Algorithms for the continuous nonlinear resource allocation problem—new implementations and numerical studies

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Abstract

Patriksson [Pat08] provided a then up-to-date survey on the continuous, separable, differentiable and convex resource allocation problem with a single resource constraint. Since the publication of that paper the interest in the problem has grown: several new applications have arisen where the problem at hand constitutes a subproblem, and several new algorithms have been developed for its efficient solution. This paper therefore serves three purposes. First, it provides an up-to-date extension of the survey of the literature of the field, complementing the survey in Patriksson [Pat08] with more than 20 books and articles. Second, it contributes improvements of some of these algorithms, in particular with an improvement of the pegging (that is, variable fixing) process in the relaxation algorithm, and an improved means to evaluate subsolutions. Third, it numerically evaluates several relaxation (primal) and breakpoint (dual) algorithms, incorporating a variety of pegging strategies, as well as a quasi-Newton method. Our conclusion is that our modification of the relaxation algorithm performs the best. At least for problem sizes up to 30 million variables the practical time complexity for the breakpoint and relaxation algorithms is linear.

1 Introduction

We consider the continuous, separable, differentiable and convex resource allocation problem with a single resource constraint. The problem is formulated as follows: Let \( J := \{1, 2, \ldots, n\} \). Let \( \phi_j : \mathbb{R} \to \mathbb{R} \) and \( g_j : \mathbb{R} \to \mathbb{R} \), \( j \in J \), be convex and continuously differentiable. Moreover, let \( b \in \mathbb{R} \) and \(-\infty < l_j < u_j < \infty, j \in J\). Consider the problem to

\[
\begin{align*}
\text{minimize} \quad & \phi(x) := \sum_{j \in J} \phi_j(x_j), \\
\text{subject to} \quad & g(x) := \sum_{j \in J} g_j(x_j) \leq b, \\
& l_j \leq x_j \leq u_j, \quad j \in J.
\end{align*}
\]

We also consider the problem where the inequality constraint (1b) is replaced by an equality, i.e.,

\[
\begin{align*}
\text{minimize} \quad & \phi(x) := \sum_{j \in J} \phi_j(x_j), \\
\text{subject to} \quad & g(x) := \sum_{j \in J} a_j x_j = b, \\
& l_j \leq x_j \leq u_j, \quad j \in J.
\end{align*}
\]

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where \( a_j \neq 0 \), \( j \in J \), and the sign is the same for all \( j \in J \). Further, we assume that there exists an optimal solution to problems (1) and (2). For brevity, in the following discussions we define \( X_j := [l_j, u_j], j \in J \).

Problems (1) and (2) arise in many areas, e.g., in search theory ([Koo99]), economics ([Mar52]), stratified sampling ([BRS99]), inventory systems ([MK93]), and queuing manufacturing networks ([BT89]). Further, these problems occur as subproblems in algorithms that solve the integer resource allocation problem ([Mje83, Section 4.7], [IK88, pp. 72–75], and [BS02b]), multicommodity network flows ([Sho85, Section 4.2]), and several others. Moreover, problems (1) and (2) can be used as subproblems when solving resource allocation problems with more than one resource constraint ([Mje83, FZ83]), and to solve extensions of problems (1) and (2) to a non-separable objective function \( \phi \) ([Mje83, DSV07]); The books [Mje83, IK88, Lus12] describe several extensions, such as to minmax/maxmin objectives, multiple time periods, substitutable resources, network constraints, and integer decision variables.

Many numerical studies of the problems (1) and (2) have been performed; for example, see [BH81, NZ92, RJL92, KL98, Kiw07, Kiw08a, Kiw08b]. Our numerical study is however timely and well motivated, since except for those by Kiwiel [Kiw07, Kiw08a, Kiw08b], where the quadratic knapsack problem is studied, none of the earlier approaches study large-scale versions of problem (1) or (2). There are also several algorithms (e.g., [NZ92, Section 1.4] and [Ste01]) which are claimed to be promising, but have not been evaluated in a large-scale study. Only one earlier study ([KL98]) evaluates the performance of algorithms for the problems (1) and (2) with respect to variations in the portions of the variables whose values are at a lower or upper bound at the optimal solution (see Section 6.2), and this is done for modest size instances \( (n = 10^4) \) only. Further, no study has been done on the computational complexity for non-quadratic versions of the problems (1) or (2). Our numerical study also incorporates improvements of the relaxation algorithm, as presented in Sections 4.3.4–4.3.5, and utilizes performance profiles ([DM02]).

As a final note on the computational tests, we only consider problem instances where the dual variable corresponding to the resource constraint (1b), respectively (2b), can be found in closed form; otherwise, we would need to implement a numerical method in some of the steps, e.g., a Newton method. We consider only customized algorithms for the problem at hand, since we presume that they perform better than more general algorithms under the above assumption.

Patriksson [Pat08] presents a survey of the history and applications of problems (1) and (2). Since its publication several related articles have been published; the survey of [Pat08] is therefore complemented in Section 2. Section 3 presents a framework of breakpoint algorithms, resulting in three concrete representatives. Section 4 presents a framework of relaxation algorithms, and ultimately six concrete example methods. In Section 5 we describe a quasi-Newton method, due to Nielsen and Zenios [NZ92], for solving the problem (2). Section 6 describes the numerical study. A test problem set is specified and the performance profile used for the evaluation is defined. In Section 7, we analyze the results from the numerical study. The structure is such that we first compare the relaxation algorithms, second the pegging process, and third the best performing algorithms among these two with the quasi-Newton method. Finally, we draw overall conclusions.

**2 Extension of the survey in [Pat08]**

We here extend the survey in [Pat08], using the same taxonomy, and sorted according to publication date.

**[Mje83]** K. M. MIELDE, *Methods of the Allocation of Limited Resources*, Section 4.7

(Problem) \( \phi_j \in C^2; \) linear equality \( (a_j = 1); l_j = 0 \)

(Methodology) The ranking algorithm of [LG75]
Applications in capital budgeting ([Han68, Shi77]), cost-effectiveness problems ([Kir68, Pac70, Mje78]), health care ([Fet73]), marketing ([LG75]), multiobjective optimization ([Geo67]), portfolio selection ([JdF75]), production (the internal report leading to [BH79]), reliability ([Bod69]), route-planning for ships or aircraft ([DBR66]), search ([CC58]), ship loading ([Kyd69]), and weapons selection ([Dan67])

Notes A monograph on resource allocation problems containing a comprehensive overview of the resource allocation problem, including extensions to several resources, non-convex or non-differentiable objectives, integral decision variables, fractional programming formulations, etcetera.

[Sho85] N. Z. SHOR, Minimization Methods for Nondifferentiable Functions, Section 4.2

(Problem) $\phi_j(x_j) = \frac{1}{2}(x_j - y_j)^2$; linear equality ($a_j = 1$); $l_j = 0$

(Methodology) Pegging

(Citations) [SI69], in which the motivating linear programming application is described

(Notes) The problem arises within the framework of a right-hand side allocation algorithm for a large-scale linear program.


(Problem) $\phi_j(x_j) = \frac{1}{2}x_j^2 - r_jx_j$; linear inequality ($a_j > 0$); $l_j = 0$

(Methodology) Pegging

(Citations) Algorithms for the problem ([PK90, MR00, BS02b, BS02a]) as well as for the case of integer variables

(Notes) A numerical illustration ($n = 6$).

[DF06] Y.-H. DAI AND R. FLETCHER, New algorithms for singly linearly constrained quadratic programs subject to lower and upper bounds

(Problem) $\phi_j(x_j) = \frac{1}{2}x_j^2 - r_jx_j$, $q_j > 0$; $g_j$ convex in $C^2$ with $g_j'(x_j) > 0$

(Methodology) A combination of a bracketing algorithm on the Lagrangian dual derivative, and a secant algorithm for the Lagrangian dual problem

(Citations) Algorithms for the problem ([HKL80, Bru84, CM87, PK90])

(Notes) The problem arises as a subproblem in a gradient projection method for a general quadratic programming problem over a scaled simplex.


(Problem) $\phi_j$ and $g_j$ increasing; $g_j$ convex in $C^2$ with $g_j' > 0$

(Methodology) Multiplier search

(Citations) Multiplier search methods ([BS95]), pegging methods ([BS02b, BS02a])

(Notes) The problem arises as a subproblem in branch–and–bound methods for the integer programming version of the problem, such as for the quadratic knapsack problem, stratified sampling, manufacturing capacity planning, linearly constrained redundancy optimization in reliability networks, and linear cost minimization in reliability networks.
Convex programming with a single separable constraint and bounded variables

(Problem) $\phi_j(x_j) = \frac{q_j}{2} x_j^2 - r_j x_j$, $q_j > 0$; $g_j$ convex in $C^2$ with $g'(x_j) > 0$; studies also the special case of a linear equality

(Methodology) Iterative descent process using strictly convex quadratic separable approximations of a non-separable original objective $f \in C^2$; subproblems solved using the pegging algorithm of [Ste01]

(Citations) General references on convex programming over box constraints; [HKL80, DFL86, PK90] for example algorithms for separable convex programming

(Notes) Numerical QP ($n = 6$, $g_j$ quadratic) illustration; numerical comparison with an augmented Lagrangian algorithm for a small problem ($n = 2$).

K. C. Kiwiel, On linear-time algorithms for the continuous quadratic knapsack problem

(Problem) $\phi_j(x_j) = \frac{q_j}{2} x_j^2 - r_j x_j$, $q_j > 0$; linear equality

(Methodology) Breakpoint search algorithm applying median search of all breakpoints

(Citations) Breakpoint search algorithms: [Bru84, CM87, PK90, MSMJ03]; sorting and searching methods: [Knu98, Kiw05]

(Notes) Develops a general $O(n)$ breakpoint algorithm; shows that the algorithms of [PK90, MSMJ03] may fail even on small examples; presents a modification of the breakpoint removal in the algorithm of [CM87]. Numerical experiments ($n \in [50 \cdot 10^3, 2 \cdot 10^6]$) for uncorrelated, weakly, and strongly correlated data; the new algorithm wins in CPU time over those in [Bru84] and [CM87] by 23%, and 21%, respectively, on average.

