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Vorwort

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Darüber hinaus bietet die Reihe ein Forum für die Berichterstattung über die zahlreichen Kooperationsprojekte des Instituts mit Partnern aus Industrie und Wirtschaft.

Berichterstattung heißt hier Dokumentation des Transfers aktueller Ergebnisse aus mathematischer Forschungs- und Entwicklungsarbeit in industrielle Anwendungen und Softwareprodukte – und umgekehrt, denn Probleme der Praxis generieren neue interessante mathematische Fragestellungen.

Prof. Dr. Dieter Prätzel-Wolters
Institutsleiter

Kaiserslautern, im Juni 2001

A NOVEL NON-LINEAR APPROACH TO MINIMAL AREA RECTANGULAR PACKING

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Abstract. This paper discusses the minimal area rectangular packing problem of how to pack a set of specified, non-overlapping rectangles into a rectangular container of minimal area. We investigate different mathematical programming approaches for this and introduce a novel approach based on non-linear optimization and the "tunneling effect" achieved by a relaxation of the non-overlapping constraints. We compare our optimization algorithm to a simulated annealing and a constraint programming approach and show that our approach is competitive. Additionally, since it is easy to extend, it is also applicable to a larger class of problems.

Keywords: rectangular packing, non-overlapping constraints, non-linear optimization, regularization, relaxation

1. Introduction

Packing problems of objects with arbitrary shapes arise in a multitude of important real world applications. In particular, packing problems of rectangular-shaped objects are intensively studied. Such problems for example occur in industry, when containers or pallets have to be loaded with packed goods, or in scheduling, where jobs that require a certain amount of resource and processing time have to be planned.

In microelectronics design, the layout of an electronic system includes the placement of its devices. Being part of the floorplanning design, the *placement problem* is to place interconnected electronic devices on a board device such that certain objectives are optimized and diverse constraints are met, e.g. to minimize the board area. As the number of devices and complex design constraints grows, so does the importance of the placement problem. An essential subproblem is the rectangular packing problem.

In this paper, we focus on the following specific optimization problem fundamental to rectangular packing:

Definition 1.1. The *minimal area rectangular packing problem* (MARPP) is to arrange a set of non-rotatable rectangles into a rectangular container of minimal area, such that the container includes all rectangles and no two rectangles overlap.

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The rectangular container is also called *bounding box*. The *non-overlapping constraint* is that no two rectangles overlap and the *containment constraint* is that all rectangles are in the container.

A large variety of models and optimization approaches have been developed and studied for rectangular packing problems. Approximation algorithms are mainly studied in the context of the theory of bin packing problems (Coffman et al., 1996; Bansal and Sviridenko, 2004). They rely on the design of clever heuristics which are also used in the application to specific packing problems. Mixed integer programming (MIP) is another method to formulate rectangular packing problems (Fasano, 2004; Goetschalckx and Irohara, 2007). In section three of this paper we discuss metaheuristics, constraint programming (CP) and non-linear approaches to rectangular packing problems in more detail. Metaheuristics and non-linear approaches are traditionally used for placement problems. CP is a relatively new programming paradigm, is strongly related to operations research and has been successfully applied to packing problems in scheduling (Hooker, 2007).

For the MARPP we propose a novel non-linear model, motivated by methods used for *general semi-infinite programming* (GSIP). As recently stated (Winterfeld, 2007), GSIP can also be used to fit several geometric objects O_i into a container C while optimizing the shape of both the objects and the container and preserving the non-overlapping constraints. In the context of MARPP the O_i correspond to the rectangles r_i to be arranged and the C to the bounding box. However, formulating the MARPP as a semi-infinite problem is not necessary as for the simple shapes of objects and container the problem can be stated directly using inequality constraints. That means, the containment constraint $O_j \subset C$ reduces to a linear condition like $Ax \leq b$ and the non-overlapping constraint $\text{int}(O_j \cap O_i) = \emptyset$ can be expressed as the maximum of two smooth functions being smaller than zero.

Since the resulting function is non-differentiable this might seem inadequate for non-linear optimization approaches. Yet, smoothing techniques to circumvent this problem are well-known. In our approach we use such a technique for approximating the maximum function by a differentiable substitute while at the same time exploiting it in order to cope with the globality of the problem. The essential point is that the approximation is a relaxation of the original problem in which the rectangles can change their relative positions more easily. We refer to this behaviour as the *"tunneling effect"*. In common numerical approaches for GSIP (Stein, 2003) it is also necessary to regularize the minimum function. Therefore our non-linear programming (NLP) solver was inspired by a solver for general semi-infinite programs.

The outline of this paper is as follows: In the second section we briefly provide the notation used in this paper. In the next section we give a broad survey of metaheuristics, CP and non-linear approaches to rectangular packing problems. In the main section we present our novel non-linear model, propose an optimization algorithm for it and discuss properties of our approach. We show experiments in which we compare our method to a simulated annealing approach and the optimal solutions given by a CP approach. We conclude the paper with perspectives and an outline for future research work.

2. Notation

Throughout this paper we use the following notation:

- $\mathcal{R} = \{r_1, \ldots, r_n\}$ denotes the set of rectangles.
- $l_1^{(i)}, l_2^{(i)}$ represent the width and the height of rectangle r_i.
- $c_1^{(i)}, c_2^{(i)}$ represent the center coordinate of rectangle r_i.
- b_1, b_2 represent the width and the height of the bounding box B.

- The area as objective function is denoted by $A = b_1 b_2$.

