Globally best results (resp. globally best median results) for each instance size are shown in boldface (resp. underlined).

Note that this process is relatively time consuming, and thus, it is only performed for the initial population and after a restart. However, at any generation, the algorithm updates the Reference Set in a way that the premise *the best ω individuals of each cluster are maintained in the Reference Set* is satisfied.

7.4 Final Experimental Results

In this section we show results for our Memetic Algorithm after the incorporation of the new features. The experiments have been performed over rulers of 14 to 16 marks, and with probability $p_{ts} = 0.1$, which we found to be one of the most consistent ones after the previous experiments; and with the same other parameters as in the last experimental results.

Regarding the diversity mechanism, we have performed three different sets of experiments varying the values of the clustering parameters. These different sets of parameters are: $\tau = 5$ $\omega = 4$, $\tau = 10$ $\omega = 2$, and $\tau = 20$ $\omega = 1$.

Table 7.2 depicts the results for these new experiments and a comparison of the results presented in section 7.2 for $p_{ts} = 0.1$. As a first result we can see that for 14 marks the algorithm MA+ **always** finds the optimal solution, which did not happen with MA0.x. Second and maybe more important is that we are now able to solve a

16 marks ruler. Also note that all the median values of MA+ are superior to those produced by MA0.1. MA+5-4 seems to dominate the rest of the instances of MA+.

7.5 Summary

To summarize our newly born algorithm we must remember that it is based on a Scatter Search ([142]) scheme, which uses GRASP features for initialization and recombination, and introduces a tabu search mechanism for improving individuals. This algorithm is enriched with a complete search procedure also used for recombination whose purpose is basically to try to reach an optimal solution at any point in the execution of the algorithm (rather than provide high quality individuals). Finally, the diversity of the population is ensured by means of a clustering algorithm that divides the individuals in different clusters, and a selection mechanism that chooses the best ω individuals from each cluster to be part of the reference set.

A different point of view is the following: A Local Search and a Complete Search mechanism feed each other through a common population whose diversity is maintained by a clustering technique. According to this, tabu search and the complete search recombination would be exchanging solutions in order to find the optimal one, obtaining and returning these solutions to a diversified population. Moreover, a GRASP mechanism helps constructing the initial population and conserving it (creating high quality and also diverse individuals). All this, sustained by a Scatter Search scheme that holds everything together.

7.5.1 Lessons learnt revisited

Here is a brief explanation of how we have dealt with some of the lessons learnt during the previous chapters, and how those lessons are reflected in this final hybrid:

- Constraint programming is especially suited for satisfaction problems; even though this is an optimization problem we have transformed it into a satisfaction one in the sense that we only ask for a feasible solution to the complete search procedure (to be found among the selected distances).

- Propagation and Heuristics are key features in the constraint programming framework; however, we have limited our heuristics here in order to take advantage of the already existent data structures, although we have maintained a form of propagation related to the available distances and to the length of the potential ruler.

- Constraint Satisfaction techniques encounter many difficulties when dealing with very large search spaces. Note that the definition of search space depends on the number of variables and also on the size of the domains. While we cannot reduce the number of variables, we have reduced the number of values that the complete search procedure has to deal with; thus, harnessing completeness for the sake of speed.

- LS greatly benefits from the introduction of constructive heuristics as initial solution generators. In this case, both the GRASP initialization procedure and the GRASP recombination operator allow the LS to init the search from high quality solutions.

- LS techniques have the major drawback of getting stuck on local optima. The introduction of clustering an the resultant diversity of the population allow the LS procedure to be fed with diverse and high quality solutions, each of which have relatively high probabilities to yield a solution or at least not to converge to the same region in the search space.

- Memetic Algorithms present the danger to quickly converge to the same region of the search space without finding optimal solutions. It is sometimes hard to decide when to restart the population in order to regenerate it. Scatter Search provides a natural way to deal with this issue: restart when no new solutions can be introduced in the reference set. This, and the new diversity mechanism ensure that the algorithm will maintain a diverse population and will restart in the exact moment in which this is not possible to achieve anymore.