K. C. Kiwiel, Breakpoint searching algorithms for continuous quadratic knapsack problem

(Problem) $\phi_j(x_j) = \frac{q_j}{2} x_j^2 - r_j x_j$, $q_j > 0$; linear equality

(Methodology) A family of breakpoint search algorithms that include several choices of breakpoints for a median search and updates of quantities used for evaluating the piecewise linear implicit constraint function at the median point

(Citations) Applications in resource allocation ([BH81, BS97, HH95]), hierarchical production planning ([BH81]), network flows and transportation ([HKL80, SM90, Ven91, NZ92, CH94]), constrained matrix problems ([CDZ86]), quadratic integer programming ([BSS95, BSS96, HH95]), Lagrangian relaxation ([HWC74]), and quasi-Newton methods ([CM87]); $O(n \log n)$ sorting algorithms for the solution of the Lagrangian dual problem ([HWC74, HKL80]), $O(n)$ algorithms based on median search ([Bru84, CM87, MdPJ89, PK90, CH94, HH95, MMP97]) and approximate median search methods with $O(n)$ average-case performance ([PK90]); primal pegging algorithms with $O(n^2)$ worst-case performance ([Zip80, BH81, Mic86, Ven91, RJL92, BSS96])

(Notes) Develops several variants of $O(n)$ breakpoint search algorithms, including some ideas earlier proposed in, e.g., [PK90, CH94, HH95, MMP97]; remarks that the more complex choices made in [MdPJ89, PK90, CH94, HH95, MMP97] also means that for some simple cases cycling may occur, and also provides convergent modifications for each of them. Numerical experiments ($n \in [50 \cdot 10^3, 2 \cdot 10^6]$) for uncorrelated and weakly and strongly correlated data, and for both exact and inexact computations of the median; comparisons made with the $O(n)$ versions from [Bru84, CM87], reporting that a version (Algorithm 3.1) using exact medians is about 20% faster than the other ones; refers to an as yet unavailable technical report from 2006 for more extensive tests and comparisons with pegging methods.
K. C. Kiwiel, Variable fixing algorithms for continuous quadratic knapsack problem

(Problem) $\phi_j(x_j) = \frac{1}{2} x_j^2 - r_j x_j, q_j > 0$; linear equality

(Methodology) Pegging

(Citations) Applications: same references as in [Kiw08a]; breakpoint search methods ([HWC74, HKL80, CM87, MdpPJ9, PK90, CH94, HH95, MMP97, MSMJ03, Kiw07]; pegging methods ([LG75, BH79, BH81, Sho85, Mic86, Ven91, RJL92, BSS96])

(Notes) Develops a basic pegging algorithm and proposes several implementational choices for the solution of the reduced problem and the updates; shows that the algorithms in [Mic86, RJL92, BSS96] fail on a small example, and that there is a gap in the convergence analysis in [BH81] (which also is closed) that affects algorithms whose analyses rest on that in [BH81] (e.g., [Ven91]); provide more efficient versions of several of these methods, including the introduction of incremental updates which reduce computations, and a more efficient stopping criterion. Numerical experiments ($n \in [50 \cdot 10^3, 2 \cdot 10^6]$) for uncorrelated and weakly and strongly correlated data; comparisons made with the breakpoint search method of [Kiw08a] which uses exact medians; on average the latter is 14% slower while at the same time it has a more stable run time; it is remarked that the advantage of pegging over breakpoint search has been reported also in [Ven91, RJL92].

B. Zhang and Z. Hua, A unified method for a class of convex separable nonlinear knapsack problems

(Problem) $\phi'_j/g'_j$ monotone and invertible, $g'_j$ positive; consider $\sum_{j=1}^n g_j(x_j) < b$ where $< \in \{\leq, =, \geq\}$

(Methodology) Pegging algorithm using binary search on the value of $\phi'_j/g'_j$

(Citations) Applications: resource allocation ([LG75, Zip80, BH81, Hoc94]), the singly constrained multi-product newsvendor problem ([HW63, Er100, AMMM04]), production/inventory problems ([BSSW94, BSS95, BS02b]), stratified sampling ([BSS95, BRS99, BS02b]), “core subproblem” ([JdF75, AHKL80, MT89, RJL92, BSS95, BSS96]); algorithms: breakpoint methods ([BS95], [Ste01], [LG75]) and relaxation methods ([KL98], [BS02b], [BS02a])

(Notes) Claims (without a proof) that the complexity of the algorithm is $O(n)$, but the algorithm presented makes use of a mean-value method for the evaluation of the breakpoints which in the worst case results in $2n - 1$ iterations. We also note that each iteration consist of $O(n)$ operations, whence the complexity is $O(n^2)$. Numerical experiments ($n \in [10, 10^4]$) ($\phi$ quadratic, $g_j$ linear, $< \in$ chosen uniformly randomly).

A. De Waegenaere and J. L. Wielhouwer, A breakpoint search approach for convex resource allocation problems with bounded variables

(Problem) $\phi_j$ and $g_j$ convex; $g_j$ strictly monotone and $g_j([\phi'_j/g'_j]^{-1})$ is either strictly increasing or strictly decreasing for all $j$

(Methodology) Breakpoint search algorithm using a refined pegging method (5-sets pegging); generalizes the quadratic breakpoint algorithm in [PK90] and its extension in [Kiw08a] such that it applies for the problem setting in [BS02b]

(Citations) Generalizes the quadratic breakpoint algorithm in [PK90] and its extension in [Kiw08a] such that it is valid for $f_j$ and $g_j$ as in [BS02b]. Applications in resource allocation [PK90, NZ92, BS95, VW95, BSS96, BS02b, DWW02, CLZ09, BSSV06, Pat08]

(Notes) Discuss their algorithms’ advantages compared to other articles presented in [Pat08].
A pegging algorithm for separable continuous nonlinear knapsack problems with box constraints

(Problem) $\phi_j$ invertible: linear equality ($a_j > 0$)

(Methodology) Pegging: improves the pegging algorithm in [BH81] by allowing the primal box constraints to be checked implicitly, using bounds on their Lagrange multipliers

(Citations) Applications to portfolio selection [Mar52], multicommodity network flows [AHKL80], transportation [OK84], production planning [Tam80]

(Notes) Compares their methodology with the method in [BH81] on random test problems. On randomized quadratic continuous knapsack problems ($n \in [5 \cdot 10^3, 2 \cdot 10^6]$) their algorithms wins by 8–10%, except for the smallest problems where the method in [BH81] wins by 12.5%. Two other types of test problems are also investigated, wherein the quadratic continuous knapsack problem arises as a subproblem: quadratic network flows, and portfolio optimization. In the former case, the algorithm (based on conjugate gradients) is taken from [Ara00]. Here, the pegging algorithm proposed wins over that in [BH81] by 10–48%, with $n \in [200, 5 \cdot 10^3]$. In the portfolio optimization algorithm, which is based on a progressive hedging method described in [Ara00], the quadratic continuous knapsack problem arises as a subproblem. Here, the range of $n$ is not completely disclosed; however, the speed-up over the method in [BH81] is reported to be 21–25%.


(Problem) $\phi_j$ strictly convex; $g_j(x_j) = x_j$

(Methodology) Pegging

(Citations) [Koo53] as an origin; [KL98] for computational examples; [Pat08] as a survey

(Notes) This book extends the resource allocation problem (discussed only in Chapter 2) in several ways, including equitable optimization through the use of minmax/maxmin objectives, multiple time periods, substitutable resources, network constraints, and integer decision variables.

Heuristic and exact solution method for convex nonlinear knapsack problem

(Problem) $\phi_j$ strictly convex; $g_j(x_j) = x_j$

(Methodology) The problem at hand is a subproblem in a branch–and–bound procedure for the solution of an integer-restricted version of the problem

(Citations) Applications to the newsvendor problem ([Erl00, AMMM04]), resource allocation ([BH81, Hoc94]), production ([BSS95]), and stratified sampling ([BRS99]); efficient methods for the continuous relaxation ([BS95, KL98, Ste01, ZH08]); heuristics for the integer program based on rounding of the solution to the continuous relaxation ([BS95, HZL06]); algorithms for the integer program based on the solution of continuous problems and branch–and–bound ([BS95, BS02b])

(Notes) Utilizing the algorithm from [ZH08] to solve the continuous relaxations (and rounding to produce feasible solutions), the authors develop a branch–and–bound algorithm. It is compared with the methods from [BS95] as well as with branch–and–bound algorithms utilizing a variety of tree search principles, on instances with quadratic objectives, according to problem generation principles from [BS02b] ($n \in \{10, 15, 500, 1000, 2000\}$).

An exact algorithm for the continuous quadratic knapsack problem via infimal convolution

[BS02b]
(Problem) $\phi_j$ strictly convex quadratic; linear equality ($a_j = 1$)

(Methodology) Sorting of breakpoints

(Citations) Previous algorithms for the problem ([MT93, CH94])

(Notes) Two numerical applications: (1) an economic dispatch problem ($n = 5$), and an academic example ($n \in \{200, 10^4\}$); in the latter example the results are favourably compared with the Matlab solver QUADPROG.


(Problem) $\phi_j(x_j) = \frac{q_j}{2} x_j^2 - r_j x_j; q_j > 0$; linear equality

(Methodology) Breakpoint search utilizing a heap data structure, based on an initial multiplier estimate using a secant Newton method

(Citations) Applications ([HKL80, CM87, SM90, NZ92, DF06]); multiplier algorithms ([HKL80, Bru84, CM87, PK90, MSMJ03]); pegging methods ([BH81, Sho85, Mic86, Ven91, RJL92, BSS96, Kiw08b]); quasi-Newton methods ([DF06, CMS14])

(Notes) Numerical experiments ($n = 6.25 \cdot 10^6$) on random test problems, examining (a) the best number of initial (secant) Newton iterations, and (b) the performance against a primal pegging algorithm. Overall, breakpoint search is favourable on its own given a good initial multiplier estimate; otherwise, 3 or 4 iterations of the secant Newton method is a good initialization procedure.


