

Some applications of global optimization and semi-on-line bin packing

”Theses of PhD Dissertation”

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Introduction

The present dissertation contains some results in the field of applications of global optimization and some on semi on-line bin packing. The four sections of this dissertation can be summarized in the following.

In Section 1 a computational approach of global optimization on Stiefel-manifolds is investigated, based on the papers [2, 5, 6, 10]. The optimization on Stiefel manifolds was discussed by Rapcsák in earlier papers. Here, some methods of global optimization are dealt with and tested on Stiefel manifolds. The structure of the optimizer points of a quadratic problem is studied for the lowest interesting dimensional case, as well as the criterion for the finiteness of the number of optimizer points. Then possible reduction tricks are examined together with a numerical study obtained by the application of global optimization tools. As the main result of the section test functions are given with known global optimum points and their optimal function values and a restriction, which leads to a discretization of the problem, which results in a problem equivalent to the well-known assignment problem.

Section 2 dealt with a stochastic global optimization algorithm, called CRS (Controlled Random Search), which originally was devised as a sequential algorithm. Our work [35] was intended to analyze the degree of parallelism that can be introduced into CRS and to propose a new refined parallel CRS algorithm (RPCRS). As a first stage, evaluations of RPCRS were carried out by simulating parallel implementations. The degree of parallelism of RPCRS is controlled by a user given parameter whose value must be tuned to the size of the parallel computer system. It is shown that the greater the degree of parallelism the better the performance of the sequential and parallel executions.

In Section 3 we applied a stochastic clustering optimization method, called GLOBAL to phase stability analysis [7, 8]. Phase stability analysis is of fundamental importance in various chemical engineering applications. Phase stability is often tested using the tangent plane criterion and a practical implementation of this criterion is to minimize the tangent plane distance function (TPDF), defined as the vertical distance between the molar Gibbs energy surface and the tangent plane for the given phase composition. In the present work we used a modified TPDF and an equation of state as the thermodynamic model. We tested the efficiency and reliability of the advocated stochastic sampling and clustering method on some benchmark problems of the related literature, tuning some parameters of the original method for this.

In Section 4 new lower and upper bounds for semi-on-line bin packing problems are given, describing the results of the papers [3, 4, 9]. Semi-on-line algorithms for the bin-packing problem allow, in contrast to pure on-line algorithms, to execute one of certain types of additional operations in each step as repacking, reordering or buffering some elements before packing them. In 1996 Ivkovič and Lloyd gave the lower bound $\frac{4}{3}$ on the asymptotic worst-case ratio for the so-called fully dynamic bin packing algorithms, where the number of repackable items in each step is restricted by a constant. We improved this result to about 1.3871. We presented our proof for a semi-on-line case of the classical bin packing, but it works for fully dynamic bin packing as well. We proved the lower bound by analyzing and solving a specific optimization problem. The bound can be expressed exactly using Lambert's W function. Some lower bound results for the special case of the problem are given as well. After this, some new upper bounds are given; we defined and analyzed a "c-repacking" semi-on-line algorithm for this semi-on-line case of the classical one-dimensional bin packing problem, where in each step it is allowed to repack at most c elements, for some positive integer c .

In the following we describe the results of the sections of the dissertation in details.

1 Some global optimization problems on Stiefel-manifolds

Optimization on Stiefel manifolds was discussed by Rapcsák in earlier papers. Here some global optimization methods were considered and tested on Stiefel manifolds. Test functions with known global optimizer points and the solution of a discretization of the problem are also given.

In 1935, Stiefel introduced a differentiable manifold consisting of all the orthonormal vector systems $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k \in \mathbb{R}^n$, where \mathbb{R}^n is the n -dimensional Euclidean space and $k \leq n$ [49]. Bolla et al. analyzed the maximization of sums of heterogeneous quadratic functions on Stiefel manifolds based on matrix theory and gave the first-order and second-order necessary optimality conditions and a globally convergent algorithm [14]. Rapcsák introduced a new coordinate representation and reformed the original one to a smooth nonlinear optimization problem. Then, by using Riemannian geometry and the global Lagrange multiplier rule [41, 42, 43], local and global, first-order and second-order necessary and sufficient optimality conditions were stated and a globally convergent class of nonlinear

optimization methods was suggested.