3. Survey of other approaches

3.1. **Formulation of the problem.** In this section we focus on MARPP formulated in the following way:

$$(\mathcal{P}) \quad \min b_1 b_2$$

subject to

$$(1) \qquad \frac{1}{2} l_k^{(i)} \le c_k^{(i)} \le b_k - \frac{1}{2} l_k^{(i)} \quad \text{for } k \in \{1,2\} \text{ and } i \in \{1,\dots,n\}$$

$$(2) \qquad (c_1^{(i)} + \frac{1}{2} l_1^{(i)} \le c_1^{(j)} - \frac{1}{2} l_1^{(j)}) \vee (c_1^{(j)} + \frac{1}{2} l_1^{(j)} \le c_1^{(i)} - \frac{1}{2} l_1^{(i)}) \vee$$
$$(c_2^{(i)} + \frac{1}{2} l_2^{(i)} \le c_2^{(j)} - \frac{1}{2} l_2^{(j)}) \vee (c_2^{(j)} + \frac{1}{2} l_2^{(j)} \le c_2^{(i)} - \frac{1}{2} l_2^{(i)})$$
$$\text{for } 0 < i < j \le n$$

We assume that the bounding box is anchored at the origin. Condition (1) guarantees that the rectangles are within the container B whereas (2) assures that no two rectangles overlap. For the discussion of metaheuristics and CP approaches, we emphasize the formulation of the non-overlapping constraints as disjunctions of linear inequalities. The non-overlapping constraints express that rectangle r_i is either left, right, in front of or behind rectangle r_j.

3.2. **Metaheuristics.** In the following we briefly overview metaheuristics and focus on simulated annealing, the predominant metaheuristic applied to placement problems. Furthermore, we show how to represent a rectangular packing in a metaheuristic and sketch how one can solve MARPP in this way.

3.2.1. *Overview of metaheuristics.* Many optimization problems appearing in real world applications are, in practice, not solvable with complete solution methods due to exponential computation times. Metaheuristics have successfully been applied to such optimization problems, especially to combinatorial optimization problems.

Metaheuristics are *local search* methods which start from an initial solution and iteratively try to replace the current solution by a better solution of the neighborhood of the current solution. *Intensification* and *diversification* are the driving forces behind these methods and have to be dynamically balanced in the local search process (Blum and Roli, 2003). "Intensification is to search carefully and intensively around good solutions found in the past search. Diversification, on the contrary, is to guide the search to unvisited regions." (Yagiura and Ibaraki, 2001) The concept of a metaheuristic is independent of any specific properties of the optimization problem. The specifics only influence the neighborhood definition and the ways neighborhoods are explored. Metaheuristics are non-deterministic and guarantee no optimal solution, but a good solution in moderate running time.

"The class of metaheuristics includes – but is not restricted to – *Ant colony optimization*, *Evolutionary computation* including *Genetic algorithm*, *Iterated local search*, *Simulated annealing* (SA) and *Tabu search*." (Blum and Roli, 2003)

Metaheuristics are categorized in *single point* and *population-based* search techniques. The search space is explored along trajectories in the former category whereas it is searched through evolution of a set of points in the latter (Blum and Roli, 2003).

3.2.2. *Application to MARPP.* In order to apply a metaheuristic to MARPP we have to encode a rectangular packing solution and define neighborhoods of the current solution. We focus on simulated annealing as it is predominant in placement problems. The encoding of a solution strongly depends on the optimization problem.

How to encode an arrangement of rectangles as a combinatorial object has been intensively studied. For placement problems, such an encoding of a packing is called a *floorplan representation*. Yao et al. (2003) gave a broad overview of the multitude of different floorplan encoding schemes and how they are related.

All these representations commonly model the geometric or topological relationship of the rectangles, but not their actual positions. Usually, the representations are built up from directed graphs, trees and/or permutations. We focus on the sequence pair, a simple and often used encoding scheme.

3.2.3. *Simulated annealing.* Simulated annealing (SA) is a metaheuristic inspired by annealing processes in metallurgy where techniques involving heating and controlled cooling of a material result in a low energy configuration of the material. The fundamental idea of SA applied to a minimization problem is to accept an intermediate solution to have a worse objective function value than the current solution. The probability of such an acceptance decreases during search (Blum and Roli, 2003). The algorithm is analogous to cooling the material and the accepted intermediate increases of the objective function correspond to revisited high energy configurations. A pseudo-code of SA is given in algorithm 3.2.3.

Algorithm 1 Pseudo code of SA

```
Initialize random starting solution sp
Initialize temperature T
while termination condition not met do
  Pick neighbour sp' ∈ N(sp) through a random move
  if f(sp') < f(sp) then
    Replace sp with sp'
  else
    Accept sp' as sp with probability p(T, sp', sp)
  end if
  Update T
end while
```

The algorithm starts by generating an initial solution (either randomly or heuristically constructed) and by initializing the temperature parameter T. Then, at each iteration a solution $sp' \in \mathcal{N}(sp)$ is randomly sampled and is accepted as new current solution depending on $f(sp), f(sp')$ and T. sp' replaces sp if $f(sp') < f(sp)$ or, in case $f(sp') \geq f(sp)$, with a probability which is a function of T and $f(sp') - f(sp)$. The probability is generally computed following the Boltzmann distribution $\exp(-\frac{f(sp')-f(sp)}{T})$. The update of the temperature T usually follows a geometrical law, i.e. $T_{k+1} = \alpha T_k$ for $\alpha \in (0,1)$. This yields an exponential decay of the temperature (Blum and Roli, 2003).

3.2.4. *Sequence pair encoding.* The floorplan representation *sequence pair* is one of the most popular encoding schemes and was proposed in Murata et al. (1996). The following definition states the sequence pair for the MARPP:

Definition 3.1 (Sequence Pair)**.** Suppose the rectangles $r_i \in R$ are to be packed. Then, a *sequence pair* $sp := (\Gamma_+, \Gamma_-)$ is a pair of rectangle sequences. Both sequences Γ_+ and Γ_- are permutations of R.

The non-overlapping constraints between each pair of rectangles are disjunctions of linear inequalities. Depending on the linear order in both sequences, the sequence pair encodes exactly one geometric relation $G \in \{$left of, right of, in front of, behind$\}$ between each pair (r_i, r_j) of rectangles of R, $i < j$. Therefore, at least one linear inequality holds. In order to satisfy more than one linear inequality, transitive relations between triples of rectangles are relevant.