(Problem) $\phi_j(x_j) = \frac{q_j}{2} x_j^2 - r_j x_j; q_j > 0$; $g_j(x_j) = x_j$

(Methodology) Compares a breakpoint algorithm with CPLEX and concludes that the breakpoint algorithm outperforms CPLEX

(Citations) Applications in resource allocation and algorithms ([Pat08])

(Notes) Presents an open source library for the continuous convex separable quadratic knapsack problem and concludes that the library can be useful for further studies of the problem at hand.


(Problem) $\phi_j(x_j) = \frac{q_j}{2} x_j^2 - r_j x_j; q_j > 0$; $g_j(x_j) = a_j x_j$

(Methodology) Pegging

(Citations) Algorithms for the more general integer version of the problem; algorithms by Brethauer and Shetty ([BS95, BS02b, BS02a]); other specialized algorithms for the problem ([BH81, PK90, RJL92, Ste01, Kiw08b])

(Notes) A detailed numerical example ($n = 8$); favourable comparisons with a Matlab solver ($n \in \{50, 100, 200\}$).


(Problem) $\phi_j(x_j) = -a_j(1 - \exp(-c_j x_j)), a_j, c_j > 0$; $X$ is a scaled unit simplex
(Methodology) The KKT conditions, as defined in (3), are relaxed into a system of non-smooth equations through the utilization of the Fischer–Burmeister ([Fis92]) smoothing function; a Newton-like algorithm is then employed for these equations for a sequence of values of the smoothing parameter. The algorithm is shown to asymptotically and superlinearly converge to the unique optimal solution.

(Citations) Survey ([Pat08]); methodologies ([Ste04]); applications ([Koo99]).

(Notes) Three sets of numerical experiments. Main experiment (\(n \in \{10^2, 10^4\}\)) on randomized problems; compares with the pegging algorithm in [Ste04], noting that the proposed algorithm is faster. The proposed methodology is however terminated based on a nonzero value of the Fischer–Burmeister smoothing function, whence the final solution need not be feasible or optimal. Second set of experiments on a problem taken from [WG69] (\(n = 4\)), showing no comparisons. Third experiment on data from the Bureau of Water Conservancy (\(n = 5\)), showing no comparisons.


(Problem) \(\phi_j\) strictly convex quadratic; linear equality.

(Methodology) An approximative Newton method for the Lagrangian dual problem utilizing a secant globalization and variable fixing.

(Citations) Applications to resource allocation ([BH81, HH95, BS97]), multicommodity network flows ([HKL80, NZ92, SM90]), Lagrangian relaxation using subgradient methods ([HWC74]), quasi-Newton updates with bounds ([CM87]), semismooth Newton methods ([FM04]); related methods ([DF06, Kiw08b]).

(Notes) Numerical experiments (\(n \in \{50 \cdot 10^3, 2 \cdot 10^6\}\)) comparing the proposed method to a secant method ([DF06]), breakpoint search ([Kiw08b]), and median search ([Kiw08a]) on problems with uncorrelated, weakly correlated, and correlated data. The proposed Newton method is overall better—about 30% better on the larger instances. A further test is made on the classification problems described in [DF06] arising in the training in support vector machines; as the Hessian is non-diagonal, a projected gradient method is used, leading to subproblems of the type considered. Here, Newton’s method is superior.


(Problem) \(\phi_j\) and \(g_j\) convex, and in \(C^2\) on an open set containing \([l_j, u_j]\). Further, \(\phi_j\) is decreasing on \([l_j, u_j]\) and \(g_j\) is increasing on \([l_j, u_j]\), and \(\sum_{j \in J} g_j(l_j) < b < \sum_{j \in J} g_j(u_j)\). Test instances include resource renewal \([\phi_j(x_j) := c_j x_j (e^{1/j} - 1)\) for \(x_j > 0\), \(\phi_j(x_j) := -x_j\) for \(x_j < 0\), and \(g_j\) linear], weighted \(p\)-norm over a ball \([\phi_j(x_j) := c_j(x_j - y_j)^p\) and \(g_j(x_j) := |x_j|^r\) with \(p, r \in \{2, 2.5, 3, 4\}\]), sums of powers \([\phi_j(x_j) := c_j|x_j - y_j|^p, g_j(x_j) := |x_j|^r\]), convex quartic over a simplex \([\phi_j\) a fourth-power polynomial, and \(g_j(x_j) := x_j\), and log-exponential \([\phi_j(x_j) := \ln(\sum_{j} \exp(a_{ij} x_j + d_{ij})], g_j\) linear].

(Methodology) A damped feasible interior-point Newton method for the solution of the KKT conditions.

(Citations) Survey ([Pat08]); application to resource renewal ([MR00]); methodologies ([Bru84, PK90, RJL92, MR00, Kiw08a]).

(Notes) The algorithm is introduced for problems where subsolutions are not available in closed form. Shows that the linear system defining the Newton search direction is solvable in \(O(n)\) time. Numerical experiments (\(n \in \{10^2, 10^6\}\)) conclude that the interior point method wins over breakpoint search, often by an order of magnitude.
3 Breakpoint algorithms

Algorithms based on the Lagrangian relaxation of the explicit constraint (1b) have an older history than the relaxation algorithms. This is probably due to the fact that the relaxation algorithm quite strongly rests on the Karush–Kuhn–Tucker (KKT) conditions, which did not become widely available until the end of the 1940s and early 1950s with the work of F. John [Joh48], W. Karush [Kar39], and H. W. Kuhn and A. W. Tucker [KT51]. Lagrangian based algorithms have been present much longer and the famous “Lagrange multiplier method” for equality constrained optimization is classic in the calculus curriculum. Indeed, Lagrange multiplier techniques for our problem (1) date back at least as far as to [Bec52]; see [Pat08] for a survey of the history of the problem.

Considering problem (1) and introducing the Lagrange multiplier $\mu$ for constraint (1b), we obtain the following conditions for the optimality of $x^*$ in (1):

\[
\begin{align*}
\mu^* &\geq 0, \quad g(x^*) \leq b, \quad \mu^*(g(x^*) - b) = 0, \quad (3a) \\
x_j^* &\in X_j, \quad j \in J, \quad (3b)
\end{align*}
\]

and

\[
\begin{align*}
x_j^* &= l_j, \quad \text{if } \phi_j'(x_j^*) \geq -\mu^* g_j'(x_j^*), \quad j \in J, \quad (3c) \\
x_j^* &= u_j, \quad \text{if } \phi_j'(x_j^*) \leq -\mu^* g_j'(x_j^*), \quad j \in J, \quad (3d) \\
l_j &\leq x_j^* \leq u_j, \quad \text{if } \phi_j'(x_j^*) = -\mu^* g_j'(x_j^*), \quad j \in J. \quad (3e)
\end{align*}
\]

For a fixed optimal value $\mu^*$ of the Lagrange multiplier the conditions (3c)–(3e) are the optimality conditions for the minimization over $x \in \prod_{j=1}^n X_j$ of the Lagrangian function defined on $\prod_{j=1}^n X_j \times \mathbb{R}_+$,

\[
L(x, \mu) := -b\mu + \sum_{j=1}^n \{\phi_j(x_j) + \mu g_j(x_j)\}.
\]

Given $\mu \geq 0$ its minimization over $x \in \prod_{j=1}^n X_j$ separates into $n$ problems, yielding the Lagrangian dual function

\[
q(\mu) := -b\mu + \sum_{j=1}^n \min_{x_j \in X_j} \{\phi_j(x_j) + \mu g_j(x_j)\}. \quad (4)
\]

By introducing additional properties of the problem, we can ensure that the function $q$ is not only concave but finite on $\mathbb{R}_+$ and moreover differentiable there. Suppose, for example, that for each $j$, $\phi_j(\cdot) + \mu g_j(\cdot)$ is weakly coercive on $X_j$ for every $\mu \geq 0$ [that is, that either $X_j$ is bounded or that for every $\mu \geq 0$, $\phi_j(x_j) + \mu g_j(x_j)$ tends to infinity whenever $x_j$ tends to $\pm\infty$], and that $\phi_j$ is strictly convex on $X_j$. In this case the derivative $q'$ exists on $\mathbb{R}_+$ and equals

\[
q'(\mu) = \phi'_j(x_j(\mu)) + \mu g'_j(x_j(\mu)),
\]

where $x(\mu)$ is the unique minimum of the Lagrange function $L(\cdot, \mu)$ over $\prod_{j=1}^n X_j$. Thanks to this simple form of the dual derivative, the maximum $\mu^*$ of $q$ over $\mathbb{R}_+$ can be characterized by the complementarity conditions (3a), and the conditions (3) are the primal–dual optimality conditions for the pair of primal–dual convex programs.

If we assume that $\mu^* \neq 0$, we search for $\mu^* > 0$ such that $q'(\mu^*) = 0$ [or, in other words, $g(x(\mu^*)) = b$], that is, we need to solve a special equation in the unknown entity $\mu$, where the function $q'$ is implicitly defined, but is known to be decreasing since $q$ is concave. This equation can of course be solved through the use of any general such procedure [for example, bisection search takes two initial values $\overline{\mu}$ and $\underline{\mu}$ with $q'(\overline{\mu}) < 0$ and $q'(\underline{\mu}) > 0$, then iteratively cancels part of the initial interval given the sign of $q'$ at its midpoint $(\overline{\mu} + \underline{\mu})/2$, but the structure of $q'$ makes specialized algorithms possible to utilize.

9
From the above optimality conditions for the Lagrangian minimization problem, we obtain that

\[
x_j(\mu) = \begin{cases} 
  l_j, & \text{if } \mu \geq \mu_j^l := -\phi'_j(l_j)/g'_j(l_j), \\
  u_j, & \text{if } \mu \leq \mu_j^u := -\phi'_j(u_j)/g'_j(u_j), \\
  x_j, & \text{if } \phi'_j(x_j) + \mu g'_j(x_j) = 0,
\end{cases} \quad j \in J.
\]  

(5)

In a rudimentary algorithm we order these indices (or, breakpoints) \(\mu_j^l\) and \(\mu_j^u\) in an increasing (for example) order into \(\{\mu_1, \ldots, \mu_N\}\), where \(N \leq 2n\) due to the possible presence of ties. Finding \(\mu^*\) then amounts to finding an index \(j^*\) such that \(q'(\mu_j^*) > 0\) and \(q'(\mu_{j^*+1}) < 0\); then we know that \(\mu^* \in (\mu_{j^*}, \mu_{j^*+1})\) and \(q'(\mu^*) = 0\). Hence from equation (5), we know for all \(j\) if \(x_j^* = l_j\), \(x_j^* = u_j\) or \(l_j < x_j^* < u_j\). Now by fixing all variables \(x_j^*\) that equal the corresponding lower or upper bound we can ignore the bound constraint (1c) and find an analytical solution of the problem.