In the dissertation, some special global optimization problems on Stiefel manifolds are investigated and test functions are given for the global optimization tools. Consider the following optimization problem:

$$\min \sum_{i=1}^k \mathbf{x}_i^T A_i \mathbf{x}_i \quad (1)$$

$$\begin{aligned} \mathbf{x}_i^T \mathbf{x}_j &= \delta_{ij}, & 1 \leq i, j \leq k, \\ \mathbf{x}_i &\in \mathbb{R}^n, & i = 1, \dots, k, \quad n \geq 2, \end{aligned} \quad (2)$$

where A_i , $i = 1, \dots, k$, are symmetric matrices and δ_{ij} is the Kronecker delta. Furthermore, let $M_{n,k}$ denote the Stiefel manifold consisting of all the orthonormal systems of k vectors in the n -dimensional Euclidean space. Hence, we deal with the optimization of a special type of quadratic functions subject to quadratic constraints. In the literature of optimization, not too many efficient methods giving a good approximate solution of this problem are known. It is also difficult to provide feasible solutions for it [31]. This is the reason why special instances of the original problem are investigated.

First, we gave the solution of problem (1)-(2) on $M_{2,2}$ and a criterion for the finiteness of the number of the optimum points in this lowest-dimensional interesting case. In the case of diagonal matrices A_i , $i = 1, \dots, k$, all coordinates of the optimum points are from the set $\{0, +1, -1\}$, (except the extreme case when all feasible points are optimum points, as well). An interesting question is how we might find the criterion for the finiteness of the number of optimizer points on $M_{n,k}$.

In Section 1.3, based on the results of the paper [10] some global optimization tools are applied to the numerical optimization of problem (1)-(2). Some reduction steps and numerical results are presented here. To illustrate them, a numerical study was attached. We studied problem (1)-(2) numerically by using a stochastic method [18] and a reliable procedure [17, 33]. The aim of the application of the last one, the GlobSol program was to obtain verified solutions. It is worth mentioning that the GlobSol software provided verified solutions only by using spherical substitutions. Without transformations like these, it has been demonstrated earlier that a simple (9-variable) problem on $M_{3,3}$ runs for more than 3 days on an average computer if we require reliable results. That is why the possible speed up improvements should be theoretically investigated both in geometrical reductions and in numerical tools. Hence, appropriate testing examples should be necessary.

Since the results can easily be non optimal as it was seen, in Section 1.3 (which based on the paper [5]), a series of test problems of arbitrary size (with n and k as parameters) are defined for the above problem. The global optimum points of the test functions and their optimal function values are known. These problems make the testing of efficiency of existing algorithms feasible; hence to define test problems belongs to an important area of global optimization (see [22] and [23]). In the provided test functions the number of optimum points is finite, although it is exponential in the size of the input.

Furthermore, a restriction, which leads to a discretization of the problem is suggested, which results in a problem equivalent to the well-known assignment problem. This special discretization of problem (1)-(2) was also considered in [5].

2 A parallelized random search global optimization algorithm

Two general models of global optimization methods exist: deterministic methods which require a certain mathematical structure and stochastic methods which are based on the random generation of feasible trial points and nonlinear local optimization procedures. A profound discussion on the classification of methods can be found in Törn and Žilinskas [51] and for a complete and rigorous mathematical description of global optimization methods, both deterministic and stochastic approaches, one may consult the Handbook of Global Optimization [31].

Roughly speaking, it could be said that deterministic methods may be more efficient than the stochastic ones, when an analytical expression of f , its derivatives, bounds and useful properties are available. However, when f is a black-box function deterministic methods cannot be applied. In contrast, stochastic methods do not require any specific structure of f , only a computational procedure to obtain the value of the function at any location of the searching domain is needed. So, most optimization problems can be solved by stochastic global optimization techniques.

For computationally expensive functions, stochastic global optimization methods have shown to be very useful because of, compared to deterministic methods, fewer function evaluations are needed to obtain the solution of their global optimization problem. In addition, stochastic methods can be applied to problems where the objective function is not differentiable or not continuous, and only a tool for evaluating the function at any

location is required.

For most of the functions, global optimization is a NP hard problem. For this reason, the global optimization problem is a suitable candidate for the use of supercomputers, mainly for those functions whose evaluation is computationally expensive.