- Finally, we have discussed about the LS being fed with diverse and high quality

solutions. In this case, diversity is maintained thanks to the clustering and selection techniques, and the quality is maintained by the GRASP recombination operator. Also, the complete procedure benefits from this diversity and high quality, it constantly considers different sets of distances with relatively high probabilities to contain a solution (this is perturbed by the random selection of a certain number of them, before they are passed to the complete procedure).

Chapter 8

Conclusions and Future Work

This last chapter is devoted to the conclusiones derived from the research developed for this thesis, and to the future work that follows from every research in every field including hybrids.

8.1 Conclusions

Throughout this thesis we have presented several approaches to solve different hard combinatorial optimization problems. We have succeeded in developing effective techniques to solve these problems, and we have also created a new hybrid that incorporates mechanisms from the Constraint Programming, Local Search and Genetic Algorithm's frameworks.

Within the CSP framework we have introduced two novel aspects in redundant modelling for multiple permutation problems:

- A novel value ordering heuristic which takes into account the primal and both dual models, and which generalizes for multiple permutation problems ideas introduced in ([35, 211] for simple permutation problems. The speedup produced by this heuristic is quite remarkable, up to three orders of magnitude in some cases.

- The use of channelling constraints linking more than a single pair of models

to provide forward checking with the same pruning power as arc consistency at a much smaller cost in constraint checks, and thus in performance, provided that ordering effects are taken into account in the min-domain variable selection heuristic.

We have also shown that SAT encodings allow for much more scalable solutions in QCP problems, in particular when compared to previous results in the literature. We have explained this performance by properties of the representation and by solver-specific features; and we have shown that those features can also be fruitfully exploited in CSP models to get much better CSP solutions than before.

In the next research work we have reconsidered the scheduling of social golfers, a highly combinatorial and symmetric application which has raised significant interest in the constraint programming community. It presented an effective local search algorithm which found the first solutions to 11 new instances and matched, or improved upon, all instances solved by constraint programming solutions but 3. Moreover, the local search algorithm was shown to find almost all solutions in less than a couple of seconds, the harder instances taking about 1 minute. The algorithm also features a constructive heuristic which trivially solves many instances of the form $odd-odd-w$.

Finding Golomb rulers is an extremely challenging optimization problem with many practical applications that have been approached by a variety of search methods in recent years. It combines hard and dense feasibility constraints and an optimization function to minimize the length of the ruler. Related to this, we have presented:

- A hybrid evolutionary algorithm GROHEA to find near-optimal Golomb rulers in reasonable time. The algorithm is conceptually simple and uses a natural modeling. It incorporates a tabu-search algorithm for mutation and a one-point crossover to cross two rulers. It optimizes the length of the rulers indirectly by solving a sequence of feasibility problems.

- We have presented a memetic approach for finding near-optimal Golomb rulers at an acceptable computational cost. The MA combines, in different stages of the algorithm, a GRASP-like procedure (for diversification and recombination)

and tabu search (for local improvement) within the general template of scatter search. The results of the MA have been particularly good, clearly outperforming other state-of-the-art evolutionary approaches for this problem. One of the aspects on which our analysis has been focused is the influence of the LS component. We have shown that lower rates of Lamarckianism achieve the best tradeoff between computational cost and solution quality.

- We have introduced several improvements to the previous algorithm (complete search and clustering) to yield outstanding results: we are able to solve a 16 marks ruler and to consistently solve every 14 mark rulers. The algorithm tested using different sets of parameters referred to the clustering mechanism is consistently superior to the previous algorithm without the improvements.

Finally, we have presented a new hybrid algorithm. This algorithm is based on a Scatter Search template and includes a complete search inherited technique to combine individuals, and a clustering procedure which we apply to our population in order to achieve a higher degree of diversity. Results of this hybrid for the Golomb Ruler Problem are superior to those presented in previous chapters in this thesis.