Two decisions thus need to be made: how to find the index \(j^*\), and how to perform the interpolation. Starting with the former, the easiest means is to run through the indices in ascending or descending order to find the index where \(q'\) changes sign. If we have access to the indices \(j^+\) and \(j^-\) for which \(q'(\mu_{j^+}) > 0\) while \(q'(\mu_{j^-}) < 0\), then we can choose the midpoint index, check the corresponding sign of \(q'\), and reduce the index set accordingly. Given the sorted list, we can also find this index in some randomized fashion.

As remarked above, algorithms such as bisection search can be implemented without the use of the breakpoints, and therefore without the use of sorting, as long as an initial interval can somehow be found; also general methods for solving the equation \(q'(\mu) = 0\), such as the secant method or regula falsi, can be used even without an initial interval; notice however that \(q \notin C^2\), whence a pure Newton method is not guaranteed to be well-defined.

While the sorting operation used in the ranking and bisection search methods takes \(O(n \log n)\) time, it is possible to lower the complexity by choosing the trial index based on the median index, which is found without the use of sorting; the complexity of the algorithm is then reduced to \(O(n)\). It is not clear, however, that the latter must always be more efficient, since the “\(O\)” definition calls for \(n\) to be “large enough”.

We also remark that in the case when the problem (1) arises as a subproblem in an iterative method, as the method converges the data describing the problem will tend to stabilize. This fact motivates the use of reoptimization of the problems, which most obviously can be done by using the previous value of the Lagrange multiplier as a starting point and/or utilizing the previous ordering of the breakpoints; in the latter case, the \(O(n \log n)\) sorting complexity will eventually drop dramatically.

In Section 3.1 we consider the breakpoint algorithm for the equality problem (2). In Section 3.2 we describe three pegging methods and in Sections 3.3–3.5 we apply these pegging methods to the breakpoint algorithm. Finally, in Section 3.6 we briefly discuss the convergence and time complexity of the breakpoint algorithm.

3.1 Equality constraints

We now consider problem (2) where the inequality of the primal constraint is replaced by an equality. For the problem to be convex, the resource constraint (2b) has to be affine, i.e., \(g(x) := \sum_{j \in J} a_j x_j - b\). Beside the resource constraint, the Lagrangian and the optimality conditions will take the same form as for problem (1) but with one important difference; \(\mu\) is unrestricted in sign, whence the condition (3a) is replaced by “\(g(x^*) = b\)”.

3.2 The pegging process

The origin of the pegging process is found in the relaxation algorithm; see, e.g., [BH81]. The purpose of pegging is to predict properties of the primal variables in the optimal solution from an arbitrary dual value. In Sections 3.2.1, 3.2.2, and 3.2.3 we show how to predict if an optimal primal variable value equals its lower or upper bound, or is strictly within any of the bounds.
3.2.1 2-sets pegging

If we can determine if a variable equals its lower bound at the optimal solution then we add its variable index to a set \( L \) and reduce the original problem. Similarly, if we know that a variable equals its upper bound at the optimal solution then we add the variable index to the set \( U \). Using the sets \( L \) and \( U \) when solving problem (1) or (2) will be referred to as 2-sets pegging.

Assume that we have a lower limit \( \underline{\mu} \) and an upper limit \( \overline{\mu} \) on the optimal dual value, that is, \( \underline{\mu} \leq \mu^* \leq \overline{\mu} \). From (5) we can define the sets \( L(\mu) := \{ j \in J \mid \mu \geq -\phi_j'(l_j)/g_j'(l_j) \} \) and \( U(\overline{\mu}) := \{ j \in J \mid \overline{\mu} \leq -\phi_j'(u_j)/g_j'(u_j) \} \). Let \( J^k := J \setminus (L(\mu) \cup U(\overline{\mu})) \) and let \( b^k := b - \sum_{j \in L(\mu)} g_j(l_j) - \sum_{j \in U(\overline{\mu})} g_j(u_j) \). Hence we can define a subproblem of problem (1) as follows:

\[
\begin{align*}
\text{minimize} \quad & \phi(x) := \sum_{j \in J^k} \phi_j(x_j), \\
\text{subject to} \quad & g(x) := \sum_{j \in J^k} g_j(x_j) \leq b^k, \\
& l_j \leq x_j \leq u_j, \quad j \in J^k.
\end{align*}
\]

Similarly we can define a subproblem of problem (2) as follows:

\[
\begin{align*}
\text{minimize} \quad & \phi(x) := \sum_{j \in J^k} \phi_j(x_j), \\
\text{subject to} \quad & g(x) := \sum_{j \in J^k} a_j x_j = b^k, \\
& l_j \leq x_j \leq u_j, \quad j \in J^k.
\end{align*}
\]

Consider problem (6). Assuming that \( \mu^* > 0 \), the constraint (1b) has to be fulfilled with equality. For any given dual variable \( \mu^k \) we can determine the primal solution \( x^k(\mu^k) \) of problem (6) from condition (5). We know from Section 3 that all optimality conditions (3) except the resource constraint (1b) are satisfied. Moreover, we know that the resource constraint has to be fulfilled with equality, in order for the solution to be optimal. Substituting \( x^k \) into the resource constraint will be referred to as explicit evaluation; this leaves us with three cases, namely

\[
\sum_{j \in J^k} g_j(x^k_j) = b^k, \quad \sum_{j \in J^k} g_j(x^k_j) < b^k, \quad \text{or} \quad \sum_{j \in J^k} g_j(x^k_j) > b^k. \tag{8c}
\]

If (8a) is fulfilled for \( x^k \) then all optimality conditions are met and \( x^* = x^k \). Consider next the case (8b); clearly \( x^k \) is not optimal but we know that \( x^* \) is such that \( \sum_{j \in J^k} g_j(x^*_j) > \sum_{j \in J^k} g_j(x^k_j) \) since \( \sum_{j \in J^k} g_j(x^*_j) = b^k \). The function \( g_j \) is convex and differentiable and can increase in one interval and decrease in another (consider, e.g., \( g_j(x_j) = x_j^2 \)), which implies that no predictions can be made of the size of \( x^*_j \) relative to that of \( x^k_j \). Hence, we need \( g_j \) to be monotone. For problem (1), Brethauer and Shetty [BS02b, Section 2] consider four cases equivalent to the following:

**Case 1:** For all \( j \in J \), \( g_j \) is decreasing and \( \mu(x_j) := -\phi_j'(x_j)/g_j'(x_j) \) is increasing in \( x_j \).

**Case 2:** For all \( j \in J \), \( g_j \) is increasing and \( \mu(x_j) \) is decreasing in \( x_j \).
Case 3: For all $j \in J$, $g_j$ is decreasing and $\mu(x_j)$ is decreasing in $x_j$.

Case 4: For all $j \in J$, $g_j$ is increasing and $\mu(x_j)$ is increasing in $x_j$.

If Case 3 or 4 holds it is possible to find a closed form of the optimal solution to the problem (1), see [BS02b, Proposition 10]. Considering problem (2), Cases 3 and 4 cannot occur, since the resource constraint is affine, i.e., $\mu(x_j) := -\phi_j'(x_j)/a_j$. Hence, only Cases 1 and 2 are of interest here.

Note that if $\mu(x_j)$ is increasing in $x_j$ then $x_j(\mu)$ is nondecreasing and vice versa. This is an essential property for the validity of the pegging process. We can indeed state the following proposition (a similar one can be stated for problem (2), but without the assumption $\mu^* > 0$):

**Proposition 1** (pegging for Cases 1 and 2). Consider problem (1) and assume that $\mu^* > 0$.

(i) If Case 1 holds, and if (8b) holds, then $x_j^* = l_j$ for all $j \in L(\mu^k)$.

(ii) If Case 1 holds, and if (8c) holds, then $x_j^* = u_j$ for all $j \in U(\mu^k)$.

(iii) If Case 2 holds, and if (8b) holds, then $x_j^* = u_j$ for all $j \in U(\mu^k)$.

(iv) If Case 2 holds, and if (8c) holds, then $x_j^* = l_j$ for all $j \in L(\mu^k)$.

**Proof.** A proof of (i) is given; the proofs for (ii), (iii), and (iv) are analogous. From (8b) we have that

$$\sum_{j \in J^k} g_j(x_j(\mu^k)) < b^k.$$

In Case 2, for all $j$, $g_j$ is increasing and $x_j(\mu)$ is nonincreasing, which implies that $g_j(x_j(\mu))$ is nonincreasing in $\mu$ for all $j$. Hence, we have that $\mu^k = \overline{\mu} \geq \mu^*$ which implies that $x_j^k \leq x_j^*$ for all $j$ since $x_j(\mu)$ is nonincreasing in $\mu$ for all $j$. Hence, for $j \in U(\mu^k)$ we know that $x_j^{k+1} = u_j = x_j^*$, i.e., we can peg $j \in U(\mu^k)$.

**3.2.2 3-sets pegging**

As in the 2-sets pegging principle of Section 3.2.1 we determine if a variable takes the value of the lower or upper bound at the optimal solution. Additionally for the 3-sets pegging we determine if a variable belongs to the open interval between the lower and upper bound, i.e., if $x_j^* \in (l_j, u_j)$. Assume that we know that $\mu^* \in (\mu^u_j, \mu^l_j)$; then it follows from (5) that $x_j^* \in (l_j, u_j)$ and there is no need to check if $x_j^k$ equals the lower or upper bound which will reduce future calculations. 3-sets pegging is used for the quadratic knapsack problem (24) in [Kiw08a, Section 3]. The method described in [Kiw08a, Section 3] can be generalized according to the following proposition:

**Proposition 2** (relax primal variables from lower and upper bounds). Assume that Case 1 or 2 in Section 3.2.1 holds and that for some values of $\underline{\mu}$ and $\overline{\mu}$, $\underline{\mu} < \mu^* < \overline{\mu}$ holds. If $\underline{\mu}, \overline{\mu} \in [\mu^u_j, \mu^l_j]$ holds for some $j \in J^k$ then $l_j < x_j^* < u_j$.