Section 2 only dealt with a stochastic global optimization algorithm called CRS and a new parallel version of CRS. CRS (Controlled Random Search) algorithm was introduced by Price [36, 37, 38]. It is based on clustering techniques and has proved to be very reliable and computationally inexpensive. The aim of this work was to describe and evaluate a parallel algorithm, called RPCRS, which is based on the CRS algorithm. Some parallel approaches of the original CRS algorithm have been proposed and evaluated using several models of parallel computers and strategies [21, 25, 27, 34, 39, 50, 54]. In [26] a parallel version of CRS (PCRS) was proposed and applied to efficiently solve a global optimization problem coming from the image processing field, whose objective function were computationally very expensive. RPCRS is a refined version of PCRS.

Our proposal only makes small modifications to the original sequential version of CRS. These modifications are aimed at increasing the degree of parallelism of CRS by creating a pile of work to feed the set of processors of a parallel computer. RPCRS allows to evaluate the objective function at several trial points, simultaneously. Nevertheless, the general strategy used in CRS remains in our parallel version.

The RPCRS algorithm was originally devised to be executed on parallel multicomputer system, but it is also shown that RPCRS outperforms CRS even when it is run on a single processor system. Our study only covers analysis of the speed up of RPCRS as compared to the original sequential CRS algorithm. Our analysis is only based on empirical results obtained from experimental executions. Although a wide set of standard test functions was used to validate our results, this work does not provide any theoretical support to demonstrate that the same results can be obtained using other functions.

Two different kinds of experiments were carried out for analyzing the speed up of RPCRS: those oriented to highlight advantages of its parallel nature and those intended to show its capability for being executed on a parallel computer system. In Section 2.2. the CRS algorithm and its parallel version RPCRS is described. Section 2.3. is devoted to show experimental results intended to evaluate the speed up of RPCRS compared to CRS, as a function of a control parameter which determines the degree of parallelism. Finally, in Section 2.4. numerical results of parallel exe-

cutions of RPCRS is shown, performed on a CRAY T3D using up to 16 processor elements.

3 Application of a stochastic method to the solution of the phase stability problem

Section 3 advocates a stochastic global optimization technique for the solution of the phase stability problem. The method proved to be capable to solve small to moderate size problems in an efficient and reliable way, and does not require a priori knowledge of the location of the possible solutions.

Phase equilibrium calculations and phase stability analysis are of fundamental importance in various chemical engineering applications, such as azeotropic and three-phase distillation, supercritical extraction, petroleum and reservoir engineering, etc. Phase stability is often tested using the tangent plane criterion, and a practical implementation of this criterion is to minimize the tangent plane distance function (TPDF), defined as the vertical distance between the molar Gibbs energy surface and the tangent plane for given phase composition.

The problem is normally solved either by finding all stationary points of the TPDF or by finding the global minimum. Because the TPDF is a highly non-linear and complex expression, global optimization methods are required for its minimization. Use of global techniques is relatively unexplored in this area of computation. The majority of the research papers discussing the numerical solution of the determination of phase stability has been critically reviewed Wakeham and Stateva in their comprehensive review [53].

Stochastic optimization techniques have often been found to be as powerful and effective as deterministic methods in many engineering applications. They require only the objective function values and are highly likely to locate the global minimum. In the present work we used a modified TPDF [46, 47, 48] and an equation of state [45] as the thermodynamic model. We advocated [7, 8] a stochastic sampling and clustering method [13, 18] to locate the minima of the TPDF.

The robustness and efficiency of our method is demonstrated by two systems only taken from the literature, namely the hydrogen sulfide + methane system, and the nitrogen + ethane + propane system. We have chosen these particular examples because it illustrates that the stability problem can be quite difficult even for very small systems and because it

provides grounds for a comparison on the basis of the found roots between our algorithm and other algorithms [1,4-7,10]. However, we would like to emphasize that a direct comparison with global optimization methods [4-6] regarding computational cost requirements cannot and will not be made. Thus, we gave the number of function evaluations and CPU time required to find all roots for a given feed composition as an information rather than as a basis for comparison. The reliability of GLOBAL expressed as the percentages of independent runs that could locate all the global minimum points can easily be tuned by the algorithm parameters.

As pointed out in the dissertation, in order to improve the efficiency and reliability of our algorithm we have changed some parameters of the global program, recommended in [16].

The method is user-friendly and not computationally demanding regarding the number of function-evaluations and CPU time.

4 Bounds for semi-on-line bin packing problems

The classical one-dimensional bin packing problem is among the most frequently studied combinatorial optimization problems. In its traditional definition a list $L = \{x_1, x_2, \dots, x_n\}$ of elements (also called items) with sizes in the interval $(0, 1]$ and an infinite list of unit capacity bins are given. Each element x_i from the list L has to be assigned to a unique bin such that the sum of the sizes of the elements in a bin does not exceed the bin capacity. The size of an element is also denoted by x_i . The *bin packing problem* consists of packing the items to the bins in such a way that as few bins as possible are used.