8.2 Future Work

There are many issue to persue within this thesis. Remember that every chapter deals with a different kind of problem and a different kind of technique. Thus, possible future work in each of these different research works will be the following:

8.2.1 CSP and SAT

Many issues remain to be explored. While we did try a number of alternatives to the presented value ordering heuristics without success, others may be more successful. There are some anomalies in the behavior of the ch3-fc approach vs ch2-ac which could be symptoms of more subtle effects than the ordering effects reported above, and which need to be explored. There is finally the issue of why CBJ and nogood

learning did not help in this problem, which may in part suggest that in a sense randomness dominates over structure in QCPs, but which should at any rate be an incentive to develop more effective implementations of these techniques so that at least they do not hurt when they do not help.

It would be interesting to see whether the combination of the ideas of this paper with either alldiff constraints or Operations Research techniques could yield further improvements in our ability to solve larger QCPs. For example, we mentioned that the same effect achieved by introducing triangular channelling constraints would be achieved by reintroducing instead the dual not-equal constraints, which in turn could be replaced by dual alldiff constraints.

On the other hand while we can explain Satz's performance and exploit its features in CSP approaches, a similar study could be carried out for satzoo. This might help in understanding the role of CBJ and learning in QCPs, as they do not help with QCPs formulated as CSPs (as mentioned above). Moreover, we plan to study the effect of many-valued models [7] as an intermediate and potentially more concise representation between SAT and CSP.

8.2.2 Local Search for Scheduling Social Tournaments

Let us first point out a number of interesting observations. First, the social golfer is a problem where the properties of the instances seem to determine which approach is best positioned to solve them. In particular, hard instances for constraint programming are easy for local search and viceversa. There are of course other applications where this also holds. What is interesting here is the simplicity of local search compared to its constraint programming counterpart and the absence of symmetry-breaking schemes in local search. Whether this observation generalizes to other, highly symmetric, problems is an interesting issue for future work. See, for instance, [180, 181] for early results along these lines.

Moreover, we are interested by the effect of the seeding heuristic. It not only constructs optimal solutions for several instances, but represents an effective starting point for the algorithm. However, we believe that a deeper study on its effects should

be performed in order to adapt the heuristic to certain instances and to develop new intensification and diversification mechanisms.

8.2.3 Golomb Rulers

We are currently exploring alternatives for some of the operators used in our algorithm. Preliminary experiments with multi-tier reference sets –i.e., including a diversity section– do not indicate significant performance changes. A deeper analysis is nevertheless required here. In particular, it is essential that the particular distance measure used to characterize diversity correlate well with the topology of the search landscape induced by the reproductive operators. Defining appropriate distance measures in this context (and indeed, checking their usefulness in practice) will be the subsequent step. However, the clustering mechanism achieves a high degree of diversity that might be sufficient.

As for the final hybrid resulting of the introduction of the new improvements, there is a very obvious observation: the SS and the LS deal with marks, while the Clustering and Complete Search deal with distances. We plan to make it uniform and possibly implement all the techniques so they can deal with distances. More efficient clustering techniques are also worth being studied.

8.2.4 Developing Hybrids

On the other hand, we are still also very interested in developing new hybrid algorithms. We are currently devoting some research on hybrid local search and constraint programming algorithms. Namely, we are experimenting with a form of Limited Discrepancy Search ([112]) for Local Search. We are also in the first stages of development of a LS algorithm which will incorporate a heuristic based on constraint propagation. Memetic Algorithms are still of great interest as well.

Conclusiones y Trabajo Futuro

Este último capítulo está dedicado a las conclusiones generadas por cada trabajo de investigación, así como al trabajo futuro a realizar en cada campo, incluyendo en el desarrollo de híbridos.

Conclusiones

En esta tesis hemos presentado diversos enfoques para resolver problemas de optimización combinatoria. Hemos tenido éxito al crear técnicas efectivas para resolver este tipo de problemas, y hemos creado también un nuevo híbrido que incorpora mecanismos de la programación con restriccciones, de la búsqueda local y de los algoritmos evolutivos.

