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Abstract

- English -

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Versuche in das Abstract folgende Punkte aufzunehmen: Fragestellung der Arbeit, methodische Vorgehensweise oder die Hauptergebnisse deiner Arbeit.

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 $A \quad \mathrm{mm^2} \quad \mathsf{Fläche}$

D - mm Werkstückdurchmesser

 $d_{\min} \quad \mathrm{mm} \quad \quad \text{kleinster Schaftdurchmesser}$

 $L_{\mathbf{1}} \hspace{0.5cm} \mathrm{mm} \hspace{0.5cm} \hspace{0.5cm} \mathsf{L\"{a}nge} \hspace{0.1cm} \mathsf{des} \hspace{0.1cm} \mathsf{Werkst\"{u}ckes} \hspace{0.1cm} \mathsf{Nr}. \hspace{0.1cm} \hspace{0.1cm} 1$

Grad Freiwinkel

Grad Keilwinkel

Abkürzungsverzeichnis

GCG Generic Column Generation

SCIP SCIP

BaPCod Branch-and-price Code

hMETIS Hypergraph METIS

strlPlib Structured Integer Program Library

MIP Mixed Integer Programming

SRT Set Refinement Tree

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Quellcodeverzeichnis

1 Introduction

Feel introduced.

1.1 Motivation and Contribution

I am motivated.

1.2 Structure

This text is well-structured.

2 Preliminaries

In this chapter, we provide sufficient background needed to understand the algorithmic details and ideas discussed in Chapter 5. First, we take a look at linear optimization as a general concept and discuss necessary basics such as Mixed Integer Programming (MIP). Afterwards, these concepts are used to take a more detailed look into the characteristics of the Dantzig-Wolfe decomposition, which represents a major component of the decomposition solver GCG. In addition, notations and basic definitions related to Graph Theory are introduced including the concept of *Partition Refinement*; an algorithmic approach used as a building block in Chapters 5 and 6.

2.1 Linear Optimization

Linear Optimization is a mathematical optimization technique used to determine the best possible values for a set of variables in a given model, whose constraints or requirements are represented by linear relationships. The goal is typically to maximize or minimize a objective function, subject to a set of equality and/or inequality constraints. Both objective and constraints must be linear.

If all variables are only allowed to take values from \mathbb{R}^n_{\geq} , i.e., only continuous values, then this optimization technique is referred to as $Linear\ Programming$. In a standard form, a linear programming problem with variable vector $\mathbf{x} \in \mathbb{R}^n$, constraint matrix $A \in \mathbb{R}^{m \times n}$, objective coefficients $c \in \mathbb{R}^n$ and right-hand side vector of the constraints $b \in \mathbb{R}^m$ can be expressed as follows:

$$z_{LP}^* = \min \quad c^T \mathbf{x} \tag{2.1}$$

s.t.
$$A \mathbf{x} \ge b$$
 (2.2)

$$\mathbf{x} \ge 0 \tag{2.3}$$



Figure 2.1: Solution space of a linear program highlighted in gray. Point highlighted in blue represent the solution space of the corresponding integer linear program.

Note that it is also possible to represent a set of equality $A'\mathbf{x} = b'$ by the two sets of inequalities $A'\mathbf{x} \ge b'$ and $A'\mathbf{x} \le b'$. Without loss of generality, we assume optimization problems to always be minimization problems, unless explicitly stated otherwise. Constraints 2.2 specify a *convex* polytope over which the Objective Function 2.1 is optimized as shown in Figure 2.1. A solution vector $\mathbf{x} \in \mathbb{R}_{\ge 0}$ is called *feasible*, iff it satisfies both both constraints 2.2 and 2.3. The linear program as a whole is called *feasible*, if there exists such a vector, otherwise it is considered *infeasible*. A feasible solution $\mathbf{x} \in \mathbb{R}_{\ge 0}$ is called *optimal* iff

$$c^T \mathbf{x} = \min\{c^T \mathbf{x} \mid \mathbf{x} \text{ is feasible}\} \iff \nexists \mathbf{y} \in \mathbb{R}_{\geq 0} : (\mathbf{y} \text{ feasible}) \land \underbrace{\left(c^T \mathbf{y} < c^T \mathbf{x}\right)}_{\mathbf{y} \text{ is "better"}}$$

If there exists a feasible solution vector, but no optimal one, then the problem is called *unbounded*, as shown in Figure 2.1.

Linear programming is widely used in various fields such as operations research, economics, engineering, and logistics, due to its efficiency in solving large-scale real-world optimization problems. Algorithms such as the Simplex Method and Interior Point Methods are commonly used to solve LP problems efficiently. The simplex algorithm in particular is widely used in practice because of its efficiency on most problems, even though its worst-case complexity is exponential-time on certain families of problems depending on the chosen pivot-rule. However, on most problems the simplex algorithm only takes a polynomial number of steps to terminate. For more information about how the algorithms work and their mathematical details we refer to [1].

unbounded on right

cite

2.1.1 Mixed-Integer Programs

$$\begin{split} z_{LP}^* &= \min \quad c^T \mathbf{x} &+ d^T \mathbf{y} \\ &\text{s.t.} \quad A \, \mathbf{x} &+ B \, \mathbf{y} \geq b \\ &\mathbf{x} &\in \mathbb{Q}_{\geq 0} \\ &\mathbf{y} \in \mathbb{Z}_{> 0} \end{split}$$

Even thought linear programs are already a powerful tool on its own, some problems require discrete bounds for some variables, e.g., the y-variables shown in the system above. These variables are usually restricted to a subset of \mathbb{Z} . If the system contains integer and continuous variables, then the model is called a Mixed Integer Program (MIP). If only discrete variables are present, the prefix "Mixed" is omitted.

MIPs are significantly more difficult to solve than pure linear programs, since the integer restrictions make the feasible region *non-convex*, eliminating a key assumption of the simplex algorithm and its optimality conditions. Standard solution approaches include branch-and-bound, branch-and-cut, and cutting-plane methods, which systematically explore and prune the search space.

It can be shown that the decision problem of whether an $\mathbf{IP!}$ with all variables restricted to the domain $\{0,1\}$ has a solution is NP-hard. Despite the higher computational complexity, MIPs are extremely powerful because they allow the modeling of a wide range of practical decision-making problems, including scheduling, routing, facility location and production planning

2.2 Dantzig-Wolfe Decomposition

The ${\it Dantzig\text{-}Wolfe}$ ${\it Decomposition}$ is a

Seite 2

Seite 3

2.3 Graph Theory

Graphs are the fundamental data structure used in almost every aspect of computer science. This section will *not* introduce new concepts not already found in standard literature about graphs and related topics. We will mainly introduce the notation used for the following sections and chapters.

A graph is a tuple G = (V, E) with $V \subseteq \{1, 2, ..., n\}$ for some $n \in \mathbb{N}$ and $E \subseteq \{(u, v) \mid (u, v) \in V \times V\}$. The elements of set V are called *vertices* or *nodes*. The elements of set are ordered pairs called *directed edges*, arcs or simply edges which connect two vertices with each other. The set of outgoing neighbors of a specific vertex $v \in V$ is denoted $E(v) = \{(v, v') \mid v' \in V, vEv'\}$. The set of incoming neighbors $E^{-1}(v) = \{(v', v) \mid v' \in V, v'Ev\}$ is defined analogously. In this thesis, we will distinguish four types of graphs: directed, un-directed and bipartite, with directed being the assumed type if not stated explicitly.

For un-directed graphs, the edge relation E must be symmetric $\forall u, v \in V : uEv \rightarrow vEu$, i.e., if vertex u is connected to v or vice versa, then the corresponding back-edge must exists as well.

Bi-partite graphs are a special kind of graph class, where the set V can be represented with two sets $L, R \subseteq V$ such that $L \cap R = \emptyset$ and $E \subseteq \{(u,v) \mid u \in L, v \in R\}$. More informally, the vertex V can be split into two disjoint subsets $L, R \subseteq V$ such that no edges exists between vertices in each corresponding set. Bi-partite graphs are especially interesting, because the relationship between variables and the constraints they participate in can be encoded as such a graph as shown in Figure 2.2. This concept will be used in Chapter 4 to algorithmically detect various underlying structures.

Wording

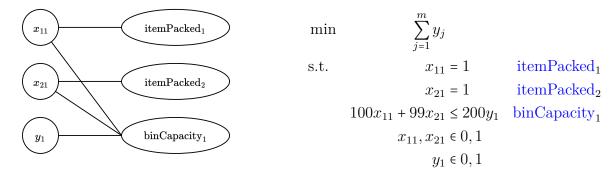


Figure 2.2: A simple binpacking problem with 2 items and 1 bin represented as graph.