**Proof.** Assume that Case 2 holds, i.e., $\mu = -\phi_j'/g_j'$ is decreasing. (The proof for Case 1 is analogous.) Assume that $\underline{\mu}, \overline{\mu} \in [\mu^u_j, \mu^l_j]$ holds for some $j \in J^k$. Since $-\phi_j'/g_j'$ is decreasing we have that $\underline{\mu}, \overline{\mu} \in [\mu^u_j, \mu^l_j]$ implies that $\mu^* \in (\mu^u_j, \mu^l_j)$, and from (5) it then follows that $l_j < x_j^* < u_j$.

**3.2.3 5-sets pegging**

As in the 3-sets pegging principle in Section 3.2.2 we determine if a variable takes the value of the lower or upper bound or if the variable strictly belongs to the interval between the lower and upper bound. For 5-sets pegging we also determine if a variable is larger than the lower bound or smaller than the upper bound. 5-sets pegging for problem (1) is used in [DWW12], generalizing a method from [Kiw08a]. Assuming that we know that $x_j^* < u_j$, there is no need to check if $x_j^k$ equals the upper bound; this might reduce future calculations. The proof of the following proposition follows from the monotonicity of $g_j$ and $x_j(\mu)$ (see [DWW12] for a proof).
If we can determine if the value of a variable \( x_j \) is strictly within the bounds for all \( \mu \) such that \( \mu < \mu < \bar{\beta} \), then we don’t have to check if \( x_j \) violates the bounds when we determine \( x_j \) from (5) in future iterations (see Proposition 2). This might save us some operations. Define a set of indices for the lower and upper limit being within the interval of the lower and upper breakpoint for a variable: \( M := \{ j \in N \mid \mu_j \in [\mu_j, \mu_u] \} \). From Proposition 2 we have that if \( j \in M \) then \( l_j < x_j < u_j \). Hence if \( j \in M \) we do not have to check if \( x_j \) violates the bounds in future iterations. But we should have in mind that to determine if \( j \in M \) requires some extra operations. If we let the initial values of the limits be \( \underline{\beta} = -\infty \) and \( \bar{\beta} = \infty \), then \( \mu \subseteq \{ \mu_j, \mu_u \} \) and we note that there is no need to check if \( j \in M \), as long as \( \underline{\beta} = -\infty \) or \( \bar{\beta} = \infty \). Hence, to avoid unnecessary operations we start by checking if

\textbf{Algorithm: Median search of Breakpoints with 2-sets pegging (MB2)}

Consider Case 1 or 2 in Section 3.2.1 for problem (1). Let \( \text{median}(\cdot) \) denote a function which provides the median of a finite vector; let \( \mu_m \) be the median breakpoint, and define the total use of the resource due to variables that equal the lower and upper bounds as \( \beta_l := \sum_{j \in \{ N \mid \mu_j < \mu_m \} } g_j(l_j) \), and \( \beta_u := \sum_{j \in \{ N \mid \mu_j > \mu_m \} } g_j(u_j) \), respectively. In the spirit of [BS02a, Section 3.1] and [Kiw07, Algorithm 3.1], we present the following algorithm:

**Initialization:**

Set \( N := J \), \( k := 1 \), and \( b^k := b \).

Compute breakpoints \( \mu_l := (\mu_{l,j})_{j \in N} \), \( \mu_u := (\mu_{u,j})_{j \in N} \) as in (5), and let \( \mu^k := (-\infty, (\mu_l)^T, (\mu_u)^T, \infty)^T \).

**Step 0** (check if \( \mu = 0 \) is optimal):

If \( \sum_{j \in N} g_j(x_j(0)) \leq b \), for \( x_j(\mu) \) is determined from (5), then \( \mu^* = 0 \), \( x_j^* = x_j(0) \) for \( j \in N \). Stop.

**Iterative algorithm:**

**Step 1** (stopping test):

\( \mu_k = 0 \)

**Step 2** (compute explicit reference):

Determine \( \delta := \sum_{j \in \{ N \mid \mu_j < \mu_m \} } g_j(x_j(\mu_m)) + \beta_u + \beta_l \), where \( x_j(\mu) \) is determined from (5).

If \( \delta > b^k \), then go to Step 3.1.

If \( \delta < b^k \), then go to Step 3.2.

Otherwise \( (\delta = b^k) \) let \( \mu^* := \mu_m \), find \( x^* \) from (5), and stop.

**Step 3.1** (update and fix lower bounds):

For all \( j \in N \):

If \( \mu_{j} \geq \mu_{l,j} \) then let \( N := N \setminus \{ j \} \) and \( x_j^* := l_j \).

Let \( \mu_{l,j}^k := (\mu_{l,j}^k)_{j \in \{ N \mid \mu_j < \mu_m \} }, b_l^{k+1} := b_k - \beta_l \), and \( k := k + 1 \).

Go to Step 1.

**Step 3.2** (update and fix upper bounds):

For all \( j \in N \):

If \( \mu_{j} \leq \mu_{u,j} \) then let \( N := N \setminus \{ j \} \) and \( x_j^* := u_j \).

Set \( \mu_{u,j}^k := (\mu_{u,j}^k)_{j \in \{ N \mid \mu_j > \mu_m \} }, b_u^{k+1} := b_k - \beta_u \), and \( k := k + 1 \).

Go to Step 1.

For problem (2), the algorithm is similar except Step 0 vanishes.

\textbf{Algorithm: Median search of Breakpoints with 3-sets pegging (MB3)}

If we can determine if the value of a variable \( x_j \) is strictly within the bounds for all \( \mu \) such that \( \mu < \mu < \bar{\beta} \), then we don’t have to check if \( x_j \) violates the bounds when we determine \( x_j \) from (5) in future iterations (see Proposition 2). This might save us some operations. Define a set of indices for the lower and upper limit being within the interval of the lower and upper breakpoint for a variable: \( M := \{ j \in N \mid \mu_j \in [\mu_j, \mu_u] \} \). From Proposition 2 we have that if \( j \in M \) then \( l_j < x_j < u_j \). Hence if \( j \in M \) we do not have to check if \( x_j \) violates the bounds in future iterations. But we should have in mind that to determine if \( j \in M \) requires some extra operations. If we let the initial values of the limits be \( \underline{\beta} = -\infty \) and \( \bar{\beta} = \infty \), then \( \mu \subseteq \{ \mu_j, \mu_u \} \) and we note that there is no need to check if \( j \in M \), as long as \( \underline{\beta} = -\infty \) or \( \bar{\beta} = \infty \). Hence, to avoid unnecessary operations we start by checking if
Remark 1. If γ is not separable then the updates of γ1 and/or γ2 in Steps 3.1 and 3.2 vanish.

3.5 Algorithm: Median search of Breakpoints with 5-set pegging (MB5)

As in the algorithm MB2 in Section 3.3 we peg the variables whose values equal the lower or upper bounds, and as in MB3 we determine if a variable is strictly within the bounds. Further, we determine if a variable is smaller than the upper bound or larger than the lower bound as in Section 3.2.3. Define a set \( L_\cdot \) of indices where the optimal solution is known to be strictly smaller than the upper bound in the optimal solution, i.e., \( L_\cdot := \{ j \in N \mid x^*_j < u_j \} \), and similarly define a set \( U_\cdot \) of indices where the variable is known to be larger than the lower bound in the optimal solution, i.e., \( U_\cdot := \{ j \in N \mid x^*_j > l_j \} \). Define, respectively, the total use of the resource due to variables whose values equal the lower and upper bounds as \( \beta_l := \sum_{j \in \{ N \cup L_\cdot \mid \mu_j \leq \mu_m \}} g_j(l_j) \) and
Remark 2. Consider iteration from earlier iteration is negligible hence some operations are repeated. Only need to check if this holds for $x$ dual variable. This differs from the algorithm in [DWW12] since that algorithm finds similar to the algorithm MB2 in Section 3.3:

Initialization:

Set $N := J$, $k := 1$, $b_k := b$, $\gamma := 0$, and $M = L_+ = U_+ := \emptyset$, $\mu := -\infty$, and $\overline{\mu} := \infty$.

Compute breakpoints $\mu^l := (\mu^l_j)_{j \in N}$, $\mu^u := (\mu^u_j)_{j \in N}$ as in (5), and let $\mu^k := \left(\begin{array}{c} \mu^l \\ \mu^u \end{array}\right)$.

Iterative algorithm:

Step 2 (compute explicit reference):

Determine $\delta := \sum_{j \in \{N \cup U_+ \cup L_- | \mu^u_j < \mu_m \}} g_j(x_j(\mu_m)) + \gamma(\mu_m) + \beta_u + \beta_l$, where $x_j(\mu)$ is determined from (5).

If $\delta > b_k$, then go to Step 3.1.

If $\delta < b_k$, then go to Step 3.2.

Otherwise ($\delta = b^k$) set $\mu^* := \mu_m$ and find optimal $\mathbf{x}^*$ from (5), and stop.

Step 3.1 (update and fix lower bounds):

Let $\mu := \mu_m$.

For $j \in N$: If $\mu \geq \mu^l_j$ then let $N := N \setminus \{j\}$ and $x^*_j := l_j$.

For $j \in L_-$: If $\mu \geq \mu^l_j$ then let $L_- := L_- \setminus \{j\}$ and $x^*_j := l_j$.

For $j \in N$: If $\mu \geq \mu^l_j$ then let $N := N \setminus \{j\}$ and $L_- := L_- \cup \{j\}$.

For $j \in U_+$: If $\mu \in [\mu^l_j, \mu^u_j)$ and $\overline{\mu} \geq \mu^u_j$ then let $U_+ := U_+ \setminus \{j\}$ and $M := M \cup \{j\}$; update $\gamma_1$, $\gamma_2$.