The consistent assignment of exactly one linear inequality for each rectangle pair can be transformed to a lower-left compacted packing. This can be formulated as a linear program or as longest path problems on two directed acyclic graphs, one for the horizontal and the vertical dimension. For further properties and details of the sequence pair we refer to Murata et al. (1996).

3.2.5. *Details of the application to MARPP.* When we represent a packing solution with a sequence pair sp and apply SA, we only have to define neighborhood structures $\mathcal{N}$ and to define our objective function f.

A *move* defines how to traverse randomly from a solution sp to a neighbourhood solution $sp' \in \mathcal{N}$. Moves for the sequence pair are based on randomly shifting or swapping rectangles in either one or both sequences. Typically, a rectangle is shifted in one sequence and pairs of rectangles are swapped in one or both sequences. In order to guarantee the diversification of the SA, moves should be chosen randomly out of several different move types. However, any sequence pair can be simply reached from any other sequence pair by consecutively applying any single move out of the described move types. More details on neighborhood definitions and their properties can be found in Berger (2006).

The objective function for the MARPP is the area $f(sp) := b_1 b_2$ of the bounding box, where $b_1(sp) = \max_{i=1,\ldots,n}(c_1^{(i)}(sp) + l_1^{(i)}/2)$ and $b_2(sp) = \max_{i=1,\ldots,n}(c_2^{(i)}(sp) + l_2^{(i)}/2)$.

3.3. **Constraint programming.** In the following we briefly overview constraint programming and how it is applied to rectangular packing. Therefore, we study how to represent the constraints of MARPP and sketch how to solve MARPP.

3.3.1. *Overview of CP.* "Constraint programming is a powerful paradigm for solving combinatorial search problems that draws on a wide range of techniques from artificial intelligence, computer science, databases, programming languages, and operations research." (Rossi et al., 2006) From the CP viewpoint, the decision or optimization problem is to satisfy relations between variables stated in the form of constraints. "A constraint between variables expresses which combination of values for the variables are allowed." (Clautiaux et al., 2007) A multitude of different generic constraints yield a powerful, expressive and flexible modeling language. In order to reduce the search effort CP develops strong inference and propagation methods for constraints.

3.3.2. *Relevant constraints for MARPP.* The containment constraint is simply expressed as bounding constraints on domain variables for the center coordinates of the rectangles. For the non-overlapping constraint, there are the following few meta-constraint formulations:

(1) The *disjunctive* constraint is for scheduling problems and may, in general, be written disjunctive$(s|p)$, where $s = (s_1, \ldots, s_n)$ are the start times of the jobs to be scheduled, and $p = (p_1, \ldots, p_n)$ are the processing times (Hooker, 2007). The constraint is satisfied when the jobs do not overlap. *Edge-finding* is a constraint propagation technique for identifying the precedence of jobs (must be first/last) and has been applied very successfully to scheduling problems (Baptiste et al., 2001).

(2) The meta-constraint *cumulative* differs from the disjunctive constraint in that several jobs may run simultaneously but can only consume a certain amount of resource. Edge finding for disjunctive scheduling can be generalized to cumulative scheduling (Baptiste et al., 2001).
(3) The *diffn* constraint was developed in order to handle multidimensional placement problems that occur in scheduling, cutting or geometrical placement problems. Its intuitive idea is to extend the *alldifferent* constraint which works on a set of domain variables all have to be assigned with different values, to a non-overlapping constraint between a set of k-dimensional rectangles defined in an k-dimensional space. The declaration of the diffn constraint may, in general, be written

$$\text{diffn}([[O_1^{(1)}, \ldots, O_k^{(1)}, L_1^{(1)}, \ldots, L_k^{(1)}], \ldots, [O_1^{(n)}, \ldots, O_k^{(n)}, L_1^{(n)}, \ldots, L_k^{(n)}]])$$

where $O_j^{(i)}$ and $L_j^{(i)}$ are respectively the origin and the length of the k-dimensional rectangle in the j^{th} dimension $i = 1, \ldots, n,\ j = 1, \ldots, k$ (Beldiceanu and Contjean, 1994). In Beldiceanu and Carlsson (2001) propose the *sweep* algorithm as a pruning and propagation algorithm for the non-overlapping constraint of rectangles.

3.3.3. *Application to MARPP.* Rectangular packing has also been a challenge for researchers form CP and several CP approaches are proposed for problems related to MARPP. Briefly, they differ in the way they model the non-overlapping constraint, how it is propagated and how search is branched. In general, branching is either done on the alternative disjuncts of the non-overlapping constraint or done on the coordinates of the rectangles.

Beldiceanu et al. (1999) proposed a CP model for the *perfect square problem* which uses the global constraints diffn and cumulative. The perfect square problem is to pack a set of squares with given different sizes into a bigger square in such a way that no squares overlap each other, all squares borders are parallel to the border of the big square, and no area of the big square is left blank.

A constraint-based scheduling model for the *two-dimensional orthogonal packing problem* can be found in Clautiaux et al. (2007). The two-dimensional orthogonal packing problem consists in determining if a set of rectangles can be packed in a larger rectangle of fixed size. They use *energetic reasoning* together with a subset-sum propagation algorithm to effectively prune the search tree in a branch-and-bound framework.

Amossen and Pisinger (2006) proposed to solve multi-dimensional bin packing problems with guillotine constraints through a depth-first search with constructive assignment of the disjuncts of the non-overlapping constraints. During search, feasibility with respect to the guillotine constraints is maintained.