2.4 Partition Refinement

Partition refinement is a fundamental concept in computer science, particularly relevant in fields such as automata theory [2], graph theory, and model checking [3]. A partition refers to a decomposition of a finite set U into disjoint, non-empty subsets $\{A_1, A_2, \ldots, A_k\}$, called *cells* or *blocks*, such that:

$$\bigcup_{i=0}^{k} A_i = U \text{ and } \forall i \neq j : A_i \cap A_j = \emptyset$$

The set of all partitions over a set U is denoted $\Pi(U)$. A partition $\pi = \{A_1, A_2, \dots, A_k\}$ of a set U is called a refinement of another partition $\pi' = \{B_1, B_2, \dots, B_m\}$, denoted $\pi \subseteq \pi'$, iff

$$\forall A_i \in \pi \ \exists B_i \in \pi' : A_i \subseteq B_i$$

As a special case, a partition is a refinement of itself. More informally, partition π' must reflect a "finer" classification of the elements than in π .

Partition refinement refers to an *iterative* process that refines a given initial partition of a set over the course of multiple iterations. In the following, let $f: P \times Q \mapsto \Pi(A)$ be a function, which partitions the elements from $P \subseteq U$ with respect to the elements in $Q \subseteq U$. The arguments P and Q are called *target cell* and *inducing cell* respectively. A partition π is called *stable* with respect to f, iff

$$\forall A_i, A_j \in \pi : |f(A_i, A_j)| = 1$$

That is, there is no cell in π which acts as a "splitter" to another cell according to f. Let π_{init} be an *initial* partition. The goal is typically to find the coarsest partition $\pi_f = \{A_1, A_2, \ldots, A_k\}$ of U such that the following properties hold:

- 1. The partition π_f is a refinement of the initial partition π_{init}
- 2. The partition π_f is *stable* with respect to f.

In the following, we define $Step: \Pi(U) \mapsto \Pi(U)$ as function performing one refinement step, i.e., it picks a splitter-cell B_j if it exists and replaces each cell B_i of the input partition with $f(B_i, B_j)$.

Algorithm 1 A simple partition refinement algorithm which refines π_{init} until a fixed-point is reached.

```
Input: Initial partition \Pi_{init} = \{A_1, A_2, \dots, A_k\}, splitter-function f : P \times Q \mapsto \Pi(P)
Output: Coarsest stable partition
```

```
function IterateRefinement(\Pi_{init}, f)
i \leftarrow 0
\Pi_0 \leftarrow \Pi_{init}
repeat
i \leftarrow i + 1
\Pi_i \leftarrow Step(\Pi_{i-1})
until \Pi_i = \Pi_{i-1}
return \Pi_i
end function
```

This process is illustrated in Algorithm 1. Note that new cells are continuously being produced in the loop which are able to act as inducing cells during the next iteration.

For the purposes of this work, f will usually represent a function structurally similar to a connection function as it used in many graph automorphism packages. Given a graph G = (V, E), then we define two types of connection function as follows:

$$f_{\text{count}}(v, X_{\text{ind}}) = |\{v' \in V \mid \forall (v, v') \in E, v' \in X_{\text{ind}}\}|$$

$$(2.4)$$

$$f_{\text{exists}}(v, X_{\text{ind}}) = \begin{cases} 1 & f_{\text{count}}(v, X_{\text{ind}}) \ge 1\\ 0 & \text{else} \end{cases}$$
 (2.5)

If Function 2.5 is used, then the problem of finding the coarsest partition with respect to f is equivalent to the *Relational coarsest partition problem* described in [4] which also contains corresponding correctness and termination proofs. For this case in particular, Algorithm 1 always maintains the invariant $\Pi_i \subseteq \Pi_{i-1}$.

Furthermore, the underlying problem structure to which partition refinement is applied, as well as the type of splitter function used, are not inherently restricted. In practice, however, many problems can be reformulated or encoded as graphs, where the function f captures a vertex property. For instance, in deterministic finite automaton (DFA) minimization, partition refinement is used to iteratively distinguish states by observing the equivalence classes of their transitions (Hopcroft's algorithm): two states are grouped

together only if, for every input symbol, their transitions lead into the same partition class; in graph isomorphism testing, it could encode vertex degrees or local neighborhood structures; and in Markov decision processes (MDPs), f might reflect the expected reward or transition behavior. These encodings allow partition refinement to exploit structural symmetries and behavioral equivalences in a wide range of domains, especially if problems in that domain can be encoded as graphs. Further domains of application include Model Checking [3] and sorting algorithms [5].

Furthermore, if the underlying graph is bipartite, the splitter-function is expressing a vertex property such as Function 2.4 or 2.5 and each vertex on one of the two sides of the graph is in its own class, then the partition refinement algorithm can be implemented more efficiently as hinted on in [6]. This is due to the fact that one of the sides is already fully refined, thus only the other side might change. Combined with the fact that the graph is bi-partite, splits that occur within one cell cannot affect other cells. Thus, we don't have to "go back" during the execution of the loop in Algorithm 2.

```
Algorithm 2 More efficient refinement, if graph G = ((U, V), E) bipartite and \forall v \in U:
|E^{-1}(v)| \le 1 or \forall v \in V : |E^{-1}(v)| \le 1. For the algorithm we assume the former.
Input: Initial partition \Pi_{init} = \{A_1, A_2, \dots, A_k\}, Bi-partite graph G = ((L, R), E)
Output: Coarsest stable partition
  function REFINEFAST(\Pi_{init}, G)
       i \leftarrow -1
       \Pi_0 \leftarrow \Pi_{init}
       for v \in R do
            i \leftarrow i + 1
            \Pi_i \leftarrow \text{REFINE}(\Pi_{i-1}, E^{-1}(v))
       end for
       return \Pi_i
   end function
  function Refine(\pi, S)
       for A_i \in \pi do
            \pi \leftarrow \pi \setminus A_i
            \pi \leftarrow \pi \cup \{A_i \cap S\} \cup \{A_i \setminus S\}
                                                                       \triangleright Set S "splits" A_i into two parts
       end for
  end function
```

2.5 Surprise and Entropy

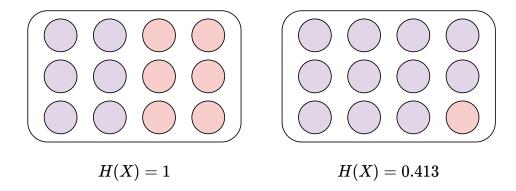


Figure 2.3: Entropy is measure of "surprise" and it increases with decreasing probability. On the left side, both colors are evenly distributed, so drawing either one is equally surprising. On the right side, drawing a red ball from the set of elements would be very surprising, because the probability is only $\frac{1}{12}$. But because this event is so unlikely, one does *not expect* to be surprised. As a result, the expected surprise - that is, the entropy - is low.

The information value or surprisal of an event E is defined as

$$I(E) = \log_b \left(\frac{1}{p(E)}\right) = -\log_b \left(p(E)\right) \tag{2.6}$$

It increases as the probability of the event p(E) decreases. Intuitively, if the probability is close to 1, then one wouldn't be surprised if this event actually occurred, so the surprisal is close to 0.

The entropy, or expected surprise, H(X) of a discrete random variable X which takes values in the set \mathcal{X} is defined by equation 2.7 [7].

$$H(X) = \sum_{x \in \mathcal{X}} p(x)I(X) = -\sum_{x \in \mathcal{X}} p(x)\log_b p(x)$$
(2.7)

where $p(x) := \mathbb{P}[X = x]$.

If not specified any further, the base b of the logarithm is assumed to be 2. In chapter these concepts will be used to define a heuristic scoring system based on constraint names.

2.6 Adjusted Rand Index

The Rand Index is a statistical measure used to compare two different partitions $\pi = \{A_1, A_2, \ldots, A_k\}, \pi' = \{B_1, B_2, \ldots, B_l\}$ of elements from the same set $U = \{1, 2, \ldots, n\}$. Let $f_{\pi}(x) : U \mapsto \mathbb{N}$ be a function mapping an element $x \in U$ to the index of its cell in partition π . Function $f_{\pi'}$ is defined analogously. Furthermore, let

$$E_{\circ_1,\circ_2} = \{(x,y) \in U \times U \mid (f_{\pi}(x) \circ_1 f_{\pi}(y)) \land (f_{\pi'}(x) \circ_2 f_{\pi'}(y))\}$$

Intuitively, e.g. the set $E_{=,\neq}$ refers to the set of pairs $(x,y) \in U \times U$ of elements which are in the same cell in π , but in different cells in π' . Now we can define the *Rand Index* as follows:

$$RI = \underbrace{\frac{|E_{=,=}| + |E_{\neq,\neq}|}{|E_{=,=}| + |E_{\neq,\neq}| + |E_{\neq,\neq}|}}_{\text{Number of all pairs}} = \frac{|E_{=,=}| + |E_{\neq,\neq}|}{\binom{n}{2}} \in [0, 1]$$
(2.8)

With appropriate data structures, e.g. a mapping between elements and cell index for each partition, Equation 2.8 can be evaluated in O(n).