Dentro del campo de los CSP hemos introducido dos aspectos novedosos en el modelado redundante de problemas de múltiples permutaciones:

- Una nueva heurística de ordenación de valores que tiene en cuenta los modelos primal y dual, y que generaliza las ideas introducidas en ([35, 211] para problemas de múltiples permutaciones. La ganancia en cuanto a tiempo de resultados es bastante notable, llegando a ser de hasta 3 órdenes de magnitud en algunos casos.

- El usar restricciones de canalización uniendo más de dos modelos para conseguir que forward checking tenga el mismo poder de poda que arco-consistencia, a un menor precio en términos de chequeos de restricciones, y, por lo tanto, en eficiencia.

También hemos mostrado como las codificaciones SAT permiten una mayor escalabilidad de soluciones en el problema de completitud de cuasigrupos, en concreto, al compararlo con resultados previos disponibles en la literatura. Hemos explicado esos resultados en términos de la representación y de los resolutores, y hemos demostrados que estas caracterísitcas pueden ser también importadas al enfoque CSP para obtener resultados superiores.

En el siguiente trabajo de investigación hemos reconsiderado la calendarización de golfistas sociales, un problema altamente combinatorio y simétrico que ha generado gran interés en la comunidad de la programación con restricciones. Hemos presentado un algoritmo de búsqueda local que encuentra la primera solución para 11 instancias, y empata con el resto, excepto por 3 instancias, con los resultados conseguidos mediante otras técnicas de programación con restricciones. Además el algoritmo de búsqueda local encuentra las casi todas las soluciones en menos de un par de segundos, mientras que instancias difíciles apenas tardan un minuto. El algoritmo también incorpora una heurística constructiva que resuelve muchas instancias de la forma $impar - impar - w$ trivialmente.

Encontrar Golomb rulers es un problema de optimización combinatoria muy difícil que tiene diversas aplicaciones prácticas y que se tratado desde diferentes enfoques en los últimos tiempos. Combina restricciones duras y densas de satisfacción con un función a minimizar que corresponde a la longitud de la regla. En relación con esto hemos presentado:

- Un algoritmo evolutivo híbrido GROHEA para encontrar reglas cuasi-óptimas en un tiempo razonable. El algoritmo es conceptualmente simple y usa un modelo natural. Incorpora una búsqueda tabu como operador de mutación y una recombinación de un punto. Optimiza la longitud de las reglas mediante la resolución de una sequencia de problemas de satisfacción.

- Hemos presentado un enfoque memético a un coste computacional aceptable. El algoritmo combina un procedimiento tipo GRASP y búsqueda local dentro del esquema del "Scatter Search". Los resultados son claramente superiores a resultados previos del estado del arte. Un aspecto en el que nos hemos centrado es en el método de mejora local y su influencia en los resultados. Hemos mostrado como tasa bajas de Lamarckianismo consiguen el mejor balance entre coste computacional y calidad en la solución.

- Hemos introducido diversas mejoras al algoritmo anterior (búsqueda completa y clustering), consiguiendo grandes resultados: siendo capaces de resolver reglas de hasta 16 marcas, y resolviendo hasta 14 marcas sistemáticamente. Este

nuevo algoritmo se ha probado usando distintos parámetros para el mecanismo de clustering siendo consistentemente superior al algoritmo previo en cada caso.

Finalmente, hemos presentado un nuevo híbrido que está basado en el esquema del Scatter Search y que incluye búsqueda completa para la recombinación y clustering para obtener un mayor grado de diversidad en la población. Los resultados obtenidos son superiores a cualquier resultado presentado en capítulos anteriores en la tesis.

Trabajo Futuro

Hay muchos temas que abordar después de esta tesis. Recordad que cada capítulo trata diferentes problemas con diferentes técnicas. Así pues, el possible trabajo futuro en cada uno de estos aspectos es:

CSP y SAT

Hay muchos aspectos a explorar. A pesar de que probamos diversas alternativas de ordenación de valor sin éxito, sería interesante utilizar otras nuevas. También hay ciertas anomalías en el compartamiento de los modelos uno frente a otro que podrían ser causados por algo más que la ordenación y que merece la pena sean estudiadas. Otro aspecto es porque CBJ y el aprendizaje de "nogoods" no es de ninguna ayuda, lo cual puede significar que la aleatoriedad domina sobre la estructura en QCPs.