Moffitt and Pollack (2006) also applied a backtracking search for constructively assigning disjuncts of the non-overlapping constraints of MARPP. They propose several new problem-specific as well as well-known problem-independent pruning and propagation techniques in order to explore consistent solutions of a reduced search tree. In their approach, all-pair shortest path matrices for the two dimensions are maintained. During search, these matrices are efficiently used to check if an assignment of a geometric relation between rectangles is consistent with respect to other constraints.
They evaluate their approach by proving optimal solutions for packing squares of consecutive size into a container of minimal area. To our knowledge, their results are the best in terms of running time for the prove of optimality. In section 5 we compare the generated solutions of our approach to the optimal solutions proven by them.

3.4. **Nonlinear approaches.** There are also several ways to use a continuous model for packing problems. Formulating the MARPP as a non-linear problem may not seem like an obvious choice. Since the non-overlapping constraints are highly non-convex, standard gradient-based approaches likely stop in a local optimum and rarely find a good global solution (Horst and Tuy, 1996). There are several strategies to come close to the global optimum nevertheless. One is to divide the solution space in subsets and chooses representatives which are used as starting solutions. Alternatively one can also generates them randomly. However, depending on the problem the number of starting solution necessary to provide a good final solution can be very large. Further strategies can be found in (Levy and Montalvo, 1985; Ali et al., 1997; Wang and Zhang, 2007).

In the context of rectangular packing problems several approaches exists: In Zhan et al. (2006) and Ababei et al. (2005) the main issue is a floorplanning algorithm. The size of the container is fixed but beside the positioning also the sizing of the rectangles is variable within a predefined range. The algorithm consists of two stages: In the first stage a uniform distribution of the rectangles is calculated which needs not be completely feasible; in the second stage the overlapping is explicitly penalized to enforce feasibility. Since the overlapping is described by an approximation of maximum and minimum functions, a final post-processing is necessary to eliminate remaining overlaps. The main objective here is to minimize the length of wires connecting the rectangles in some predefined way.

In Birgin et al. (2006) the container is supposed to be convex but need not be box shaped. The algorithm consists of an iterative loop where in each iteration the number of rectangles is increased and the violation of the containment and non-overlapping constraints is minimized. If the violation is not close to zero the algorithm terminates. For the containment constraints it is enough to check the four corners of a rectangle, for the non-overlapping constraints a smooth approximation of the maximum function is used.

In Dorneich and Sahinidis (1995) a mixed integer non-linear programming approach is used. The shape of the rectangles can be changed to a certain amount and there are further constraints like some pairs of rectangles have to share a common border. A combination of a non-linear solver and a branch-and-bound algorithm is proposed to solve the problem.

In Herrigel and Fichtner (1989) the model also allows 90° rotations and several other objectives. However, the resulting non-linear program has a structure which is not very easy to handle. The way the non-overlapping constraints are smoothed is similar to our approach, except that the regularization parameter is constant. As a consequence, the error introduced by the regularization is not driven to zero which leaves a slight infeasibility in the end of the algorithm.

Alon and Ascher (1988) also deal with a placement problem. Here the non-overlapping constraints are enforce by lower bounds on the Euclidean distance of the rectangle's midpoints. This is a significant overestimation, however, it allows the rotation by any degree without much extra work. The main objective is again minimal length of wires and constraints are added as a penalty term.

Also related is the problem of packing circles with different or identical sizes in a rectangle as for instance in George et al. (1995). Since the non-overlapping constraints have a simple structure non-differentiable functions can be avoided.

3.5. **Remarks on the different approaches.** Naturally the question arises when which of the generic approaches, CP, metaheuristics and non-linear formulation is most appropriate.

Obviously CP is the first choice if an exact optimum is needed, the problem is highly constrained and it is hard to find a feasible solution, or the problem instance is small. It is most effective when specific properties or constraints of the problem can be efficiently used to deduce information and prune the search tree. Yet, the implementation of such propagation algorithms can be laborious. If the problem instance is large, this approach applied with a complete search is obviously inadequate.

Metaheuristics can also deal with large-scale problems. The basic algorithms are easy to adapt and implement. The main issue is to design mechanisms for intensification and diversification. When the structure of a problem is hardly known, it is rarely possible to apply metaheuristics well. However, if an encoding of a problem is well-designed, these techniques may have the ability to handle global optimization problems.

Finally, formulating a given problem using differentiable functions and solving it with methods from continuous optimization can be a very flexible approach, since changes in the objective or constraints can easily be adapted without changing the solver. For instance, it is easy to add a continuous formulation of the objective "minimize the wire length" or "make heat distribution uniform". Gradient-based methods usually improve the objective in each iteration. But then, one has to develop techniques to avoid bad local optima. Furthermore, the design of a good solver, which can deal with a large class of problem instances is an art. Often enough, it is necessary to tune the solver for a new class based on trial and error, since it is sometimes not obvious how the structure of the problem influences the behaviour of the solver.

In any case the possibilities to express a given problem in formulae making it comprehensible for computational evaluation limits the choice of methods. Yet for the MARPP we can use methods from each of the three generic approaches and compare them.

4. The novel non-linear approach

4.1. **Reformulation of the problem.** An equivalent formulation of $\mathcal{P}$ is the following:

$$(\mathcal{P}') \qquad \min b_1 b_2$$

subject to

$$\frac{1}{2}l_k^{(i)} \leq c_k^{(i)} \leq b_k - \frac{1}{2}l_k^{(i)} \text{ for } k \in \{1,2\} \text{ and } i \in \{1,\dots,n\}$$

$$\max_{k\in\{1,2\}} \left(|c_k^{(i)} - c_k^{(j)}| - \frac{1}{2}(l_k^{(i)} - l_k^{(j)}) \right) \geq 0 \text{ for } 0 < i < j \leq n \tag{3}$$

It is easy to see that (3) is just a reformulation of (2). Even though (3) avoids the disjunctions of (2) it is still non-linear, non-convex and non-differentiable. Since differentiability is an essential precondition for most NLP solvers, we approximate the constraints by differentiable functions, a procedure which is known as *smoothing* or *regularization*.