The Adjusted Rand Index is a chanced-adjusted version of the regular Rand Index which accounts for similarities that might occur by random chance. It is one of the most popular measures for comparing partitions or clusters and can be computed by using Equation 2.9 [8].

$$ARI = \frac{RI - Expected RI}{Max RI - Expected RI} = \frac{\sum_{ij} {v_{ij} \choose 2} - \left[\sum_{i} {a_i \choose 2} \sum_{j} {b_j \choose 2}\right] \div {n \choose 2}}{\frac{1}{2} \left[\sum_{i} {a_i \choose 2} + \sum_{j} {b_j \choose 2}\right] - \left[\sum_{i} {a_i \choose 2} \sum_{j} {b_j \choose 2}\right] \div {n \choose 2}}$$
(2.9)

The values v_{ij} , a_i and b_j are taken from the so called Contingency Table shown in Figure 2.1.

The notation of Table 2.1 makes it seem like that $l \cdot k$ set intersection operations have to be computed in order to compute the full contingency table. Computing the intersection $A \cap B$, with $A, B \subseteq U$ being of roughly similar size, can be quite an expensive operation, depending on the precise data structures used. However, when there is an efficient data structure available mapping each element to the index of its containing cell, then the

contingency table can be computed in one pass over all elements as shown in Algorithm 3.

$\pi' \setminus \pi$	A_1	A_2		A_k	sums
B_1	v_{11}	v_{12}	•••	v_{1k}	a_1
B_2	v_{21}	v_{22}	•••	v_{2k}	a_2
:	:	:	٠.	÷	:
B_l	v_{l1}	v_{l2}	•••	v_{lk}	a_l
sums	b_1	b_2		b_k	

Table 2.1: Contingency Table of partitions π and π' . Entry v_{ij} denotes the number of elements sets A_i and B_j have in common, i.e., $v_{ij} = A_i \cap B_j$.

Algorithm 3 A simple algorithm computing the contingency table with one pass over all elements of U.

```
Input: Partitions \pi = \{A_1, A_2, \dots, A_k\}, \pi' = \{B_1, B_2, \dots, B_l\}, function f_C : U \mapsto \mathbb{N} for C = \{C_1, C_2, \dots\} \in \Pi(U) mapping u \in U to C_i iff u \in C_i
```

Output: Contingency Table of partitions π, π' and sums of columns and rows

```
function COMPUTECONTINGENCYMATRIX(\Pi_{init}, G)
A \leftarrow 2 \text{D Array with } l \text{ rows and } k \text{ columns}
sumsOfColumns \leftarrow 1 \text{D Array with } k \text{ entries}
sumsOfRows \leftarrow 1 \text{D Array with } l \text{ entries}
\text{for } u \in U \text{ do}
column \leftarrow f_{\pi}(u)
row \leftarrow f_{\pi'}(u)
A[row, column] \leftarrow A[row, column] + 1
sumsOfColumns[column] \leftarrow sumsOfColumns[column] + 1
sumsOfRows[row] \leftarrow sumsOfRows[row] + 1
\text{end for}
\text{return } (A, sumsOfRows, sumsOfColumns)
end function
```

We refer to [9] for a more detailed discussion on different similarity measures and their mathematical derivation.

3 Related Work

4 Generic Column Generation (GCG)

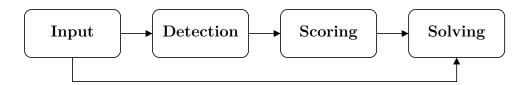


Figure 4.1: A simplified overview of the four major stages of solving a model with GCG.

In this chapter, we introduce Generic Column Generation (GCG), a decomposition solver which is based on the open-source MIP-Solver SCIP (SCIP) [10]. Readers already experienced with GCG and its capabilities may still find some details and observations interesting. For a given problem, GCG is able to perform an automatic Dantzig-Wolfe reformulation which is then solved using a branch-price-and-cut algorithm. Alternatively, GCG support a special *Benders-Mode* which reformulated the problem using Benders decomposition.

In contrast to other open-source solvers like BaPCod (Branch-and-price Code) [11] or commercial software such as SAS [12] which rely solely on user-provided decompositions, GCG is able to automatically detect different kinds of structures algorithmically, including but not limited to

- Single-Bordered structures
- Arrowhead structures using the third-party tool hMETIS (Hypergraph METIS) [13].
- Staircase structures

The solving process in divided into multiple consecutive stages as shown in Figure 4.1. Each stage will be explained in more detail in the following section as needed. The detection in particular aims to make GCG more accessible to a wider range of users which do not necessarily have the required theoretical background and practical experience to reformulate linear programs on their own. For more details about individual features and capabilities, we refer to the official documentation [14].

Entfernen und auf Kapitel vorher ref

Kurz
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Schritte
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einen
Satz

4.1 Detection

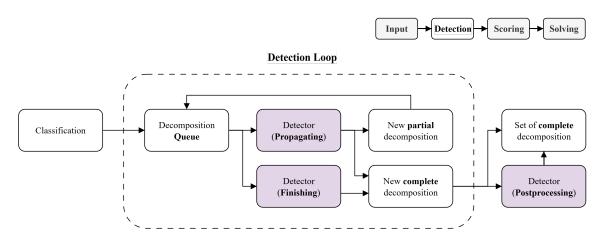


Figure 4.2: A simplified overview of the detection process and its detection loop.

As mentioned in the introduction to this chapter, one integral part and distinguishing feature of GCG is its detection framework. A simplified overview of the detection currently ¹ implemented in GCG is shown in Figure 4.2. For a more detailed visualization including additional information about how pre-solving is handled we refer to the official documentation [14]. The framework consists of two major parts:

- 1. A classification step, in which a set of classifiers is partitioning the constraints (and variables) according to a certain property, producing one partition each. The goal of this step is to detect different underlying structures of the constraint matrix, which can be used during the detection loop to make more informed decisions about which constraints to assign to which block or master. Important classifiers for the remainder of this thesis are discussed in more detail in Section 4.2.
- 2. The **detection loop**, which consists of a set of detectors which are responsible for assigning constraints either the master or to individual blocks. In round n + 1 a detector receives a partial decomposition, that is, a decomposition in which not all constraints are assigned yet, from round n as input and pushes a set of newly created (partial) decompositions to a queue. In case the user did not provide a partial decomposition as input in round 0, the loop is initialized with a decomposition in which no constraint is assigned yet.

¹GCG version 3.5, as of 2025-07-18.

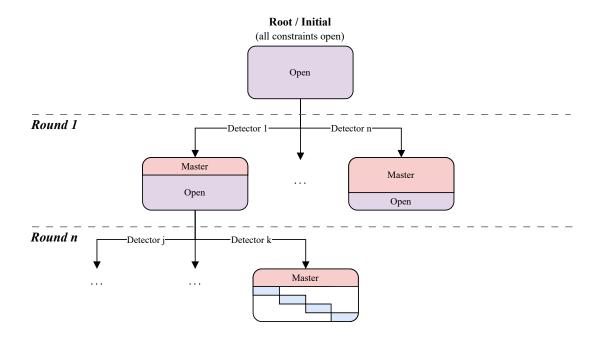


Figure 4.3: Visualization of the induced tree of propagated partial decompositions.

The concept of detecting structures in different rounds is visualized in Figure 4.3. Starting from a root decomposition in which all constraints are still unassigned or "open", different detectors produce a set of new partial decomposition. Depending on the configuration, a detector is not allowed to work on a certain partial decomposition or its decedents twice. A very simple but concrete example of how such a tree might look like in practice can be found in Section 4.4.

Furthermore, if no detector found any new decomposition in round k, or k exceed the maximum number of rounds, the detection loop is stopped and all complete decomposition are collected, scored and exactly one is chosen for which the solving is started. The scoring and selection stage is of particular interest in practice, because the tree in Figure 4.3 might grow beyond thousand of decompositions, of which the best in terms of solving time or a different metric must be selected. Because the scoring of decompositions is not of major interest for *this* thesis, we refer to the official documentation for details [14].

Grammati Wortwahl

4.2 Classifiers

As mentioned in the introduction to this chapter, classifiers are responsible for detecting different underlying structures of the constraint matrix, which can be used during the detection loop to make more informed decisions about which constraints to assign to which block or master. Given a set of constraints $C = \{c_1, c_2, \ldots, c_m\}$, classifiers can be seen as a *injective* function $f: C \mapsto \mathbb{Z}$, i.e., a function that assigns each constraint to exactly one number or class. Note that in GCG, classifiers are allowed to only classify a subset $C' \subseteq C$, leaving $C \setminus C'$ unassigned to any class 2 . In the current version of GCG, however, all classifiers always assign every constraint to some class.

Furthermore, each classifier is identified with an unique *name* and an integral priority, influencing the order in which the classifiers are being executed by the framework.

4.2.1 Name Classifiers

The names of constraints and variables are, if provided, a strong indicator to which constraints or variables are related to each other. The names usually consist of two parts:

- 1. The semantic group name, such as "capacity" or "link" for e.g. a Bin-Packing model.
- 2. A *modifier*, which usually consists of numbers, capital letters or a combination of both. Typically, the modifier is separated from the semantic group name via. non alpha-numeric characters such as "_" or "#".

Constraints in the same group typically share similar names, with the *modifier* being the only differentiating factor. For example, in a Bin-Packing problem, capacity constraints such as "capacity_1", "capacity_2", ... usually vary only in the index indicating the bin. This similarity can be quantified using metrics like the *Levenshtein Distance*, which is the minimum number of single-character edits required to change one word into the other.