Sería también interesante ver si la combinación de otras ideas como la restricción alldiff o técnicas de investigación operativa pueden ayudar a mejorar los resultados. Por ejemplo, hemos mostrado que el efecto de introducir las restricciones de canalización triangulares es el mismo que reintroducir las desigualdades duales, lo que se podría reemplazar por alldiff duales.

Por otro lado, tras explicar la eficacia de Satz y aprovechar sus características, sería interesante realizar el mismo estudio para el resolutor Satzoo. Esto podría ayudar a entender el efecto de CBJ y aprendizaje en QCPs. Además, planeamos estudiar el efecto de modelos multi-valuados [7] como un método intermedio y potencialmente más conciso.

Búsqueda Local para Calendarización de Torneos Sociales

Antes de nada hay que indicar una serie de observaciones interesantes. Primero, el golfista social es un problema donde las propiedades de las instancias parecen determinar que enfoque es mejor para resolverlas. En concreto, instancias difíciles para CSPs con búsqueda completa son fáciles para la búsqueda local y viceversa. Hay otros dominios en los que esto también ocurre. Lo interesante aquí es la sencillez de la búsqueda local comparada con la completa, en la que se encuentran mecanismos de rotura de simetrías muy complejos. El hecho de que esta observación pueda generalizarse para problemas altamente simétricos es para estudiar en el futuro. Consultad, por ejemplo, [180, 181] para trabajo en esta línea.

Además, estamos interesados en el efecto de la heurística constructiva. No solo construye soluciones óptimas para varias instancias, sino que además constituye un punto de partida efectivo para el algoritmo. Sin embargo, habría que realizar un estudio más detallado para poder adaptar la heurística a otras instancias y desarrollar nuevos métodos de intensificación y diversificación.

Golomb Rulers

Actualmente estamos estudiando alternativas a ciertos operadores. El uso de subconjuntos de más de dos individuos para la recombinación es una posibilidad a investigar. De momento, el incluir una zona de diversidad no cambia los resultados. En cualquier caso sería importante hacer un estudio más detallado de la medida de distancia que caracteriza la diversidad de la población y que debe hallarse correctamente relacionada con la topología del espacio de búsqueda. Sería interesante definir otros tipos de medidas distancia más apropiadas. Sin embargo, parece que el uso de clustering como mecanismo para conseguir diversidad es suficientemente efectivo.

En cuanto al híbrido final resultante de la introducción de las nuevas mejoras, hay una observación directa: Scatter Search y tabu manejan marcas mientras que clustering y la búsqueda completa utilizan distancias entre marcas. Sería conveniente conseguir que esto sea uniforme y posiblemente, traducir todo a distancias entre marcas. También sería interesante estudiar otros mecanismos de clustering más eficientes.

Desarrollo Híbridos

Por otro lado, todavía estamos muy interesados en la creación de nuevos algoritmos híbridos. Actualmente estamos desarrollando híbridos de búsqueda completa y local para CSPs. Por ejemplo, estamos experimentando con una forma de "Limited Discrepancy Search" ([112]) para búsqueda local. También estamos en las primeras etapas de desarrollo de un algoritmo de búsqueda local que incorporará un heuristica basada en la propagación de restricciones. Además, los algoritmos meméticos siguen siendo de interés.

Appendix A

GRASP and Clustering

In this appendix we are going to briefly introduce two techniques that have been used in the last hybrid developed for this thesis. Since this techniques are not the focus of our research, but only tools we have utilized to improve the efficiency of our technique, we believe that a brief appendix is better suited to introduce them.

A.1 Greedy Randomized Adaptive Search Procedures (GRASP)

The GRASP (Greedy Randomized Adaptive Search Procedure) metaheuristic can be viewed as an iterative process, each iteration consisting of two phases: construction and local search ([78]). The construction phase builds a solution whose neighborhood is investigated by the local search procedure. During the whole process, the best solution is updated and returned at the end of a certain number of iterations. Figure A.1 illustrates the basic GRASP procedure.