4.2. **Regularization of the problem.** Our approach is based on a variant of the Chen-Harker-Kanzow-Smale function $f(a,b) = \frac{1}{2}(a + b - \sqrt{(a-b)^2}\,)$ which is equivalent to the minimum function (Chen and Harker, 1993). The counterpart for the maximum function is $f(a,b) = \frac{1}{2}(a + b + \sqrt{(a-b)^2}\,)$. There are a few similar functions (Sun and Qi (1999), Chen et al. (2000)) which are known as non-linear complementary problem (NCP) functions[1]. As indicated by the name they are used to express the complementarity constraints which appear for instance in

[1] We do not have any evidence that one of the functions is preferable. The comparison of the numerical behaviour of different NCP functions in our context could be subject to further research.

the Karush-Kuhn-Tucker optimality conditions. For primal-dual and interior point methods these conditions arise explicitly and need to be regularized. This is usually done by inserting a regularization parameter τ in an appropriate way such that when τ goes to zero the regularized function converges to the original function (Wright, 1997; Ye, 1997; Burke and Xu, 2000).

By introducing the function $g_{l^{(1)},l^{(2)}}(x,y) := (x-y)^2 - \frac{1}{4}(l^{(1)}+l^{(2)})^2$ we get the new formulation of the non-overlapping constraints:

$$f\left(g_{l_1^{(i)},l_1^{(j)}}(c_1^{(i)},c_1^{(j)}), g_{l_2^{(i)},l_2^{(j)}}(c_2^{(i)},c_2^{(j)})\right) \geq 0 \text{ for } 0 < i < j \leq n \tag{4}$$

The regularized form[2] of the Chen-Harker-Kanzow-Smale function f is $f_\tau(a,b) := \frac{1}{2}(a+b+\sqrt{(a-b)^2+4\tau}\,)$. For $\tau > 0$, f_τ is differentiable everywhere and the regularized problem is

$(\mathcal{P}_\tau)$ min $b_1 b_2$
subject to

$$\frac{1}{2}l_k^{(i)} \leq c_k^{(i)} \leq b_k - \frac{1}{2}l_k^{(i)} \text{ for } k \in \{1,2\} \text{ and } i \in \{1,\ldots,n\} \tag{5}$$

$$f_\tau\left(g_{l_1^{(i)},l_1^{(j)}}(c_1^{(i)},c_1^{(j)}), g_{l_2^{(i)},l_2^{(j)}}(c_2^{(i)},c_2^{(j)})\right) \geq 0 \text{ for } 0 < i < j \leq n \tag{6}$$

Note that $f_0 \equiv f \equiv \max$ and $f_\tau(a,b) \geq f(a,b)$. Therefore, the set of feasible solutions of $(\mathcal{P})$ is contained in the one for $(\mathcal{P}_\tau)$. That means that replacing the condition (4) by (6) causes not only a smoothing but also a relaxation of the problem. The relaxation has a specific interpretation: Depending on the size of τ condition (6) allows partially overlapping or even containment of the rectangles. In the context of the global optimization problem this can be used to get away from local minima. The effect of this mechanism is illustrated in figure 3 in section 5.1. Winterfeld (2007) describes an analog observation in the context of semi-infinite programming.

4.3. **Analysis of the tunneling effect.** In order to give a proper analysis of the effect caused by the relaxation we need a stricter notion of the overlapping. To ease the presentation we restrict ourselves now to squares, i.e. we assume $l_1^{(i)} = l_2^{(i)}$ and omit the subscript. In this way, we can concentrate on the main idea without having to take care of several sub-cases.

Definition 4.1. Given two squares with midpoints $c,\ e \in \mathbb{R}^2$ and side lengths $l^{(1)}$, $l^{(2)}$, respectively. The *degree of overlapping* is given by $d(c,e) = \max\{0, \frac{1}{2}(l^{(1)}+l^{(2)}) - \max_{k\in\{1,2\}}\{|\ c_k - e_k\ |\}\}$.

Note that $d(c,e) > 0$ if and only if the corresponding squares overlap, i.e. the interior of their intersection is non-empty. Furthermore, $d(c,e) \leq \frac{1}{2}(l^{(1)}+l^{(2)})$ and equality holds when the midpoints coincide. In figure 1 the degree of overlapping is indicated by o.

Lemma 4.2. *Given two squares with side lengths $l^{(1)}$ and $l^{(2)}$. For $r := \frac{1}{2}(l^{(1)}+l^{(2)})$, any $o \in [0,r]$ and $\tau_0 := (2ro - o^2)r^2$ equation (6) guarantees a degree of overlapping smaller or equal than o.*

Proof. Assume that the midpoints c and e of the two squares have a distance of δ_1 and δ_2 in the corresponding dimension and $d(c,e) > o$. Furthermore without loss

[2]Often also stated as $f_\tau(a,b) := \frac{1}{2}(a+b+\sqrt{(a-b)^2+4\tau^2}\,)$

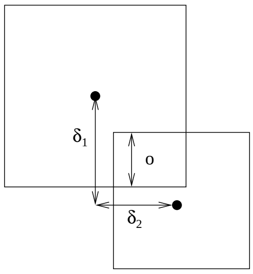


FIGURE 1. Illustration of the meaning of the variables

of generality $\delta_1 \geq \delta_2$. Then $\delta_1 < r - o$, $g_r(c_k, e_k) = \delta_k^2 - r^2$ for $k \in \{1, 2\}$ and we have

$$\begin{aligned} f_{\tau_0}(g_r(c_1,e_1), g_r(c_2,e_2)) &= \frac{1}{2}\left(\delta_1^2 - r^2 + \delta_2^2 - r^2 + \sqrt{(\delta_1^2 - \delta_2^2)^2 + 4(2ro - o^2)r^2}\right) \\ &\leq -r^2 + \frac{1}{2}\left(\delta_1^2 + \sqrt{\delta_2^4 + 4(2ro - o^2)r^2}\right) \\ &< -r^2 + \frac{1}{2}\left((r-o)^2 + \sqrt{(r-o)^4 + 8r^3o - 4r^2o^2}\right) \\ &= -r^2 + \frac{1}{2}\left(r^2 - 2ro + o^2 + \sqrt{(-r^2 - 2ro + o^2)^2}\right) \\ &= 0 \text{ using that } -r^2 - 2ro + o^2 \leq 0 \end{aligned}$$

which contradicts equation (6). □

Corollary 4.3. *For the setup of Lemma 4.2 and given $\tau \in [0, r^4]$ the equation (6) guarantees a degree of overlapping smaller or equal than $r - \sqrt{r^2 - \frac{\tau}{r^2}}$.*