²When using GCG as a library, this can be checked via. IndexPartition::isIndexClassified.

Because there is no standardized naming scheme for either variables or constraints, name classifiers usually operate under the assumption that the modeler provided *reasonable* names, if any at all. A non-exhaustive collection of different naming schemes observed is provided in Appendix . If the modelers provided no names of it's own, then the underlying solver usually chooses a default prefix such as "c" or "cons" for constraints, followed by an increasing number, resulting in constraint names "c0" - "c4999" for a model with 5000 constraints.

Appendix

Given a alphabet Σ , words $w, v \in \Sigma^*$, then the *Levenshtein* distance between those two words can be computed as:

$$\operatorname{lev}(w,v) = \begin{cases} |w| & \text{if } v = \epsilon \\ |v| & \text{if } w = \epsilon \\ |\operatorname{lev}(\operatorname{prefix}(w), \operatorname{prefix}(v)) & \text{if head}(w) = \operatorname{head}(v) \\ 1 + \min \begin{cases} \operatorname{lev}(\operatorname{prefix}(w), v) \\ |\operatorname{lev}(w, \operatorname{prefix}(v)) & \text{otherwise} \end{cases} \end{cases}$$

$$(4.1)$$

Equation 4.1 can be computed in $O(|w| \cdot |v|)$ using a dynamic programming approach. Let $B = (\text{lev}(\text{name}(c_i), \text{name}(c_j)))_{1 \le i,j \le m}$ the pair-wise Levenshtein Distance between constraint names, $k \in \mathbb{N}$ the connectivity and G = (V, E) with $V = \{c_1, c_2, \dots, c_m\}, E = \{\{u, v\} \mid u, v \in V, u \neq v, \text{lev}(\text{name}(u), \text{name}(v)) \le k\}$. Furthermore, let reach(v) be the set of reachable vertices from vertex $v \in V$ which is defined as the fix-point of the following function for s = v:

$$reachEventually_t(T) = \{u \in V \mid \exists v \in T : v \in E(u) \} \cup \{t\}$$

Then two constraints $c_i, c_j \in V$ are in the same class iff $c_j \in reach(c_i)$. A small example of this concept is shown in Figure 4.4. This idea can also be applied to variable names.

WIP 5000

 $\frac{\text{cons}}{\text{limit}}$

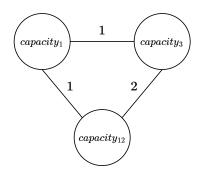


Figure 4.4: The graph of pair-wise Levenshtein weights for three capacity constraints. For k = 1, the edge between $capacity_3$ and $capacity_{12}$ vanishes, but because they is still a connecting path via. $capacity_1$, both constraints are assigned to the same class.

4.2.2 Numeric Classifiers

Nonzero

$$A = \begin{array}{c} cons_1 \\ cons_2 \\ cons_3 \\ cons_4 \end{array} \begin{pmatrix} 1 & 5 & -1 & -1 \\ 20 & 0 & 0 & 20 \\ 20 & 10 & 10 & 0 \\ 0 & 100 & -100 & 100 \end{pmatrix} \begin{array}{c} 4 \\ 2 \\ 3 \\ 3 \\ \end{array}$$

Figure 4.5: A constraint matrix with coefficients for each variable. Each constraint is assigned to a class corresponding to its number of non-zero entries.

The nonzero classifier classified constraints according to their number of non-zero variable coefficients as shown in Figure 4.5. Many types of models including Bin-Packing and Cutting-Stock consist only of constraint groups with a rather "stable" internal structure, i.e., the capacity constraint for each bin in model 4.4 consist of the same number of variables, because each constraint is just a sum over all items differing only in index for the respective bin. In general, constraint groups that are suited for this type of classifiers usually involve summations over fixed-sized sets (e.g. a set of items or bins) whose choice is not dependent on any quantified variable. Example for the latter include problems whose formulation is based on graphs and usually contains flow-conservation constraints

Wrong ref shown in Equation 4.2.

$$\sum_{u \in E(v)} x_{uv} - \sum_{u \in E^{-1}(v)} x_{vu} = 0 \quad \forall v \in V$$

$$\tag{4.2}$$

The amount of non-zeros in these constraint is entirely dependent on the number of outgoing and incoming edges for each vertex.

Objective Function

A simple classification for variables can be done using information from the objective function, such as:

- 1. Partition variables according to the sign of their coefficient in the objective function. This approach yields three classes in total Positive, Negative and Zero.
- 2. Partition them according to the actual value of the coefficient.

Partitioning variables according to the first approach is sufficient for models such as Bin-Packing, in which only the y-variables appear in the objective function.

The second approach might partition the variables in too many small cells when e.g. different costs are associated with variables in the objective function. This behavior can be observed on model types such as Multi-Commodity-Flow and Unit-Commitment.

4.2.3 Type Classifiers

Type classifiers examine the constraint matrix to infer a higher-level *type* for each individual constraint. A key objective of such classifiers is ensuring or at least improving *robustness*. Even minor modifications to a single constraint - such as the removal of one variable - can lead to a different classification, as seen with the previously discussed nonzero classifier. Moreover, the likelihood of such changes increases when pre-processing is enabled.

SCIP Types

When using GCG as a library, the type of a variable or constraint can be retrieved via. SCIPconsGetType (cons) or SCIPvarGetType (cons) respectively. The former function is not provided by SCIP itself, but is implemented in GCG instead. The implementation compares the name of the handler the constraint is assigned to and compares it to a known list of constraint handlers. The list of supported handlers includes Knapsack, Set Partitioning, Set Covering, Set Packing, Varbound and General, in case no special structure was detected. Variables can be classified as Integer, Binary or Continuous ³.

the

Check List

The clear downside of this classification is its important precondition. In order to use this feature properly and retrieve a meaningful type via. the two methods, pre-solving must have been executed prior to detection. When GCG reads the problem as e.g. an .1p file, all constraints are added as linear constraints to the underlying SCIP model. These constraints are usually "upgraded" if possible, that is, their structure is analyzed and assigned to the correct constraint handler during pre-solving. This is done in order to take advantage of properties only possessed by certain types of constraints, e.g. a solution to a set of Knapsack constraints can be computed more efficiently by using an algorithm based on dynamic programming. For more detailed information we refer to the official documentation [15]. Preliminary testing showed that it is not trivial to configure the pre-processing in such a way that only the upgrade mechanism is triggered and variables and constraints remain unchanged.

Add test config to appendix

³There are more types of variables in newer versions of SCIP such as *Implicit Integer*, but these three basic types are sufficient for the purpose of this discussion.

MIPLIB Constraint Types

Nr.	Type	Linear Constraint	Notes
1	Empty	Ø	-
2	Free	$-\infty \le x \le \infty$	No finite side.
3	Singleton	$a \le x \le b$	-
4	Aggregation	ax + by = c	-
5	Precedence	$ax - ay \le b$	x, y have same type.
6	Variable Bound	$ax + by \le c$	$x \in \{0, 1\}$
7	Set Partitioning	$\sum 1x_i = 1$	$\forall i: x_i \in \{0, 1\}$
8	Set Packing	$\sum 1x_i \le 1$	$\forall i: x_i \in \{0, 1\}$
9	Set Covering	$\sum 1x_i \ge 1$	$\forall i: x_i \in \{0, 1\}$
10	Cardinality	$\sum 1x_i = b$	$\forall i: x_i \in \{0, 1\}, b \in \mathbb{N}_{\geq 2}$
11	Invariant Knapsack	$\sum 1x_i \le b$	$\forall i: x_i \in \{0, 1\}, b \in \mathbb{N}_{\geq 2}$
12	Equation Knapsack	$\sum a_i x_i = 1$	$\forall i: x_i \in \{0, 1\}, b \in \mathbb{N}_{\geq 2}$
13	Bin Packing	$\sum a_i x_i + ay \le a$	$\forall i: x_i, y \in \{0, 1\}, b \in \mathbb{N}_{\geq 2}$
14	Knapsack	$\sum a_i x_i \le b$	$\forall i: x_i \in \{0, 1\}, b \in \mathbb{N}_{\geq 2}$
15	Integer Knapsack	$\sum a_i x_i \le b$	$\forall i: x_i \in \mathbb{Z}, b \in \mathbb{N}$
16	Mixed Binary	$\sum a_i x_i + \sum p_j s_j \{\leq, =\} b$	$\forall i : x_i \in \{0, 1\}, \forall j : s_j \text{ continuous}$
17	General Linear	$\sum a_i x_i \ \{\leq,\geq,=\} \ b$	No special structure.

Table 4.1: The structure of all 17 constraint types MIPLIB keeps track of.

In contrast to the automatic constraint classification performed by SCIP during presolving, the MIPLIB benchmark set provides its own static classification scheme [16]. This classification assigns constraints to a set of well-defined structural types such as knapsack, set-partitioning and others as shown in Table 4.1. Since it is based solely on the syntactic form of the constraints in the original model, it can be applied *independently* of solver presolving. Because all types shown in Table 4.1 are deducible only from *local* information such as type of variables and right hand side coefficient, the types can be detected with one pass over the constraint matrix.