It is well-known that finding an optimal packing is *NP-hard* [28]. Consequently, a large number of papers have been published which look for polynomial time algorithms that find feasible solutions with an acceptable approximation quality.

For measuring the efficiency of algorithms there are two general methods: the investigation of the worst-case behavior or – assuming some probability distribution of the elements – a probabilistic analysis. In this dissertation we concentrated on the asymptotic worst-case ratio of an algorithm. For a given list L , denoted by $A(L)$ and $OPT(L)$ the number of bins used by algorithm A and the number of bins used in an optimal packing, re-

spectively. Then the *asymptotic worst-case ratio* (*AWR*) of algorithm A is

$$R_A := \limsup_{l \rightarrow \infty} \left\{ \max_L \left\{ \frac{A(L)}{l} \mid OPT(L) = l \right\} \right\}.$$

In the dissertation we dealt with semi-on-line (SOL) bin packing problems. The so called *semi-on-line algorithms* [15, 19] are between the well-known on-line and off-line ones. For such algorithms at least one of the following operations is allowed: repacking of some items [24, 32], lookahead of the next several elements [29], or some kind of preordering.

To discuss the considered subclasses of semi-on-line bin packing, we need to introduce the role of the "scheduler" and the role of the "packer". The role of the scheduler is to produce the input list, while the role of the packer is to pack the items (that is, to realize the packing algorithm).

In the above mentioned problem classes the rule of the scheduler is trivial: to give the elements one by one (let say this is the Insert operation) and to mark the end of the (whole) list.

In *batched bin packing* (BBP) problems (see [30]) the scheduler splits the input list into a number of batches. In every step the scheduler either gives a new element, or marks the end of the current batch. The algorithm has to pack each batch as an offline one (that is, a lookahead is possible within the current batch). However, batches have to be packed in an on-line manner: during the packing of a new batch the elements of the earlier batches can not be moved. In other words, lookahead is not allowed outside the current batch.

Another special variant of bin packing, the *dynamic bin packing* problem is defined in [16]. In this case, one of the following two possibilities is allowed for the scheduler in each step: giving a new element (Insert operation) or deleting an earlier given element (Delete operation). In this version the number of bins used by the algorithm is defined as the maximum number of non-empty bins used at any step of the packing procedure.

A special case of the dynamic bin packing problem is the so-called *fully dynamic bin packing* (FDBP, [24]) problem. The difference from the dynamic bin packing problem is that the packer is allowed to perform repacking. If the repacking is restricted, i.e. in every step the packer can repack at most c number of elements, then we speak about a *c-repacking fully dynamic bin packing problem* (*c-repacking FDBP*).

The classical on-line bin packing can be also relaxed by allowing the repacking of at most c elements in each step. This version of the problem is called *c-repacking semi-on-line bin packing* (*c-repacking SOL*). Obviously, the case $c = 0$ gives back the pure on-line bin packing problem.

In Section 4.2. we improved the lower bound to 1.3871 for the c -repacking SOL algorithms, but it follows from the construction that this lower bound is also valid for c -repacking fully-dynamic bin-packing algorithms. The results obtained are valid for every c . During our analysis we used different instruments: LP-techniques were combined with results from linear algebra, and finally a non-linear optimization problem was solved.

In Section 4.3 we investigated a special case of the c -repacking SOL bin packing problem, where the number of different element sizes is bounded by p ($p \geq 0$ fixed integer). This means that the scheduler can give at most p different element sizes in the list; however, the number of elements with a specific size is not bounded.

In Section 4.3 we first showed that our construction generalizes the construction of [32]. It is the particular case of $p = 2$. After that, we showed that for any fix p value we can also generalize the construction of [30] and with this new lower bounds can be derived for the c -repacking SOL problem for every different p values. Note that the construction in [30] was similar, but the main point is different: they used only equidistant element sizes, while we can consider any (not only equidistant) point system for this. Although we dealt with this special version of the c -repacking SOL bin packing problem, it was also pointed out that our construction can be used for deriving the same lower bound for the c -repacking FDBP with at most p number of different element sizes.