Let $\mu^{k+1} := (\mu^l_j)_{j \in \{N \cup U \cup L_- \cup U_+ | \mu_m < \mu^u_j\}}$, $b^{k+1} := b_k - \beta_l$, and $k := k + 1$.

Go to Step 1.

Step 3.2 (update and fix upper bounds):

Let $\overline{\mu} := \mu_m$.

For $j \in N$: If $\overline{\mu} \leq \mu^u_j$ then let $N := N \setminus \{j\}$ and $x^*_j := u_j$.

For $j \in U_+$: If $\overline{\mu} \leq \mu^u_j$ then let $U_+ := U_+ \setminus \{j\}$ and $x^*_j := u_j$.

For $j \in N$: If $\overline{\mu} \leq \mu^u_j$ then let $N := N \setminus \{j\}$ and $U_+ := U_+ \cup \{j\}$.

For $j \in L_-$: If $\overline{\mu} \in [\mu^l_j, \mu^u_j)$ and $\mu \leq \mu^l_j$ then let $L_- := L_- \setminus \{j\}$ and $M := M \cup \{j\}$; update $\gamma_1$, $\gamma_2$.

Let $\mu^{k+1} := (\mu^u_j)_{j \in \{N \cup M \cup L_- \cup U_+ | \mu_m > \mu^l_j\}}$, $b^{k+1} := b_k - \beta_u$, and $k := k + 1$.

Go to Step 1.

Note that when we determine $x_j(\mu_m)$ for $j \in U_+$ we do not need to check if $x_j = l_j$, and for $j \in L_-$ we do need to check if $x_j = u_j$. This will in some cases save us some operations. Further when we determine if $x_j \in M$ we only need to check if this holds for $j \in U_+$ or $j \in L_-$ depending on if we update the lower or upper bound of the variable. This differs from the algorithm in [DWW12] since that algorithm finds $M$ from $U_+ \cup L_-$. Note that we make use of information from earlier iterations when updating $\delta$. When updating $\delta$ in [DWW12] information from earlier iteration is negligible hence some operations are repeated.

Remark 2. Consider iteration $k$. In Step 3.1 we only need to check if $\mu_m \in [\mu^l_j, \mu^u_j)$ and $\overline{\mu} \geq \mu^u_j$ for $j \in U_+$ since we know from earlier iterations that if $j \in N$ then $\overline{\mu} \notin \mu^l_j$. Similar holds for Step 3.2.

3.6 Convergence and time complexity of breakpoint algorithms

Similar to [Kiw08a] and [DWW12] it is possible to show that the breakpoint algorithms converge to the optimal solution. Consider the time complexity for algorithm MB2, MB3 and MB5. Assuming that the median function $\text{median}(\cdot)$ is linear, we have $C_i n$ operations in each of the Steps 0 through 3.2 for some constants $C_i$ for $i \in$
{0; 1; 2; 3.1; 3.2} corresponding to Step 0 through 3.2 respectively. Since we use a median search function the number of iterations will terminate in $\log_2(n)$ iterations (in the worst case). Hence the time complexity of the algorithm is $O(n \log_2(n))$. However in [Bru84] a proof for a time complexity of $O(n)$ is given for the breakpoint algorithm solving the quadratic knapsack problem (24).

4 Relaxation algorithms

In a relaxation algorithm for the problem (1) we iteratively solve the problem relaxed from constraints (1c), i.e.,

$$
\text{Problem:} \quad \min \phi(x) := \sum_{j \in J^k} \phi_j(x_j),
\text{subject to} \quad g(x) := \sum_{j \in J^k} g_j(x_j) \leq b.
$$

From problem (9) we obtain a solution $\hat{x}$. Together with $\hat{x}$ we also obtain an estimate $\hat{\mu}$ of the multiplier value $\mu^*$ from the optimality condition. Then we adjust the solution $\hat{x}$ for constraints (1c) by determining $x_j$ from

$$
x_j := \begin{cases}
  l_j, & \text{if } \hat{x}_j \leq l_j, \\
  u_j, & \text{if } \hat{x}_j \geq u_j, \\
  \hat{x}_j, & \text{if } l_j < \hat{x}_j < u_j.
\end{cases}
$$

At the beginning of the algorithm we must determine whether constraint (1b) is satisfied with equality at an optimal solution. From the optimality condition (3a) we have that if the inequality constraint (1b) is satisfied then $\mu^* = 0$. Hence, for $\hat{\mu} = 0$ we find $\hat{x}$ by solving $\phi_j(\hat{x}_j) + \hat{\mu}g_j(\hat{x}_j) = 0$; if $\sum_{j \in J} g_j(x_j) \leq b$, where the value of $x_j$ is determined from (10), then we have found the optimal solution to problem (1). Otherwise, we know that $\mu^* > 0$ and that the inequality constraint (1b) can be regarded as an equality. Hence, we solve the problem (9), obtaining a solution $\hat{x}$. Let

$$
L(\hat{x}) := \{ j \in J^k \mid \hat{x}_j \leq l_j \}, \quad U(\hat{x}) := \{ j \in J^k \mid \hat{x}_j \geq u_j \}
$$

denote the sets of variables that are either out of bounds at $\hat{x}$ or equal a lower, respectively an upper, bound.

In order to simplify the remaining discussion, we consider Case 2 in Section 3.2.1, i.e., $\mu(x_j)$ to be monotonically decreasing and $g_j$ is increasing; Case 1 is treated analogously. Calculate the total deficit and excess at $\hat{x}$, respectively, as

$$
\nabla := \sum_{j \in L} (g_j(l_j) - g_j(\hat{x}_j)), \quad \Delta := \sum_{j \in U} (g_j(\hat{x}_j) - g_j(u_j)).
$$

Now, if $\Delta > \nabla$ then we set $x_j^* = u_j$ for $j \in U(\hat{x})$; if $\Delta < \nabla$ we set $x_j^* = l_j$ for $j \in L(\hat{x})$; otherwise $\Delta = \nabla$ and we have found the optimal solution. If $\Delta \neq \nabla$, then we reduce the problem by removing the fixed variables, and adjusting the right-hand side of the constraint (1b) to reflect the variables fixed. If any free variables are left, we re-solve problem (9) and repeat the procedure, otherwise we have obtained an optimal solution.

The rationale behind this procedure is quite simple and natural: Suppose that $\Delta > \nabla$ holds. We have that $\hat{\mu} = -\phi_j'(\hat{x}_j)/g_j'(\hat{x})$ for $j \in J^k \setminus \{L \cup U\}$. Let $s \in U(\hat{x})$ and $i \in J^k \setminus U(\hat{x})$. Since the functions $-\phi_j'/g_j'$ are decreasing, it follows that

$$
-\frac{\phi_s'(u_s)}{g_s'(u_s)} \geq -\frac{\phi_i'(\hat{x}_i)}{g_i'(\hat{x}_i)} = \hat{\mu} = \frac{\phi_i'(\hat{x}_i)}{g_i'(\hat{x}_i)} \geq \frac{\phi_s'(u_s)}{g_s'(u_s)}.
$$
Denote by \( b \) the right-hand side in the following iteration given that \( \Delta > \nabla \) holds: \( b_+ := b - \sum_{j \in U(\hat{x})} g_j(u_j) \).

Also let \((\hat{x}', \hat{\mu}')\) denote a pair of relaxed optimal primal–dual solutions in the following iteration. We must have that \( \hat{\mu}' \leq \hat{\mu} \), since

\[
\sum_{j \in J \setminus U(\hat{x})} g_j(\hat{x}_j) = b - \sum_{j \in U(\hat{x})} g_j(\hat{x}_j) \leq b - \sum_{j \in U(\hat{x})} g_j(u_j) = b_+ = \sum_{j \in J \setminus U(\hat{x})} g_j(\hat{x}_j);
\]

hence, for at least one \( j \in J \setminus U(\hat{x}) \) we have that \( \hat{x}_j' \geq \hat{x}_j \), and therefore,

\[
\hat{\mu}' = -\frac{\partial f_j'(\hat{x}_j')}{g_j'(\hat{x}_j')} \leq -\frac{\partial f_j'(\hat{x}_j)}{g_j'(\hat{x})} = \hat{\mu}
\]

follows. This derivation was first described by Bitran and Hax [BH81].

Since in each iteration at least one variable is pegged to an optimal value, the algorithm is clearly finite. The most serious disadvantage of the algorithm may be the requirement that the problem without the variable bounds present must have an optimal solution. The computational efficiency of this method is also determined by whether or not it is possible to provide an explicit formula for each \( \hat{x}_j \) in terms of the multiplier.

### 4.1 Explicit/Implicit evaluation

For the breakpoint algorithm we determine \( x \) from (5) for an arbitrary multiplier \( \mu \); then we explicitly evaluate the optimality of \( x \) by substituting it into the resource constraint (1b). The explicit evaluation leaves us with one out of three possible scenarios: (8a)–(8c). For the relaxation algorithm the traditional method to evaluate a solution to the problem (9) is to calculate the total deficit and excess at \( \hat{x} \) (see Section 4). Also this evaluation leaves us with 3 possible scenarios, namely

\[
\Delta = \nabla, \quad \Delta > \nabla, \quad \Delta < \nabla.
\]

Evaluating the optimality from (12a)–(12c) will be referred to as an implicit evaluation. For the relaxation algorithm we next show that the implicit and explicit evaluations are equivalent. Propositions 4 and 5 below state the relations between explicit and implicit evaluation. The proof of Proposition 5 is similar to the proof of Proposition 4.

**Proposition 4** (relation between explicit and implicit evaluation for \( g_j \) monotonically increasing). If for all \( j \in J \) \( g_j \) is monotonically increasing, then the explicit evaluation (8a)–(8c) is equivalent to the implicit evaluation (12a)–(12c), i.e., (12a) \( \iff \) (8a), (12b) \( \iff \) (8b), and (12c) \( \iff \) (8c).