This type of classifier shares some issues related to robustness with numeric classifiers. Constraint types such as Singleton, Aggregation or Variable Bound depend on the number of non-zeroes, leading to potential miss-classifications on graph based models. Furthermore, the only differentiating factor for more "complex" types such as *Bin Packing* and *Knapsack* is the presence of a variable which happens to have the same coefficient as the right-hand of that constraint.

4.3 Existing Detectors

Bild

4.4 Example

min
$$\sum_{j=1}^{m} y_{j}$$
s.t.
$$\sum_{j=1}^{m} x_{ij} = 1 \qquad \forall i \in \mathcal{I} \qquad (4.3)$$

$$\sum_{i=1}^{n} a_{i}x_{ij} \leq Cy_{j} \qquad \forall j \in \mathcal{J} \qquad (4.4)$$

$$x_{ij} \in 0, 1 \qquad \forall i \in \mathcal{I}, \forall j \in \mathcal{J}$$

$$y_{j} \in 0, 1 \qquad \forall j \in \mathcal{J}$$

Figure 4.6: Bin-Packing Model with items $\mathcal{I} = \{1, ..., n\}$, item sizes $a_i \in \mathbb{Z}_{\geq 0}$, bins $\mathcal{J} = \{1, ..., m\}$ and capacity C.

 Nr.
 Master
 Open

 1
 (4.3)
 (4.4)

 2
 (4.4)
 (4.3)

 3
 (4.3), (4.4)

Table 4.2: For each classifier, the *cons class* detector will produce $2^k - 1$ new partial decompositions with k being the number of classes.

In order to illustrate the detection with a concrete example, we revisit the textbook Bin-Packing model shown in Figure 4.6. Constraints 4.3 enforce that every item is packed in exactly one bin, while inequalities 4.3 ensure that the capacity of each bin is respected if some item is packed in it. The objective is to minimize the number of bins.

Without pre-solving enabled, a classifier such as MIPLIB would assign constraints 4.3 and 4.4 to the classes *Set Partitioning* and *Bin-Packing* respectively. If unique, this classification is added to a list provided to the detection stage.

If no further classifications are found, the *cons class* detector will yield 3 new partial decompositions as shown in Table 4.2, first assigning constraints 4.3, then 4.4 and finally both 4.3 and 4.4 to the master. The constraint group not assigned to the master remains *open*.

During the next round of detection, a detector such as Connected Base will receive the partial decomposition with only the packing constraints assigned to the master as input. Here, the induced constraint adjacency graph of the $q \ge 0$ open capacity constraints consists of q isolated connected components, forming the desired block-diagonal structure. This process is illustrated in Figure 4.7.

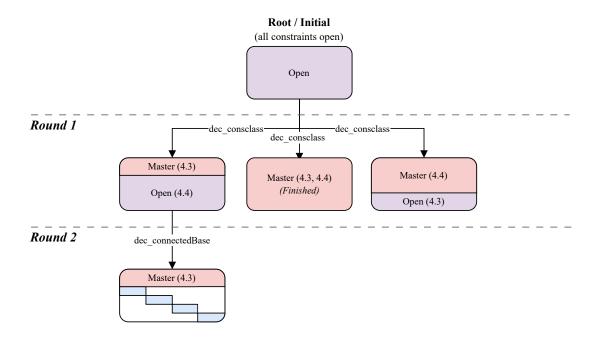


Figure 4.7: text

5 Tree Refinement

With the existing capabilities of GCG presented in the previous chapter, we continue with the main contributions of this thesis:

- A new module which is integrated into the detection framework of GCG for reverse engineering semantic groupings of the original formulation. This can be seen as a generalization of the approach presented in [6]
- Additional auxiliary classifiers which implement constraint and variable classification based on information not currently used including examples of when they are crucial detecting semantics.

This chapter is divided into three main section:

- 1. A short summary about the available information we have access to.
- 2. What the motivation and goals are why and how we aim to process this information.
- 3. The concrete algorithm and its most integral parts.

Some concrete details about the implementation itself are not subject of the following sections, but are discussed in Chapter 6.

5.1 Motivation

In [6], the implemented approaches can be seen as a three-step process:

- 1. Transform a given model to a graph-based representation.
- 2. Select a suitable initial partitioning.
- 3. Choose *one* splitter-function and run the standard partition refinement algorithm until a stable partition is reached.

Depending on the type of model, running the refinement with different initial partitions and splitter-functions might be necessary, which was already recognized in [6]. Furthermore, we suspect that for some models it might even be required to use different splitter-functions on different parts of the model.

In the following, we will generalize this process by adopting a similar approach as the one shown in Chapter 4. Instead of choosing *one* way of refining the constraints or variables based on an initial partition, we try different *strategies* to explore a more broader search space. Afterwards, the found partitions are scored and the most promising ones are selected. Note that the overall goal remains unchanged: Based on an initial partition, we aim to iteratively refine the cells in such a way, that ultimately the constraints or variables in each cell belong to the same semantic grouping as the modeler intended to.

In order to achieve this, we propose multiple strategies which form the basic building blocks of the algorithm and are discusses in Section 5.4. Each strategy takes a single cell C_i as input and computes a partition $\pi_{C_i} \in \Pi(C_i)$ as output, thereby refining the cell. In the following, the process of refining a cell according to a certain strategy is sometimes referred to as "expanding a cell". The partitions of the cells are organized in a Set Refinement Tree (SRT) as shown in Figure 5.1, i.e., each node, with exception of the root node, corresponds to a possible partitioning of its parent cell, which was computed by a strategy. The root node and its cells correspond to the initial partition and it is the only node for which the union of its cells corresponds to the whole set of constraints or variables. The cells of all other nodes only partition its immediate parent cell in the tree. This process implies that an additional post-processing step is required which translates the tree of cell-refinements to actual partitions. This step is discussed in Section 5.5.

In order to use a unified notation in the following sections, we will define the SRT and its associated information more formally. A SRT can be formalized as a tuple T = (V, E, U, R, S) with universe U corresponding to the set of all constraints or variables, designated root node $R \in V$ and set of strategies $S \subseteq \mathbb{N}$. The tuple (V, E) must induce an directed acyclic graph. Each node $v \in V \setminus R$ of the tree is associated with a parent cell ParentCell_v $\in 2^U$, a set of cells Cells_v $\in \Pi(\text{ParentCell}_v)$ and the strategy Strategy_v that was used to compute v from its parent. For the root node it holds that Cells_R $\in \Pi(U)$.

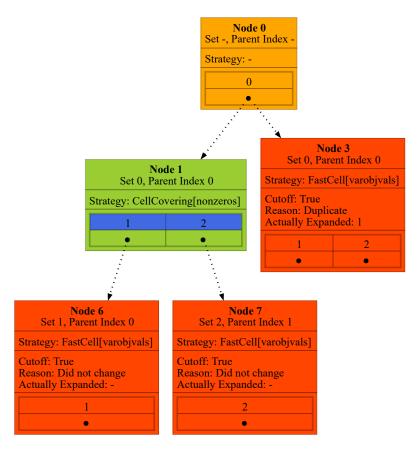


Figure 5.1: WIP WIP A example of a simple refinement tree for the Bin-Packing Problem.

5.2 Information

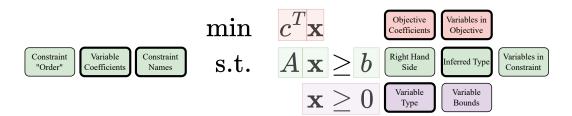


Figure 5.2: All parts of a model that contain useful information for semantic grouping of constraints and variables. Elements with a thick border are already used as a key concept in one of the existing detectors.

Before we present any algorithmic details, we give an overview about the available information which might be used to define suitable strategies.

- 1. **Objective**: For the objective functions, information about the participating variables and their coefficients is available. For some models e.g. for Bin-Packing, this information alone is sufficient to partition the variables.
- 2. **Coefficients**: The use of coefficients to classify constraints and variables was already in discussed in Section 4.2.
- 3. **Bounds**: For all variables $lb \le x \le ub$ information about their lower- and upper-bounds is available. Furthermore, the left- and right-hand-side of linear constraints $lhs \le \sum_i a_i x_i \le rhs$ are available as well.
- 4. **Types**: Variable types such as *Integer* are usually stated explicitly in the input format. If not, then information about the variable bounds can be used to deduce a type, e.g. $0 \le x \le 1$ is a strong indicator that x is a *Binary* variable.
- 5. **Names**: If specified by the modeler, then variables and constraints might have meaningful names which can be used as a strong indicator which constraints and variables belong to the same group.
- 6. **Order**: In contrast to other kinds of information, the constraint "order" is no intrinsic property of the model itself. With the term "order", we refer to the order of the constraints as specified in the input format. When a model is created e.g. via. a script, constraints are usually added in *blocks* by the modeler. This information is used in Section 5.3.3 to conceptualize a classifier based on that.