Any local search algorithm can be incorporated to improve a solution: tabu search and simulated annealing ([54, 147]), large neighborhoods ([4]) or variable neighborhood search ([161]). However, we are interested in the greedy construction phase, where a tentative solution is built in a greedy fashion.

Randomly generated solutions are usually of a poor quality, while greedy generated

```
procedure GRASP(maxIt,seed)
  1. Read_Input()
  2. for k=1,..., maxIt do
  3.     Solution ← Greedy_Randomized_Construction(seed);
  4.     Solution ← Local_Search(Solution);
  5.     Update_Solution(Solution);
  6. end;
  7. return Best_Solution;
  end GRASP
```

Figure A.1: The GRASP pseudocode

solutions tend to be attracted by local optimum[1], due to the less amount of variability. A *semi-greedy heuristic* ([77]) adds variability to the greedy algorithm. A certain greedy function yields a ranked candidate list, which is called *restricted candidate list* (RCL). An element from that list is randomly selected and added to the solution.

The procedure to construct the *semi-greedy* solution is depicted in Figure A.2. A key step in this pseudocode is the selection of an attribute from the RCL. This can be performed using a qualitative or quantitative criterion. In the former, the element is selected among the k best elements; while in the latter, the element is selected among the elements with a quality $\alpha percentage$ of the greedy value, where $\alpha \in [0, 100]$. Note that $k = 1$ or $\alpha = 100$ yields a pure greedy selection.

A.1.1 Reactive GRASP

As can be seen in the procedure described below, the selection of the k parameter is problematic. The use of a fixed value for this parameter could hinder high quality solutions([174]). A learning-based strategy named *reactive* GRASP was introduced in [175], selecting a different value in each iteration from a finite set of values. The selection of a certain value in a given iteration can be chosen on the basis of the goodness of the best solution generated by this parameter. A possibility is to maintain

[1]Local optima are points in the search space from where a local search algorithm cannot escape, and thus a restart is necessary in order to explore other regions.

procedure Greedy_Randomized_Construction(seed)
1. Solution $\leftarrow \emptyset$
2. Evaluate the incremental costs of candidate elements
3. **While** Solution is not complete **do**
4. Build the restricted candidate list RCL
5. Select element s from RCL at random
6. Solution $\leftarrow$ Solution $\cup \{s\}$;
7. Reevaluate the incremental costs;
8. **end**;
9. **return** Solution;
end Greedy_Randomized_Construction

Figure A.2: The Greedy Randomized Construction pseudocode

a vector of parameter values to use in each iteration, where a position p_i denotes the value of the parameter that serves to choose the $i-th$ candidate. We refer to this vector as *GRASP parameters vector*.

For example, a certain position of the GRASP parameters vector $p_i = 3$ makes us choose a random candidate among the four best candidates, for the $i-th$ decision, in the RCL list (From now on we will consider that the first value in the RCL is in position 0 and the last one $n-1$, where n would be the length of the RCL).

A.2 Clustering

Clustering deals with finding a structure in a collection of unlabeled data, and it can be considered the most important unsupervised learning mechanism; a loose definition of clustering could be "the process of organizing objects into groups whose members are similar in some way". A cluster is therefore a collection of objects which are "similar" among them and are "dissimilar" to the objects belonging to other clusters.

The goal of clustering is to determine the intrinsic grouping in a set of unlabeled data. In general, there is no absolute *best* criterion which would be independent of the final aim of the clustering. It is ultimately the user who has to provide the criteria that will yield results to better suit his needs.

However, when implementing a clustering algorithm, several requirements should be satisfied: scalability, possibility of dealing with different types of attribute, discovering clusters with arbitrary shape, ability to deal with noise, insensivity to order of input records, high dimensionality, interpretability and usability (among others).

Current clustering techniques suffer from the following drawbacks:

- They do not usually address all the requirements adequately and concurrently.
- Time complexity is a major problem when dealing with large number of data.
- In many occasions, the effectiveness depends on the definition of *distance*.
- Distance has to be define when it is not obvious, which might be difficult, especially when dealing with multi-dimensional spaces.
- The result of the clustering algorithm can be interpreted in different ways.