**Proof.** For all \( j \in J \), let \( \hat{x}_j \) be the solution to (9). Let \( \nabla \) and \( \Delta \) be defined as in (11). We have from (10) that

\[
\sum_{j \in J} g_j(x_j) = \sum_{j \in J \setminus \{U \cup L\}} g_j(\hat{x}_j) + \sum_{j \in L} \{g_j(l_j) - g_j(\hat{x}_j) + g_j(\hat{x}_j)\}
+ \sum_{j \in U} \{g_j(u_j) - g_j(\hat{x}_j) + g_j(\hat{x}_j)\}
= \sum_{j \in J \setminus \{U \cup L\}} g_j(\hat{x}_j) + \sum_{j \in L} \{g_j(l_j) - g_j(\hat{x}_j)\} + \sum_{j \in U} g_j(\hat{x}_j)
- \sum_{j \in U} \{g_j(u_j) - g_j(\hat{x}_j)\} + \sum_{j \in U} g_j(\hat{x}_j)
= \sum_{j \in J} g_j(\hat{x}_j) + \nabla - \Delta
= b + \nabla - \Delta.
\]
where the last equality follows from the fact that $\hat{x}$ is the solution to the relaxed problem. Hence, $\hat{x}$ must satisfy the resource constraint. We know that $\Delta, \nabla \geq 0$ since $g_j$ is increasing. Hence, if $\Delta = \nabla$ then (8a) holds, if $\Delta > \nabla$ then (8b) holds, and if $\Delta < \nabla$ then (8c) holds.

**Proposition 5** (relation between explicit and implicit evaluation for $g_j$ monotonically decreasing). If $g_j$ is monotonically decreasing for all $j \in J$, then the explicit evaluation (8a)–(8c) is equivalent to the implicit evaluation (8a)–(8c), i.e., (12a) $\iff$ (8a), (12c) $\iff$ (8b), and (12b) $\iff$ (8c).

### 4.2 Primal/Dual evaluation of boundaries

In the breakpoint algorithms in Section 3, we use the dual variable to determine if $x_j$ equals a bound or if it lies in between the bounds; see (5). In relaxation algorithms the traditional way to solve the problem (1) is to determine the primal optimal solution $\hat{x}_j$ of the relaxed problem (9) and then simply check if $\hat{x}_j$ is within the lower and upper bounds; see (10). An alternative is to find the optimal dual variable $\hat{\mu}$ of the relaxed problem (9) and then (similar to the breakpoint algorithm in Section 3) determine the primal variables from (5). Of course this requires us to determine the breakpoints. However, for the variables that violate the bounds (1c) we don’t have to determine $x_j$ from the relation $\phi_j(x_j) + \mu g_j(x_j) = 0$. Hence, instead of evaluating $L(\hat{x})$ and $U(\hat{x})$ from the primal variable as in Section 4, we can evaluate $L(\hat{\mu})$ and $U(\hat{\mu})$ from the dual variable as in Section 3.2.1.

Define $\Phi_j(x_j) := \phi_j'(x_j)/g_j'(x_j)$ and assume that there exists an inverse to $\Phi_j$. It follows from the optimality conditions (5) that $\Phi_j(\hat{x}_j(\hat{\mu})) = -\hat{\mu}$, $\Phi_j(l_j) = \phi_j'(l_j)/g_j'(l_j)$ and $\Phi_j(u_j) = \phi_j'(u_j)/g_j'(u_j)$. Hence we have that:

$$L(\hat{\mu}) := \{ j \in J \mid \hat{\mu} \geq -\phi_j'(l_j)/g_j'(l_j) \} \iff L(\hat{x}) := \{ j \in J \mid \hat{x}_j \leq l_j \}$$

and

$$U(\hat{\mu}) := \{ j \in J \mid \hat{\mu} \leq -\phi_j'(u_j)/g_j'(u_j) \} \iff U(\hat{x}) := \{ j \in J \mid \hat{x}_j \geq u_j \}.$$  

### 4.3 Implementation choices for the relaxation algorithm

Considering the performance of a relaxation algorithm two decisions need to be made: should the relaxed solution of the problem be evaluated implicitly from $\nabla$ and $\Delta$ or explicitly from $\sum g_j$ (see Section 4.1)? Should the algorithm solve the primal or dual relaxed problem (see Section 4.2)? An overview of the relaxation algorithm and its possible realizations is shown in Figure 1. The leftmost path in the figure is the classic primal relaxation algorithm of Bitran and Hax [BH81], the rightmost path in the figure is implemented in [Ste01], and the algorithm that applies the right path in Step 1 and the left path in Step 2 is implemented in [KW12]. Beside these two paths no other paths have been explored. Our intention is to evaluate the theoretically and practically best performing paths. Since no earlier studies have applied 3- or 5-sets pegging for the relaxation algorithm, our intention is to apply these two more sophisticated pegging methods.

In Section 4.3.1 we present an algorithm corresponding to the leftmost path in Figure 1; in Section 4.3.2 we present an algorithm which utilizes the rightmost path in Step 1 of Figure 1 and then changes to the left path in Step 2 of the figure; in Section 4.3.3 an algorithm corresponding to the rightmost path of Figure 1 is presented; and in Section 4.3.4 an algorithm that utilizes the rightmost path in Step 1 of Figure 1 and then utilizes the theoretically best path in Step 2 is presented. All algorithms in Sections 4.3.1–4.3.4 utilize 2-sets pegging. In Section 4.3.5 we describe how 3- and 5-sets pegging can be utilized in these.

#### 4.3.1 Algorithm: Primal determination with Implicit evaluation of the Relaxed problem (PIR2)

We first assume that Case 1 in Section 3.2.1 holds for problem (1). Define parameters to calculate the total deficit and excess, as $\alpha^k_+ := \sum_{j \in U^k} g_j(\hat{x}_j)$, $\alpha^k_- := \sum_{j \in L^k} g_j(\hat{x}_j)$, $\beta^k_- := \sum_{j \in L^k} g_j(l_j)$ and $\beta^k_+ := \sum_{j \in U^k} g_j(u_j)$.
Hence we have that $\Delta^k = \alpha_+^k - \beta_-^k$ and $\nabla^k = \beta_+^k - \alpha_-^k$. In the next iteration when we reduce the resource $b^k$ we hence don’t have to re-calculate the part of the pegged variables which define $\beta_+^k$ or $\beta_-^k$ (see Steps 3.1 and 3.2).

We present an algorithm for problem (1) which is similar to the algorithm in Section 2 of [BS02b]:

**Initialization:** Set $k := 1$, $J^k := J$, and $b^k := b$.

**Step 0** (check if $\mu = 0$ is optimal):
- Let $\mu = 0$ and find the solution $\hat{x}$ to the relaxed problem (9), i.e., solve $\phi_j'(\hat{x}_j) + \mu g_j'(\hat{x}_j)$, $j \in J^k$.
- If $\sum_{j \in J^k} g_j(x_j) \leq b$, for $x_j$ determined from (10), then $\mu^* = 0$, $x^*_j = x_j$ for $j \in J^k$, and stop.

**Iterative algorithm:**

**Step 1** (solve relaxed primal problem):
- For $j \in J^k$, find $\hat{x}^k_j$ by solving the relaxed problem (9).
- Set $L := \emptyset$ and $U := \emptyset$.

**Step 2** (implicit evaluation):
- Determine $U(\hat{x}^k)$ and $L(\hat{x}^k)$ while computing $\Delta^k := \alpha_+^k - \beta_-^k$ and $\nabla^k := \beta_+^k - \alpha_-^k$.
- If $\Delta^k > \nabla^k$, then go to Step 3.1.
- If $\Delta^k < \nabla^k$, then go to Step 3.2.
- If $\Delta^k = \nabla^k$, then set $x^*_j := l_j$ for $j \in L(\hat{x}^k)$, $x^*_j := u_j$ for $j \in U(\hat{x}^k)$, $x^*_j := x^k_j$ for $j \in J^k \setminus \{L(\hat{x}^k) \cup U(\hat{x}^k)\}$, and stop.

**Step 3.1** (peg lower bounds):
- Set $x^*_j := l_j$ for $j \in L$, $b^{k+1} := b^k - \beta_-^k$, and $J^{k+1} := J^k \setminus L$.
- If $J^{k+1} = \emptyset$ then stop, else set $k := k + 1$ and go to Step 1.

**Step 3.2** (peg upper bounds):
- Set $x^*_j := u_j$ for $j \in U$, $b^{k+1} := b^k - \beta_+^k$, and $J^{k+1} := J^k \setminus U$.
- If $J^{k+1} = \emptyset$ then stop else set $k := k + 1$ and go to Step 1.

We need to clarify some of the steps of the algorithm. In Step 1, we find $\hat{x}^{k+1}$ from, or partly from, $\hat{x}^k$. Assume,
Remark 3. For the equality problem (2), $\mu$ is unrestricted; hence the algorithm for problem (2) will be similar to the above, except we ignore Step 0.

Remark 4. In Step 1 we have to calculate $\hat{x}_j |J^k|$ times. In Step 2 we need to find $x_j$ which needs at most $2|J^k|$ comparisons. We also have to calculate $\nabla^k$ and $\Delta^k$, which implies $2|L \cup U|$ operations.

4.3.2 Algorithm: Dual determination with Implicit evaluation of the Relaxed problem (DIR2)

Instead of evaluating the primal variables in Step 1 as in the algorithm PIR2 in Section 4.3.1, we can evaluate the dual variable $\mu$. Note that if we evaluate the dual variable, then we have to determine the breakpoints in the initialization. Our modification of the algorithm in Section 4.3.1 takes the following form (Steps 0 and 3 are same as in PIR2 and are therefore not repeated):

Initialization:
Set $k := 1$, $J^k := J$, and $b^k := b$.
Calculate breakpoints $\mu^l := (\mu^l_j)_{j \in J^k}$, and $\mu^u := (\mu^u_j)_{j \in J^k}$ as in (5).

Step 1 (solve relaxed dual problem):
Find the optimal dual variable $\hat{\mu}^k$ of the relaxed problem (9).