5.3 Classifiers

In the following Sections we describe different classifiers which are not yet implemented in GCG but could potentially provide new information about the model. Adding new classifiers has, in addition to practical implications such as higher maintenance overhead, additional side-effects regarding runtime and memory requirements. Each new classifier provides new opportunities for existing detectors to find new partial decompositions. This can prove especially useful for detectors like consclass, which directly depend on the found classifications. On the other hand, this dependence can result in a sub-optimal runtime investment if the found classifications provide no new information, because the generated partial decompositions based on that will most certainly be of bad quality as well.

wording

Therefore, we will refrain from mentioning all missing model properties for which a classifier *could* be built, and only focus on promising candidates.

5.3.1 Bounds

When considering bounds, we differentiate between variables and constraint respectively.

Variable bounds

The classifier for variable bounds can be considered as a simple mapping from pairs of bounds to a unique class index. More formally, given a list of all unique pairs of lower and upper bounds for variables $B = (b_1, b_2, \ldots, b_k)$, with $b_i \in \mathbb{Q} \times \mathbb{Q}$, we map each variable to the index of its bounds in B. This mapping trivially unique.

Mapping the variables in the described way has the side-effect that $0 \le x \le 1$ and $y \in \{0, 1\}$ are mapped to the same class. This behavior is able to account for missing declarations of variables as binary in the input format read by GCG. The classification is wrong if x is truly meant to be a continuous variable, but this is offset by the fact that GCG already includes a classifiers based on SCIP types, which will correctly classify both variables in this case.

container loading example

Constraint bounds

A classifier for constraint bounds works in a similar manner as for variables. By collection all bounds and assigning a class to each constraint based on that list, we obtain a unique mapping. Note that for inequalities the absolute value either of the two bounds will always be infinity. For equalities which were not replaced with equivalent inequalities, both bounds will be equal.

cap. lot sizing example

5.3.2 Relaxed MIPLIB types

Nr.	Type	Linear Constraint	Notes
1	Empty	Ø	-
2	Free	$-\infty \le x \le \infty$	No finite side.
3	Singleton	$a \le x \le b$	-
4	Aggregation	ax + by = c	-
5	Precedence	$ax - ay \le b$	x, y have same type.
6	Variable Bound	$ax + by \le c$	$x \in \{0, 1\}$
7	Set Partitioning	$\sum 1x_i = 1$	$\forall i: x_i \in \{0, 1\}$
8	Set Packing	$\sum 1x_i \le 1$	$\forall i: x_i \in \{0, 1\}$
9	Set Covering	$\sum 1x_i \ge 1$	$\forall i: x_i \in \{0, 1\}$
10	Cardinality	$\sum 1x_i = b$	$\forall i: x_i \in \{0, 1\}, b \in \mathbb{N}_{\geq 2}$
11	Invariant Knapsack	$\sum 1x_i \le b$	$\forall i: x_i \in \{0, 1\}, b \in \mathbb{N}_{\geq 2}$
12	Equation Knapsack	$\sum a_i x_i = 1$	$\forall i: x_i \in \{0, 1\}, b \in \mathbb{N}_{\geq 2}$
13	Bin Packing	$\sum a_i x_i + ay \le a$	$\forall i: x_i, y \in \{0, 1\}, b \in \mathbb{N}_{\geq 2}$
14	Knapsack	$\sum a_i x_i \le b$	$\forall i: x_i \in \{0, 1\}, b \in \mathbb{N}_{\geq 2}$
15	Integer Knapsack	$\sum a_i x_i \le b$	$\forall i: x_i \in \mathbb{Z}, b \in \mathbb{N}$
16	Mixed Binary	$\sum a_i x_i + \sum p_j s_j \{\leq, =\} b$	$\forall i : x_i \in \{0, 1\}, \forall j : s_j \text{ continuous}$
17	General Linear	$\sum a_i x_i \ \{\leq,\geq,=\} \ b$	No special structure.

Table 5.1: The structure of all 17 constraint types MIPLIB keeps track of.

5.3.3 Voting (ordered)

As mentioned earlier, the motivating idea behind each individual classifier is to group constraints according to some property, while the type of this property can vary greatly between classifiers. Under the assumptions that groups of constraints share at least *some* of these properties and are thus assigned to the same classes, we can define a new type of classifier. Note that this classifier can be equivalently conceptualized as an additional *strategy*, which are the basic building blocks of the refinement algorithm and explained in Section 5.4. This assumption is, at least on examples that can be observed in practice, a reasonable one.

Voting (unordered)

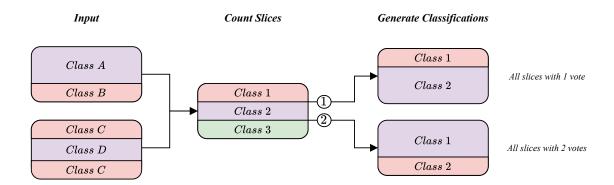


Figure 5.3: text

In order to derive a simple and efficient algorithmic approach to this problem, we can make an additional assumptions not based on the model itself, but on its representation in common input formats like .1p and .mps files. A lot of models are generated via. scripts and written to such files for portability and interoperability with other solvers. One exploitable property which can be observed in a lot of models is, that groups constraints are usually added in bulk. This results in consecutive blocks of constraints which are semantically related, which is illustrated in the "Input" column of Figure 5.3. If a class of constraints is split into two non-consecutive groups like the second partition from Figure 5.3, then we can deduce that they are meant to be two different groups.

Voting (unordered)

If the read model does not have the property of properly ordered constraint blocks, a more involved algorithmic approach can be used. Here, the general problem can be reduced to group constraints with each other which are often assigned to the same class. ___ WIP

5.4 Strategies

Strategies are the central building block of the algorithm and are responsible for refining sets of constraints or variables. Let U be a the total set of constraints or variables. Each strategy gets a single set $S \subseteq U$ as input and produces a partition $\pi_S \in \Pi(S)$ of that set as output. Each set $A_i \in \pi_S$ corresponds to one child node. Conceptually, each strategy can be seen as a materialization of a specific splitter function as defined in Section 2.4. In the following, we differentiate between re-callable and non re-callable strategies. The former type may be called more than once in any given sub-tree, as the result may depend on the set that is being refined.

5.4.1 Slice (Partition)

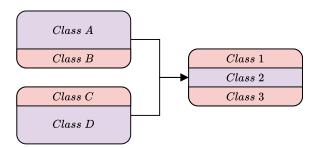


Figure 5.4: A simplified illustration assuming that constraint in both partitions can be rearranged into continuous blocks, thus "slicing" the partitions into different-sized chunks. The output partition inherits all these slices.

Slicing strategies are the most simple type of strategy. Given two partition $\pi, \pi' \in \Pi(U)$, we define the *combined partition* $\pi \sqcap \pi'$ as follows:

$$\pi \sqcap \pi' = \{ A_i \cap B_j \mid A_i \in \pi, B_j \in \pi' \} \setminus \emptyset$$
 (5.1)

This concept is illustrated in Figure 5.4. Because strategies only refine single sets and not whole partitions, Equation 5.1 always degenerates to $\pi_{slice} \sqcap \{S, U \setminus S\}$ for some partition $\pi_{slice} \in \Pi(U)$ and a set S we want to refine. The result is then restricted to elements of S, which yields a partition of S. More formally, this strategy can be expressed as Function 5.2 and computed efficiently using Algorithm 4.

$$f(\pi_{splitter}, S) = \{A_i \cap S \mid A_i \in \pi_{splitter}\} \setminus \emptyset$$
 (5.2)

Note that the operator \sqcap is trivially associative, i.e., $(\pi \sqcap \pi') \sqcap \pi'' = \pi \sqcap (\pi' \sqcap \pi'')$:

$$X \in (\pi \sqcap \pi') \sqcap \pi'' \iff \exists Z \in (\pi \sqcap \pi'), C \in \pi'' : X = Z \cap C$$

$$\iff \exists A \in \pi, B \in \pi', C \in \pi'' : X = (A \cap B) \cap C$$

$$\iff \exists A \in \pi, B \in \pi', C \in \pi'' : X = A \cap (B \cap C)$$

$$\iff X \in \pi \sqcap (\pi' \sqcap \pi'')$$

end function

In conjunction with commutativity, this fact can be used to e.g. eliminate part of the search space by pruning duplicated nodes in the tree and only expanding one instance of any given sub-tree.