Corollary 4.4. *There exists a τ such that the relaxed problem holds if and only if the containment constraints are fulfilled.*

The above statements show how to control the maximal overlapping for a given pair of rectangles explicitly. However, this depends also on the specific sizes of the two rectangles.

4.4. **The novel algorithm.** The algorithm consists of three nested loops. In the outer loop we determine the starting solution and in the middle loop an initial τ is fixed. The inner loop is within the regularized NLP solver, there the actual problem is solved.

Algorithm 2 Pseudo code of the novel algorithm

```
for i := 1 to n_1 do
  Initialize random starting solution
  for j := 1 to n_2 do
    Initialize τ_1^(j)
    Run regularized NLP solver
    if no significant improvement was achieved then
      leave inner loop
    end if
  end for
end for
```

4.4.1. *The regularized NLP solver.* The non-linear solver used here is based on penalty successive linear programming (PSLP, Zhang et al. (1985)) extended by a strategy to reduce the regularization parameter τ to zero[3]. The essential ingredients of PSLP are:

- The non-linear constraints are handled as a penalty term for the objective (multiplied by a penalty factor μ).
- In each iteration the new interim solution is calculated by solving a linearization of the problem at the current solution within a trust region.
- The trust region is adapted depending on the ratio of the improvement of the objectives of the linearized model and of the non-linear model. If the ratio is close to one, the trust region size is increased. If it is not too far from zero the trust region size is decreased. If it is nearly zero or negative, the interim solution is rejected and the current iteration is repeated with a smaller trust region.
- The stopping criterion is that the gradient of the penalized objective is close to zero and there is no change in the objective value.

If the initial solution is feasible and μ is chosen large enough, this algorithm terminates with a Karush-Kuhn-Tucker point which is usually a local optimum.

For the extension to handle the regularization, τ is considered as another variable with a separate kind of trust region. τ also appears as an additional term in the extended objective weighted by a factor. In this way, it is automatically driven to zero during the iterations.

4.4.2. *The starting solution.* The quality of the final solution depends significantly on the starting solution. Yet, the dependency seems to be arbitrary. We cannot expect to find starting solutions in a general way such that our algorithm always converges to a final solution close to a global optimum.

Therefore, we did not use sophisticated heuristics, but rather arranged the rectangles in such a way that the lower right corner of the i-th box touches the upper right corner of the $i+1$-th box. The order of the rectangles is subject to randomization. In the first iterations of the inner loop the rectangles are pushed together without any bias to a particular arrangement, which is a necessary requirement for good starting solutions.

It is worth noting that the starting solution need not be feasible for $\mathcal{P}$ but only for $\mathcal{P}_{\tau_1^{(0)}}$. If $\tau_0^{(1)}$ is chosen large enough, one could even put all rectangles on top of each other.

4.4.3. *The choice of parameters of the regularized NLP solver.* The behaviour of the solver depends on the values of a few parameters. Those which proved to be most influential are:

- $\tau_1^{(1)}$
- α which determines the adaptation of τ: $\tau_1^{(j+1)} = \alpha\tau_1^{(j)}$
- The penalty factor μ

Since the behaviour of the problem changes depending on the size of the problem instance, we did not expect to find values for this parameters which suits all problem instances equally well. Instead, we used an evolutionary algorithm (Hanne, 2007) to determine the values for several sizes of problem instances. The results are shown in table 2.

[3]In our implementation this means actually $\tau < 10^{-6}$

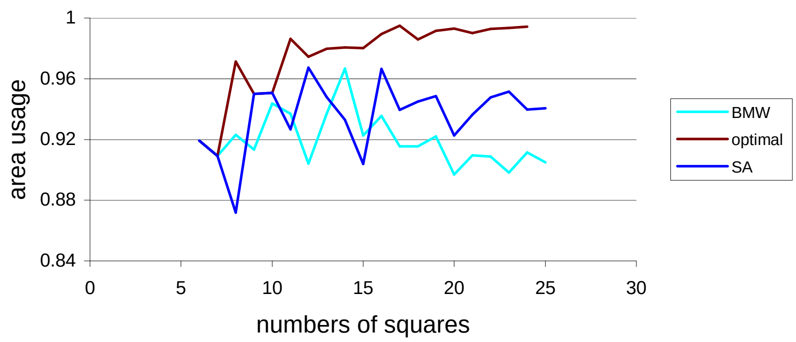


FIGURE 2. Comparison of the three different methods.

5. NUMERICAL RESULTS

To enable the comparison with an optimal solution we used the same problem setup as Moffitt and Pollack (2006), that is, n squares of consecutive sizes.

For our algorithm refered to as BMW the runtimes are the needed CPU times in seconds which are more reliable than the time span from start to termination. The actually elapsed time was a fraction of it since the calculations for different starting solutions were done in parallel. For the SA algorithm which was not parallelized the ellapsed time was measured. Table 1 shows the different parameter configurations

Variant	# starting solutions	$\tau_1^{(1)}$	α	μ
A	128	372	0.48	240835
B	128	394	0.68	76827
C	32	380	0.63	46084
D	16	270	0.77	100000

TABLE 1. Choice of parameters for table 2

used for our approach. The corresponding results for different problem instance sizes are given in table 2.