The improved lower bounds are obtained by solving the special cases of the nonlinear optimization problem, derived in Section 4.2. This nonlinear optimization problem is particularly interesting, because their solutions answer some questions raised in [30] for the two batched bin packing problem (2 -BBP). In [30] it was shown that the lower bound given there is the best possible for the case of $p = 2$, but it was not clear whether the bounds given for the cases $p \geq 3$ are the best possible bounds. With our improved bounds we disprove the conjecture regarding the optimality of those earlier bounds.

It is proved that the above mentioned lower bounds are valid in every d dimension.

In Section 4.4 we examined a family of c -repacking semi-on-line algorithms. It is clear that these types of algorithms are only worthwhile to be considered, if they perform better than pure on-line algorithms. We proved that the asymptotic worst-case ratio for a given c is not larger than $\frac{3}{2} + \frac{b_c}{1-b_c}$ where b_c is in the interval $(0, \frac{1}{6c})$. So, with increasing values of c the asymptotic competitive ratio of our algorithm quickly converges to $\frac{3}{2}$.

Our algorithms improve on-line results already for small c values. Of particular interest are two cases.

- In case $c = 2$, for the *HFR-2* algorithm $AWR(HFR-2) = 1.5728\dots$ holds, which is better than the asymptotic ratio $1.58889\dots$ of the best known on-line algorithm [44].
- In case $c = 4$, $AWR(HFR-4) = 1.5389\dots$, which is smaller than the best known lower bound $1.5401\dots$ for on-line algorithms published in [52].

This shows that our algorithm is capable of exploiting the additional flexibility gained by the possibility of repacking elements. Our algorithm does not improve the bound of the best known online algorithm of Seiden [44] for $c = 1$, but it can be mentioned that in this case our simple algorithm uses only 6 bin classes, while the very sophisticated Harmonic++ of [44] uses a complicated interval-structure: around 70 subclasses.

5 Summary

Subsequently the summary of the results of the dissertation is given, in order by sections:

1. The dissertation discussed a computational approach for an optimization problem defined on Stiefel manifolds. Some supports of this are provided, special cases of the problem are investigated, and illustrative examples are given, theoretically and by numerical methods, as well.
 - 1.1. First we gave some examples and the solution of the problem on $M_{2,2}$.
 - 1.2. The attached numerical study made by global optimization tools dealt with some motivations and reduction possibilities for the numerical investigation of the problem. Numerical results are presented here for the numerical optimization of (1)-(2).
 - 1.3. Global optimization test problems are given in order to test the efficiency of the numerical are given, which are defined on each Stiefel-manifold and has exponential number (2^k) of known optimizer points.
 - 1.4. A discretization of the problem is proved to be equivalent to the assignment problem.

2. A parallel version of a heuristic, clustering global optimization method was described and tested. The empirical investigation of this was completed in a sequential and multiprocessor environment, as well. The analysis performed on some standard test functions of the literature pointed out the efficiency of its asynchronous implementation.
3. The application of a stochastic global optimization tool was suggested for the solution of the phase stability problem. The application of the method was investigated thorough benchmark problems of the literature. The robustness of the method on this problem was tuned and with this the efficiency is improved by some parameter set.
4. Investigating a relaxation of the classical on-line bin packing problem, in which the repacking of at most c number of elements is allowed in each step:
 - 4.1. A new lower bound construction is given. The solution of the given model is derived after the application of different techniques. The obtained lower bound value (1,3871) improves the earlier known best lower bound value ($4/3$) published by Ivkovič and Lloyd in 1996. As well as the earlier bound, the new improvement is also valid for the c -repacking semi-on-line and c -repacking fully dynamic bin packing problem as well.
 - 4.2. A special case of the same problems is analyzed when p number of different element sizes is allowed, where p is fixed positive integer number. Furthermore, the results negatively answered a question raised by the authors of the paper [30] in 2005 regarding to the optimality of their lower bound values for the cases $p \geq 3$.
 - 4.3. The validity of the obtained lower bounds is extended for all d dimension number — i.e. the value 1,3871 and the lower bound given for the case when the number of different elements is restricted, as well.
 - 4.4. A family of c -repacking semi-on-line algorithms is given, more precisely one algorithm is constructed for every c -value. Analyzing the algorithms it is proved that the series of their asymptotic worst-case ratio tends to 1,5 when c tends to the infinity. In the case when $c = 4$, the regarding HFR-4 algorithm has the first ratio which is below 1,5401 which means that it is better in the worst case than any on-line algorithm.

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