Algorithm 4 If a lookup table represented by function f is available, then Function 5.2 can be implemented in O(|S|).

```
can be implemented in O(|S|).

Input: Partition \pi = \{A_1, A_2, \dots, A_k\}, set S \subseteq U, function f_C : U \mapsto \mathbb{N} for C = \{C_1, C_2, \dots\} \in \Pi(U) mapping u \in U to C_i iff u \in C_i

Output: Partition of S according to Function 5.2.

function STRATEGYSLICE(\pi, S)

\pi_{out} \leftarrow \text{list of } k \text{ empty sets } B_1, B_2, \dots, B_k

for s \in S do

i \leftarrow f_S(s)

B_i \leftarrow B_i \cup \{s\}

end for

Remove empty sets from \pi_{out}

return \pi_{out}
```

5.4.2 Slice (Covering)

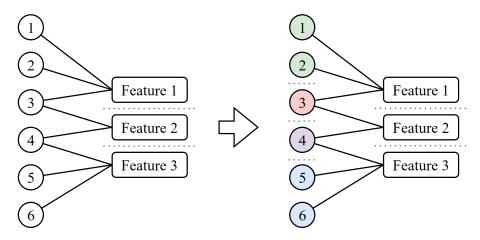


Figure 5.5: Given $U = \{1, \ldots, 6\}$, and $S = \{\{1, 2, 3\}, \{3, 4\}, \{4, 5, 6\}\} \subseteq 2^U$, with each $C \in S$ corresponding to one feature. Each element $x \in U$ is part of at least one set $C \in S$, thus possessing at least one feature. This example can be encoded as a graph, where the right side "the features" are pre-partitioned into individual cells. By applying the standard partition refinement framework from Section 2.4 with function 2.5, we obtain a partition $\pi \in \Pi(U)$ in which the elements any given cell possess the same features.

Let U be an arbitrary set. Then a covering can be defined as a set $S \subseteq 2^U$, where S^U denotes the power set, such that:

$$U = \bigcup_{C \in S} C$$

The definition is equivalent to a set partitioning without the condition that sets of S must be pairwise disjuct. Each set $C \in S$ corresponds to one feature, with the elements $x \in C$ considered to possessing said feature. The goal of the covering version of the slicing strategy is to partition the elements of a given set in such a way, that elements in the same cells all possess the same features. In order to obtain such a partition from a set covering S, we can encode the underlying problem as a graph and use the standard partition refinement framework. Afterwards, the resulting partition can be used to slice the given set as described in Section 5.4.1.

The strategy can be used to e.g. partition constraints according to the types of variables that they contain. It is functionally equivalent to the refinement method "fast" from [6]. The name most likely stems from an algorithm informally described a fast algorithm based on bucket sort to implement such a partition refinement algorithm.

5.4.3 Recursive

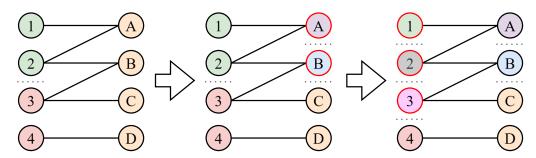


Figure 5.6: An example of a graph for which the partition refinement algorithm takes multiple iterations to yield a stable partition (Function 2.5). Red circles around the vertices highlight changes to the cells in the respective iterations. The algorithm is initialized with $\pi_{init} = \{\{1,2\}, \{3,4\}, \{A,B,C,D\}\}$. During the first iteration, all vertices on the right side are in the same cell so no changes can happen on the left side. Vertices A, B are not connected to cell $\{3,4\}$. A similar reasoning applies for the second iteration.

The recursive strategy is the the only strategy which needs to utilizes the full blown partition refinement framework. The strategy is based on the canonical constraint-variable un-directed graph already shown in Figure 2.2. Each variable and constraint corresponds to exactly one vertex, while an edge between a constraint and variable node exists iff the variable is part of the constraint. More formally, given a set of constraints $C = \{c_1, \ldots, c_m\}$ and a set of variables $X = \{x_1, \ldots, x_n\}$. Let a_{ij} be the coefficient of variable $x_i \in X$ in constraint $c_j \in C$. Then we can define the graph as follows:

$$G = (V, E) = (X \cup C, \{\{x_i, c_j\} \mid x_i \in X, c_j \in C, a_{ij} \neq 0\})$$

The size of the graph in terms of it's edges and vertices depends entirely to the underlying problem. A partition is obtained by running the algorithm with either Function 2.4 or Function 2.5. Afterwards, the partition is used to slice a given set according to the method described in Section 5.4.1. Note that even thought the generated graph is always bi-partite, it does not necessarily fulfill the conditions mentioned in Section 2.4 for the fast variant of the refinement algorithm, i.e., that all nodes on one of the two sides of the bi-partite graph are all in their own cell. As a consequence, one full execution of the recursive strategy might take orders of magnitude longer than an execution of one of the two slice variants explained previously.

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5.5 Scoring

Up until this point we have only described how the algorithm refines sets based on different strategies, despite the goal being a list of promising partitions. Before we describe how to select such partitions, we have to define how we actually *get* a list of partitions from the refinement tree.

Let G = (V, R, E) the set refinement tree with vertex set V, designated root node $R \in V$ and edges $E \subseteq V \times V$.

Let $Recombine_k(U_1, U_2, \dots, U_k) : U_1 \times U_2 \times \dots \times U_k \to 2^{U_1 \cup U_2 \cup \dots \cup U_k}, k \in \mathbb{N}$ be a Function defined as follows:

$$Recombine_{k}(U_{1}, U_{2}, \dots, U_{k}) = \begin{cases} \emptyset & k = 0 \\ U_{1} & k = 1 \\ \{\{u\} \cup r \mid u \in U_{1}, r \in Recombine_{k-1}(U_{2}, U_{3}, \dots, U_{k})\} & else \end{cases}$$

More informally, $Reombine_k$ takes a total of k arbitrary sets U_1, \ldots, U_k and computes a set containing all possible k-tuples (u_1, u_2, \ldots, u_k) with u_i restricted to elements from U_i . Thus, the set of all partitions constructible from a sub-tree rooted at vertex $v \in V$ can be computed using Function 5.3.

$$Partitions(v) = \begin{cases} Sets(v) & \text{if } v \text{ is leaf node} \\ \left\{ Recombine_{|Sets(v)|} \right\} & else \end{cases}$$
 (5.3)

It is clear that setting v = R gives the set of all possible partitions.

One can deduce from the definition of Function 5.3 that the number of partitions depends on the depth and maximum out-degree of any given node of the tree. Therefore, it will be of vital interest to only consider "interesting" sets. Ideas and possible implementations are discusses in Chapter 6.

WIP

Add simple proof

5.5.1 Constraint Names

One important piece of information that usually reflects the modelers *intent* when it comes to the semantic difference are the names of the constraints or variables, in the following abbreviated with just "names". As discusses in Section 4.2.1, names usually consist of multiple parts, with one part containing all the information related to *semantics*. Extracting this part of the name can be done heuristically using Algorithm 5. The heuristic consist of four major steps:

- 1. Remove *modifies* which are usually enclosed in either brackets or some other special character combination which consists of an *opening* and *closing* character.
- 2. "Normalize" the string by replacing any non-alpha-numeric separators such as spaces, tabs, ... with a single character c such as " $_$ ".
- 3. Split the string according to c and try to detect the part with the relevant semantics.
- 4. (Optional) Remove any left-over non-alpha characters such as numbers.

Step 4 is explicitly marked as optional, because sometimes numbers are integral part of the name, sometimes they are not. Both of these cases can actually be observed in the same model ¹. For this model in particular, the constraints "cut1" to "cut4" are of interest. The constraints with the prefix "cut1" and "cut2" are structurally identical, i.e, the they all share the same number of non-zeros and the same type of variables, while "cut3" and "cut4" do not. Here, "cut1" and "cut2" would have to belong to the same group, while "cut3" and "cut4" belong in a group their own. With the heuristic as is, this case is not detected with or without step 4 because additional information about the actual structure of constraint is required.

Note that the Algorithm makes some implicit key assumptions, such as:

- That the name actually carriers any semantically relevant information at all.
- The names adhere to a "common" format, i.e., the modifier comes *after* the semantics part. Here, constraint names such as "capacity_bin_k", "out_flow_k" qualify, but the same names in reverse do not.

 $^{^{1}}$ StrIPlib UUID: d48c9568-e0ea-4c77-9a3b-b7f4dc530d5f

These assumptions proved reasonable for almost all models observed in practice which had proper names available. Still, there cases where this approach fails .

Give MI-PLIB examples

Algorithm 5

Input: Name of a constraint

Output: Relevant semantics of the constraint name if the name adheres

```
function EXTRACTSEMANTICPART(name)

name_{new} \leftarrow name

name_{old} \leftarrow name

repeat

name_{old} \leftarrow name

start \leftarrow Position of opening character e.g. [, {, (, ... end \leftarrow Position of corresponding closing character e.g. ], }, ), ...

name_{new} \leftarrow name_{old} without characters in range [start, end]

until name_{new} = name_{old}

end function
```

WIP

As soon as the semantic part of all names is extracted, constraints and variables can be grouped based on this information. Possible post-processing steps might include an application of the mentioned Levenshtein-Distance from Chapter 4. Even thought the Algorithm has quadratic time complexity and is therefore unlikely to be used with the full set of original constraint or variable names, a reasonable assumption is that

```
{ EXTRACTSEMANTICPART(Name(c)) | c \in Cons } \ll { Name(c) | c \in Cons }
```

Analogously, the assumption is made for variable names as well. Thus, an Algorithm for the Levenshtein-Distance, even under worst-case considerations, might be applicable and thus resulting in a better partitioning.