Variant	# squares	best area	average area	usage	runtime
A	15	1344	1495	0.92	257
B	15	1350	1478	0.92	239
C	15	1363	1489	0.91	88.0
D	15	1363	1475	0.91	40.0
A	25	6106	6621	0.90	$1.29 \cdot 10^3$
B	25	6138	6561	0.90	$1.27 \cdot 10^3$
C	25	6084	6565	0.91	427
D	25	6203	6518	0.89	255
A	100	398750	689093	0.85	$2.13 \cdot 10^5$
B	100	385541	1028145	0.88	$2.86 \cdot 10^5$
C	100	386640	426158	0.87	$8.15 \cdot 10^4$
D	100	396500	674944	0.85	$5.43 \cdot 10^4$
A	150	1444114	4708489	0.79	$7.08 \cdot 10^5$
C	150	1390212	6399340	0.88	$3.08 \cdot 10^4$

TABLE 2. Comparison for different choices of parameters

In Figure 2 the optimal values taken from Moffitt and Pollack (2006), the SA implementation and our approach are compared. Here we used variant A as parameter configuration. For larger problem instances table 3 presents results using

# squares	area SA	usage SA	time SA	area BMW	usage BMW	time BMW
10	408	0.944	1.71	425	0.906	25.6
25	5772	0.957	11.9	6084	0.908	266
50	45045	0.953	31.3	48585	0.884	$3.60 \cdot 10^3$
75	149946	0.957	86.9	163710	0.876	$2.22 \cdot 10^4$
100	356136	0.950	193	386640	0.875	$8.15 \cdot 10^4$
125	690336	0.954	489	755094	0.873	$1.76 \cdot 10^5$
150	1193865	0.952	588	1390212	0.817	$3.08 \cdot 10^5$

TABLE 3. Results for larger number of squares

variant C. To our knowledge, optimal solutions are not available for these cases.

The SA implementation proved to be less sensitive regarding the choice of the starting solution and of the moves. Different runs did not yield significant differences in the quality of the solutions. Therefore, we abstained from presenting different results for this method.

For problem instances with up to 19 squares the BMW algorithm yields results of similar quality as SA, even though it needs more time. For larger instances the outcome is not as good any more. As table 1 indicates, the critical point is the number of starting solutions. A possibility to allow more starting solution by decreasing the runtime is shown in section 6.

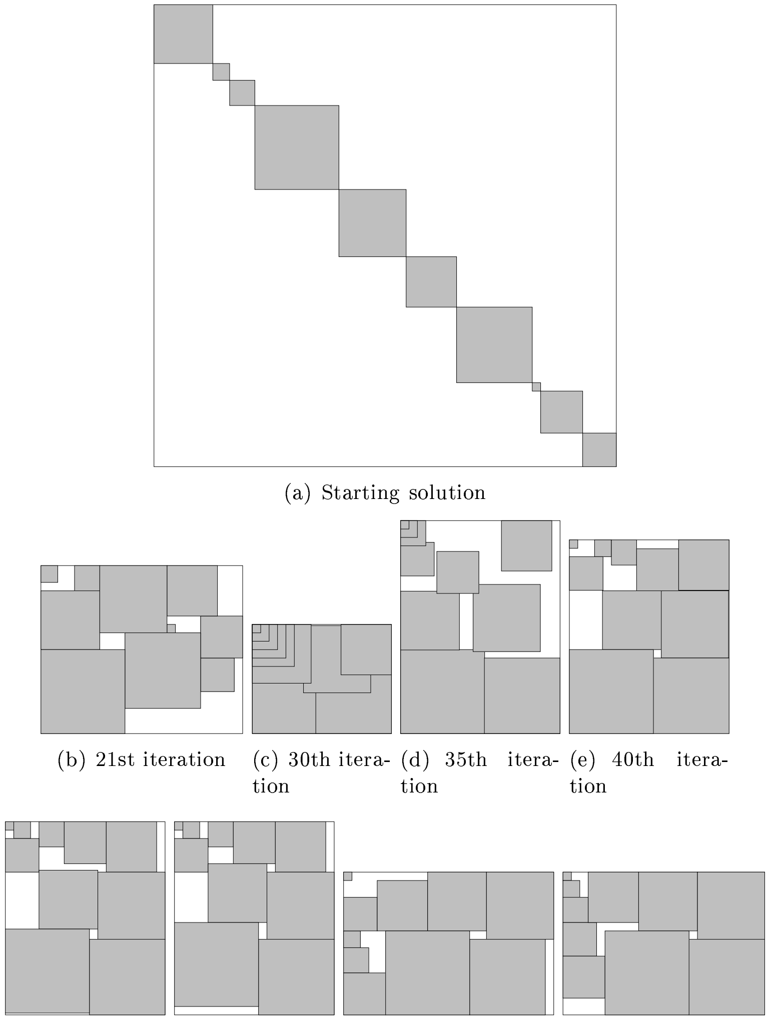
We tried to adapt τ for each non-overlapping constraint in such a way that the degree of overlapping is bounded from above. For this we used $\max\{\tau, \tau_{i,j}\}$ instead of τ where $\tau_{i,j}$ is given for each pair of rectangles (r_i, r_j). Thus, complete containments like in figure 3(d) are avoided. However, our tests did not show any significant improvement.

In contrast to other non-linear approaches the final solution is a feasible one and no further post-processing is necessary. This is an highly desirable property as we do not need a second model which focuses on feasibility and may have to deteriorate the objective function value.

The choice of parameters effects the runtime and the quality of the solution. The influence of most of the parameters on that two properties of the optimization is unapparent. However, for the most essential parameter, the number of starting solutions, the following is observed: The larger the number of starting solutions, the longer takes the algorithm but the better is the resulting final solution.