A.2.1 Clustering Algorithms

Clustering Algorithms can be classified as follows:

- Exclusive Clustering.
- Overlapping Clustering.
- Hierarchical Clustering.
- Probabilistic Clustering.

In the first case data are grouped in an exclusive ways, this means that every individual piece of information is included in one cluster and cannot be include in another one. On the contrary, the second type uses fuzzy sets to cluster data, so every point belongs to different clusters with a certain degree of memebership. The hierarchical clustering algorithm is based on the union between the two nearest clusters; the beginning condition is performed by setting every point as a cluster, and after a few iterations it reaches the final cluster. Finally, the last type of clustering algorithm relys on a completely probabilistic approach.

K-Means Algorithm

This is one of the most popular clustering algorithms that fall in the category of Exclusive Clustering. Since this is the clustering method used in our hybrid, we are going to briefly detail it here.

It is indeed one of the simplest unsupervised learning algorithms ([149]). The procedure follows a simple and easy way to classify a given data set through a certain number of clusters k fixed a priori. The main idea is to define k centroids, each one corresponding to each clustering. The next step is to associate each point to its nearest centroid. This yields a first grouping of the data. At this point we need to re-calculate the k new centroids as barycenters of the clusters resulting from the previous step. After the new centroids have been calculated, each point needs to be re-associate to a centroid again. The algorithm now iterates this process until either no cluster changes for any point occur or a stopping criterion is reached.

This algorithm aims at minimizing an *objective function*, in this case a squared error function:

$$J = \sum_{j=1}^{k} \sum_{i=1}^{n} \|x_i^{(j)} - c_j\|^2 \tag{A.1}$$

where $\|x_i^{(j)} - c_j\|^2$ is a chosen distance measure between a data point $x_i^{(j)}$ and the cluster centroid c_j, indicating the distance of the n data points from their respective cluster centres.

A.2.2 Distance Measure

As we have previuosly stated, defining the distance measure is a problematic task. If the components of the data instance vectors are all in the same physical units (metric), then it is possible that the simple Euclidean distance metric is sufficient to group similar distances. However, even in this case, the Euclidean distance can be misleading. It is dependant from the range: if one metric spans the range $[0.0, 0.5]$ and another spans $[0.0, 100.0]$, the maximum deviation in the first would have little effect on the total distance, while even a modest separation in the second would have a much larger effect. To remove this dependency it is important to *standarize* the

values. In order to achieve this, the following steps must be taken:

1. Sum the values of the metric over all objects and divide the sum by the number of objects.

2. Substract this average value from the metric in all objects.

3. Sum the squares of these new values, divide the sum by the total number of objects and take its square-root. This is the standard deviation of the new values.

4. Divide the metric by the standard deviation in each object.

Assume now that each object is described by a real-valued array of metrics of length K, the i-th object x_i has the array x_{ki} for $k = 1, 2, \ldots, K$. The general form for the distance, which is called the L_N norm, between object i and centroid j is

$$L_{Nij} = [\sum_{k=1}^{K} \mid x_{ki} - x_{kj} \mid^p]^{1/p} \tag{A.2}$$

When $p = 1$ this distance measure is known as the Manhattan distance, while for $p = 2$ it is known as the Euclidean distance.

Binary Data

When dealing with binary arrays of data, the distance measures defined so far are not valid. Even though there are many possibilities, the simplest one is to use the cosine similarity function ([196]). The cosine similarity function CS_{ij} between object i and j treats the objects as vectors and it calculates the cosine of the angle between these vectors. This similarity, which is also known as the Ochini coefficient, is given by the expression

$$CS_{ij} = \frac{\sum_{k=1}^{K} x_{ki} x_{kj}}{\sqrt{\sum_{k=1}^{K} x_{ki}^2 \ \sum_{ki=1}^{K} x_{kj}^2}} \tag{A.3}$$

Note that as the objects become more similar, CS_{ij} approaches 1.0.

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