5.5.2 Ground Truth based

As discusses in the previous Sections, the algorithm starts with a set in which all constraints or variables are in the same cell. In order to *guide* the search towards a plausible semantic partitioning, the existence of a ground-truth partition which approximates the desired partition reasonably well can be used to terminate the search or select promising partitions after the search-space has been explored. Terminating the search can, in practice, be very useful, because preventing the algorithm from expanding a node not only prevents unnecessary work being done for this particular node, but also prevents the generation of the entire sub-tree below; reducing the number of potential candidate partitions and overall runtime and space requirements of the algorithm.

Potential sources for a suitable ground-truth partitions include

- Constraint names using the heuristic from Section 5.5.1.
- Variable information, i.e., given a ground-truth of semantic groupings of variables, one could obtain a corresponding ground-truth partition for constraints by assigning two constraints to different groups iff they contain different kinds of variables according to the ground-truth.

Without the availability of a reasonably ground-truth, it is currently unclear how to know when to terminate the search and more importantly, what structured the desired target partitions should have. Here, the term "structure" refers to all relevant properties of the target partition, including but not limited to, the number and size of the cells.

Assuming a reasonable ground-truth has been obtained, a partition-comparing score such as the Rand-Index already discussed in Section 2.6 can be used a number of promising candidates. Furthermore, the refinement can be terminates for sets which are already homogeneous according to the ground-truth partition. The idea being is that by refining the set further we do not gain any new information.

 $rac{ ext{completen}}{ ext{missing}}$

5.5.3 Connected Components Score

The ground-truth based scoring from Section 5.5.2 scores candidates based on a partition π , which is assumed to resemble a semantic grouping reasonable close to the real partitioning in order to "guide" the search and find promising candidates. In case this assumption is not true, it can be expected that the selected partitions provide no useful information about the model.

In the following, let $A \in \mathbb{Q}^{m \times n}$ be a constraint matrix, G = (V, E) with $V = \{1, 2, ..., m\}$ and $E = \{\{u, v\} \in V \times V \mid \exists i : A_{ui} \neq 0 \land A_{vi} \neq 0\}$ a graph with the constraints as its vertices. There exists an edge between two constraints iff they share at least one variable with non-zero coefficient. Furthermore, let $cc(v) : V \to 2^V$ be a function mapping every vertex to its connected component in G. It is a well known result from graph-theory that every graph can be decomposed into its connected components, so the function is unique.

In order to get to a score based on connected components, we define the relation $\sim_{\pi} = \{(B_i, B_j) \in \pi \times \pi \mid (cc(B_i) \mid cc(B_j)) \vee (cc(B_j) \mid cc(B_i))\}$, where $a \mid b$ with $a, b \in \mathbb{N}$ denotes the standard divisibility relation defined on natural numbers. Given a partition $\pi = \{B_1, B_2, \ldots, B_k\}$, we can compute a "connected components score" as follows:

connectedScore(
$$\pi$$
) = $|\pi/\sim_{\pi}|$

The score corresponds to the amount of connected components of "different" sizes. Here, two sizes $a, b \in \mathbb{N}$ are considered different, if a is not divisible by b and vice-versa.

motivating example consequen

6 Implementation

Building upon the algorithmic descriptions of Chapter 5, we want to discuss how such an algorithm can be efficiently implemented and practice and how the component is integrated into GCG as a detector. The Chapter is divided into multiple sections, each describing a different aspect of the implementation:

- 1. Section 6.1 contains a high-level overview about the architecture of the detector and its relation with other components in GCG.
- 2. In Sections 6.1 6.4, we will give a brief overview about a few custom data structures required to implement the refinement more efficiently and how the tree is represented in memory.
- 3. Sections 6.5 and 6.6 conclude the Chapter with two practical considerations:
 - Is it possible to reduce to the number of candidate partitions before scoring?
 - For larger and more complicated models, can we ensure a reasonable runtime?

This Chapter does not include actual numbers concerning space and runtime, we only look at the underlying concepts which are widely used in other algorithms to achieve e.g. a better practical runtime.

6.1 Architecture

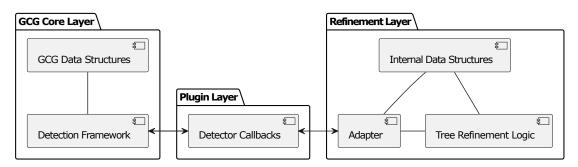


Figure 6.1: text

As mentioned in the introduction to Chapter 5, the approach is implemented as a *Detector* in GCG, contrary to the fact that the algorithm outputs a one or multiple partitions of constraints or variables. Generating such partitions is more aligned with the concept of a *classifier* from Section 4.2, but this comes with an important drawback. Because we want to incorporate information about variables for partitioning constraints and vice-versa for constraints, we have to delay the execution of the algorithm to a point in time *after* the classification has finished, i.e., all relevant data is available. Circumventing this problem by potentially implementing the algorithm as a classifier and assigning the lowest priority possible to it is not an option as well, because this would introduce additional maintenance overhead in case changes to the overall classification/detection framework are made. An implementation as a detector *ensures* that all classification step are done beforehand.

An overview about the relationship between the GCG and the detector is shown in Figure 6.1. When implementing an detector, GCG provided a set of callbacks that have to implemented such as

- Set-up/Tear-down, i.e., for allocation and deallocation of data-structures
- A handler for propagation, which takes a partial decomposition and assigns all or a subset of the remaining open constraints to either a block or the master. This concept was already shown in Figure 4.3.

The callbacks take GCG-internal data structures as input and must provide the result as such. In order to ensure better maintainability, the logic realizing the tree refinement should be mostly *independent* of the concrete framework it is being used in. Furthermore, relying on custom data structures increases control about runtime and space considerations. This decoupling is being realized by an *Adapter*, as shown in Figure 6.1, which translates between the two "worlds" of data-structures and ensures compatibility.

Wording

6.2 Metadata

6.3 Data Structures

6.4 Hashing

6.5 Cutoff Conditions

We implemented several cutoff conditions which ensure that we only explore relevant parts of the search space. The conditions can be divided into two groups:

- 1. Local Conditions, which can be evaluated by only considering information about one singular node or its immediate predecessor.
- 2. Global Conditions, whose evaluation requires information about e.g. the precise path to the node, i.e., its position in the tree and therefore information about its ancestors, or requires knowledge about other nodes or completely distinct sub-trees.

6.5.1 Local Conditions

With access only to local information, these conditions are restricted to the information that is stored within one single TreeNode data structure.

Refined Set Size

Assuming a proper ground-truth is available or any heuristic information about the potential size of the target partition, many found nodes can be excluded from the scoring a-priori.

WIP

Depth

Under the assumption that most of the "interesting" sets are found early on, it could be beneficial to abort the search for a sub-tree as soon as a certain depth has been reached. Information about the *depth* of a given node can be extracted from the data-structure itself, or by traversing the graph towards the root node.

No Changes

As soon as the algorithm expands a set S with a strategy, we get a partition $\pi \in \Pi(S)$ as a result. If $S \in \pi$, this implies that $\pi = \{S\}$ and the strategy did not refine S any further and we can terminate the search for the current sub-tree.

6.5.2 Global Conditions

As mentioned before, global conditions are more flexible and allow for more involved logic to be executed.

Sub-Tree Duplication

Most Optimistic Partition Size

6.6 Multi-Threading

7 Evaluation

7.1 Setup

Type	Name	Metric
CPU	AMD Ryzen 3700X	3.8 GHz
RAM	-	16GB

Table 7.1: Consumer-grade components used to run all experiments.

All experiences were run on a system with components as specified in Table 7.1.

7.2 StrlPlib

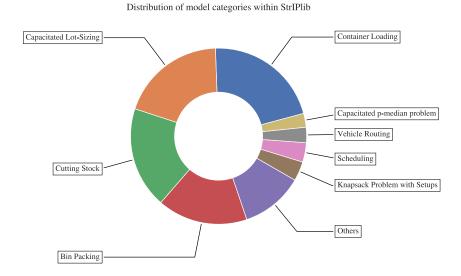


Figure 7.1: The distribution of different categories of model within strIPlib. Most problems are part of "common" categories like Bin-Packing, Scheduling and Routing. The category "Others" includes e.g. Fantasy Football, Train Scheduling and different types for which only a small number of model files are available.

The Structured Integer Program Library (strIPlib) is a collection of over 21000 mixed-integer programs with an exploitable structure such as Block-Diagonal and Staircase . All instances are assign to exactly one of the 33 main categories as highlighted in Figure 7.1. Each categories is further sub-divided into a number of smaller sub-categories, because each kind of problem can be modeled (e.g. three-index vs. four-index) or decomposed in a variety of different ways.

The number of available instances per category ranges from as low as 2 for Binary/Ternary Code Construction and up to ≈ 4700 for Container Loading, which makes the data-set in-balanced with respect to available models per main category. This is only of theoretical concern and is further discussed in section . Furthermore, the largest four categories account for $\approx 80\%$ of the total instance count with the remaining 20% distributed across 29 categories. One singular category "Haplotype Inference" with 40 instances is excluded from all tests, because the problem files are not readable by either GCG or SCIP. This behavior can be traced back to the used variable names in these models, which all contain the special character "^".

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7.3 Stuff

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