Besides the specific choices of the parameters, our algorithm is not restricted to the characteristics of MARPP. Even though the result are not better than what we get from SA, the great strength of our approach is its expressiveness and extensibility. As far as the runtime is concerned, the possibilities for improvement are not exhausted:

- For large problem instances most of the non-overlapping constraints are not active. Therefore, if such non-overlapping constraints for rectangles that are far apart are ignored, the number of constraints is significantly reduced without risking infeasibility. However, the "being-far-apart-property" has to be rechecked by the algorithm from time to time. The trust region size can be a good indicator when to recheck this property. This *ϵ-active set strategy* certainly leads to a improvement of the runtime, since the size of the non-linear program is considerably reduced.



(a) Starting solution

(b) 21st iteration (c) 30th iteration (d) 35th iteration (e) 40th iteration

(f) 77th iteration (g) 80th iteration (h) 106th iteration (i) final solution after 132 iterations

FIGURE 3. Selected iterations of one optimization run with ten squares.

- One could use different τ for each non-overlapping constraint. Since for a given τ the degree of overlapping depends on the sizes of the rectangles the effect of τ is different for each such constraint.
- The way τ is reduced within the regularized NLP solver can be designed more adaptively. Especially the speed of reduction seems to have some influence on the solution finally found. Alternatively, one could also add the condition $\tau = 0$ to the set of constraints and start with a solution which is infeasible with respect to this condition.

5.1. **Detailed study of the behaviour of the BMW Algorithm.** Figure 3 demonstrates how the outer loop of the algorithm works. Starting from the initial solution a local optimum is reached quickly which cannot be improved directly. When the NLP solver is restarted and the non-overlapping constraints are relaxed, situations like in figure 3(c) occur. The relative positions of the larger squares are maintained but for the smaller squares the relaxation is so strong that the non-overlapping constraints are completely suppressed. When the allowed relaxation is reduced, overlaps of squares disappear as it can be seen in figures 3(d) and 3(e). Then, another local optimum is reached in 3(g) and the relaxation yields a change in the relative positions of the squares. This change leads to a reduced objective value. This behaviour reoccurs twice until the last relaxation does no longer yield an improvement and the algorithm terminates.

The figures show that some squares moved to the left upper corner. This phenomenon is not related to any change in the objective. It is caused by the underlying non-linear solver and cannot be controlled directly. This is undesirable since it gives the solution some bias. Since there is no influence in the objective one way to eliminate this property is to change the non-linear solver. Alternatively, a bound on the maximal degree of overlapping can prevent this phenomenon.

5.2. **Similarities between the BMW algorithm and SA.** Using SA for global optimization of a continuous function is not a new idea (Ali et al., 1997). Recently, Wang and Zhang (2007) explicitly combined SA with a gradient-based optimization method. Interesting in our approach is that aspects from SA appear naturally through the formulation of the problem in two different perspectives.

The regularized NLP solver is analogous to SA if we consider the regularization parameter τ as the temperature and the infeasibility as the energy configuration.

A low energy configuration is achieved when no rectangles overlap and is enforced for $\tau = 0$. By corollary 4.3 we can interpret the reduction of τ as cooling the system, since we reduce the allowed degree of overlapping. The difference to SA is that a worse state is not accepted according to a probability function. Rather any improvement of the actual objective, the area of the bounding box, is accepted which does not violate the limit of overlapping determined by τ. In practice it turns out that in each iteration the current solutions achieve the maximal degree of non-overlapping allowed by the current value of τ.

Also the middle loop has a similar interpretation. Again we can consider τ as the temperature. Now, the inner loop can be seen as a move which changes the current solution. The degree of the change is determined by τ, with which the regularized NLP solver is initialized. However, so far this analogy is not carried out completely. The middle loop does not stop when τ is small enough but when no further improvements were achieved. Also, deteriorations are not accepted in any case. However, the algorithm can easily be adapted to represent this strategy.

Putting both loops together one can consider the outer loop as a kind of reheating, which is an idea well known for SA (Kolonko, 1999; Anagnostopoulos et al., 2006).

6. Conclusion and future research

We presented a novel approach to solve the MARPP based on a continuous model and a regularization of the maximum function. We compared our approach with SA and it turned out that it is competitive, even though the improvement of the performance of the solver remains an issue. The special features of this algorithm are that it always provides a feasible solution and the tunneling effect. This technique uses the relaxation of the non-overlapping constraints to excape from local optima and shows similarities to metaheuristic concepts. Finally, the major strength of our model is that it can be easily extended with other continuous objectives and constraints. Such extensions may expecially benefit from the tunneling effect. For instance, when minimizing the length of wires the gradient of the objective yields more information. These are useful in particular when the relaxation causes a large degree of freedom.

Another interesting topic is to exchange the underlying NLP solver. Alternatives to PSLP may be sequential quadratic programming, other Newton-like methods or interior point algorithms.

Furthermore, one could make use of the possibilities offered by the non-linear, continuous formulation of the problem. For example, in microelectronics, the rectangles correspond to modules which are interconnected by wires in a predefined way and one important goal is to keep the length of the wire as short as possible. This leads intuitively to a continuous objective function.

Extending this approach to three (or higher) dimensions may be interesting. The main issue for this is that instead of smoothing something like $\max\{a(x), b(x)\}$ one has to consider $\max\{a(x), b(x), c(x)\}$. To do so, another regularization function is needed which probably behaves numerically slightly worse. However, the underlying algorithm stays the same, whereas SA or CP approaches have to deal with a significantly higher combinatorial complexity.

Hybridization of our approach with other approaches like SA or CP might yield improvements. They could complement each other in a framework which unifies the robust sampling of the solution space from metaheuristics, the strong propagation mechanisms from CP and the flexible relaxation from global non-linear optimization. For example, considering simulated annealing one could switch between SA moves and iterations of the NLP solver as described in Wang and Zhang (2007). Also, it should be possible to use CP with its strong methods to investigate arrangements of a subset of the rectangles on which additional constraints are imposed. When dealing with CP applied in a complete search one can use the NLP solver to get upper bounds for the problem and propagate this information during search.

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