Step 2 (implicit evaluation):
Determine $L(\hat{\mu}^k)$ and $U(\hat{\mu}^k)$ while computing $\Delta^k := \alpha^k_+ - \beta^k_+$ and $\nabla^k := \beta^k_+ - \alpha^k_-$.
If $\Delta^k > \nabla^k$, then go to Step 3.1.
If $\Delta^k < \nabla^k$, then go to Step 3.2.
If $\Delta^k = \nabla^k$, then set $x^*_j := l_j$ for $j \in L(\hat{\mu}^k)$, $x^*_j := u_j$ for $j \in U(\hat{\mu}^k)$,
\[ x^*_j := x^*_j \text{ for } j \in J \setminus \{L(\hat{\mu}^k) \cup U(\hat{\mu}^k)\}, \text{ and stop.} \]

Remark 5. In Step 1 we need to find the optimal dual solution $\hat{\mu}^k$ to the relaxed problem. In Step 2 we need at most $2|J^k|$ comparisons but we only need to calculate $\hat{x}_j(\mu)$ for $j \in \{L \cup U\}$. For the evaluation we need to calculate $\nabla^k$ and $\Delta^k$, which implies $2|L \cup U|$ operations.
4.3.3 Algorithm: Dual determination with Explicit evaluation of the Relaxed problem (DER2)

As in the algorithm DIR2 in Section 4.3.2 we evaluate the dual variable but instead of evaluating the relaxed solution implicitly we do it explicitly. Define $\beta_t := \sum_{j \in L} g_j(l_j)$ and $\beta_u := \sum_{j \in U} g_j(u_j)$. The algorithm follows (Steps 0 and 3 are same as in PIR2 in Section 4.3.1 and are therefore not repeated):

**Initialization:**

Set $k := 1$, $J^k := J$, and $b^k := b$. Calculate breakpoints $\mu^l := (\mu_j^l)_{j \in J^k}$, $\mu^u := (\mu_j^u)_{j \in J^k}$ as in (5).

**Step 1** (solve relaxed dual problem):

Find the optimal dual variable $\hat{\mu}^k$ of the relaxed problem (9).

**Step 2** (explicit evaluation):

Determine $U(\hat{\mu}^k)$ and $L(\hat{\mu}^k)$ and calculate $\delta(\hat{\mu}^k) := \sum_{j \in J^k \setminus \{L(\hat{\mu}^k) \cup L(\hat{\mu}^k)\}} g_j(x_j(\hat{\mu}^k)) + \beta_t + \beta_u$.

If $\delta(\hat{\mu}^k) > b^k$, then go to Step 3.1.

If $\delta(\hat{\mu}^k) < b^k$, then go to Step 3.2.

If $\delta(\hat{\mu}^k) = b^k$, then set $x_j^k := l_j$ for $j \in L(\hat{\mu}^k)$, $x_j^k := u_j$ for $j \in U(\hat{\mu}^k)$, $x_j^k := x_j^2$ for $j \in J \setminus \{L(\hat{\mu}^k) \cup U(\hat{\mu}^k)\}$, and stop.

The algorithm uses the principle of the algorithm in [Ste01, Algorithm 1].

**Remark 6.** In Step 1 we need to find the value of $\hat{\mu}^k$ from the relaxed problem. In Step 2 we need at most $2|J^k|$ comparisons and we need to calculate $x_j^k$ for $j \in J^k \setminus \{L \cup U\}$. For the evaluation we need to calculate $\delta(\hat{\mu}^k)$, which implies $|J^k|$ operations.

4.3.4 Algorithm: Dual determination modification with blended evaluation of the Relaxed problem (DBR2)

Consider the implicit evaluation in Section 4.3.2. We calculate $\nabla^k$ and $\Delta^k$ from $\nabla^k := \sum_{j \in L(\hat{\mu}^k)} g_j(l_j) - \sum_{j \in U(\hat{\mu}^k)} g_j(x_j^k)$ and $\Delta^k := \sum_{j \in L(\hat{\mu}^k)} g_j(x_j^k) - \sum_{j \in L(\hat{\mu}^k)} g_j(u_j)$, which implies $2P|L^k \cup U^k|$ operations, where $P$ is an integer associated with the number of operations it takes to calculate $g_j(x_j)$. Moreover, we have to determine $\hat{x}_j$ for $j \in \{L^k \cup U^k\}$, which implies $Q|L^k \cup U^k|$ operations, where $Q$ is an integer associated with the number of operations it takes to determine $x_j(\hat{\mu})$.

Now consider the explicit evaluation: We have to calculate $\delta(\hat{\mu}^k) := \sum_{j \in J^k \setminus \{L(\hat{\mu}^k) \cup L(\hat{\mu}^k)\}} g_j(x_j(\hat{\mu}^k)) + \sum_{j \in L(\hat{\mu}^k)} g_j(l_j) + \sum_{j \in U(\hat{\mu}^k)} g_j(u_j)$, which implies $P|J^k|$ operations. Moreover, we have to determine $\hat{x}_j$ for $j \in J^k \setminus \{L^k \cup U^k\}$, which implies $Q|J^k \setminus \{L^k \cup U^k\}$ operations.

Hence, if $(P + Q)|J^k| < (2P + 2Q)|U(\mu^k) \cup L(\mu^k)|$ or, equivalently, $|J^k| < 2|U(\mu^k) \cup L(\mu^k)|$, then using the explicit evaluation of the relaxed solution $\hat{x}$ in Step 2 would require less operations, and it would be more successful to use the algorithm in Section 4.3.3. If however $|J^k| > 2|U(\mu^k) \cup L(\mu^k)|$, then there will be less operations if we use the algorithm in Section 4.3.2. So, we propose a new algorithm that utilizes the cardinalities of the sets $J^k$, $U(\hat{\mu}^k)$ and $L(\hat{\mu}^k)$: from the cardinalities we make the decision whether to use an explicit or implicit evaluation in Step 2. We consider the following modification of the algorithm PIR2 in Section 4.3.1:
Initialization:

Set \( k := 1, J^k := J, \) and \( b^k := b. \)
Calculate breakpoints \( \mu^l := (\mu^l_j)_{j \in J^k}, \mu^u := (\mu^u_j)_{j \in J^k} \) as in (5).

Step 1: (solve relaxed dual problem):

Find the optimal dual variable \( \hat{\mu}^k \) of the relaxed problem (9).

Step 1.1: (implicit or explicit evaluation?):

- Determine \( U(\hat{\mu}^k) \) and \( L(\hat{\mu}^k). \)
- If \( |J^k| < 2|U(\hat{\mu}^k) \cup L(\hat{\mu}^k)| \) then use explicit evaluation (continue with algorithm DER2 in Section 4.3.3), otherwise use implicit evaluation (continue with algorithm DIR2 in Section 4.3.2).

### 4.3.5 3- and 5-sets pegging for relaxation algorithms

From the proof of convergence of the relaxation algorithm (see Section 4.4) we have that the algorithm improves the lower or the upper bound for the dual variable in each iteration. Hence, similar to the breakpoint algorithm (see Sections 3.4 and 3.5) it is possible to apply 3- and 5-sets pegging for the dual relaxation algorithms DIR2, DER2 and DBR2. Similar to the relaxation algorithm we will denote a relaxation algorithm that uses 3-sets-pegging with a suffix "3", e.g., DBR3, and one that uses 5-sets-pegging with a suffix "5", e.g., DBR5. The implementation of 3- and 5-sets pegging is similar for the three dual relaxation algorithms; therefore only DIR3 and DIR5 are given (Step 0 is similar as for PIR in Section 4.3.1):

**DIR3:**

**Initialization:**

Set \( k := 1, J^k := J, M^k := \emptyset, b^k := b, \mu = -\infty, \) and \( \overline{\mu} = \infty. \)
Calculate breakpoints \( \mu^l := (\mu^l_j)_{j \in J^k}, \mu^u := (\mu^u_j)_{j \in J^k} \) as in (5).

**Step 1** (solve relaxed dual problem):

Find the optimal dual variable \( \hat{\mu}^k \) of the relaxed problem (9).

**Step 2** (implicit evaluation):

Determine \( L(\hat{\mu}^k) \) and \( U(\hat{\mu}^k) \) from \( J^k \) and compute \( \Delta^k = \alpha^k_+ - \beta^k_- \) and \( \nabla^k = \beta^k_- - \alpha^k_+ \).

- If \( \Delta^k > \nabla^k \), then go to Step 3.1.
- If \( \Delta^k < \nabla^k \), then go to Step 3.2.

If \( \Delta^k = \nabla^k \), then set \( x^*_j = l_j \) for \( j \in L(\hat{\mu}^k) \), \( x^*_j = u_j \) for \( j \in U(\hat{\mu}^k) \)

- \( x^*_j = x_j(\hat{\mu}^k) \) for \( j \in \{ J^k \cup M^k \} \setminus \{ L(\hat{\mu}^k) \cup U(\hat{\mu}^k) \} \), and stop.

**Step 3.1** (peg lower bounds):

Update lower bound, \( \mu := \hat{\mu}^k \), and resource \( b^{k+1} := b^k - \beta^k_- \).
Set \( x^*_j := l_j \) for \( j \in L^k \), \( J^{k+1} := J^k \setminus L^k \) and \( M^{k+1} := M^k \).
For \( j \in J^{k+1} \):
- If \( \mu, \overline{\mu} \in [\mu^l_j, \mu^u_j] \) then \( J^{k+1} := J^{k+1} \setminus \{ j \}, M^{k+1} := M^{k+1} \cup \{ j \} \).
If \( J^{k+1} = \emptyset \) then find optimal solution and stop, else set \( k := k + 1 \) and go to Step 1.

**Step 3.2** (peg upper bounds):

Update upper bound, \( \hat{\mu} := \hat{\mu}^k \), and resource \( b^{k+1} := b^k - \beta^k_+ \).
Set \( x^*_j := u_j \) for \( j \in U^k \), \( J^{k+1} := J^k \setminus U^k \) and \( M^{k+1} := M^k \).
For \( j \in J^{k+1} \):
- If \( \mu, \overline{\mu} \in [\mu^l_j, \mu^u_j] \) then \( J^{k+1} := J^{k+1} \setminus \{ j \}, M^{k+1} := M^{k+1} \cup \{ j \} \).
If \( J^{k+1} = \emptyset \) then find optimal solution and stop, else set \( k := k + 1 \) and go to Step 1.

In Steps 3.1 and 3.2, if \( J^{k+1} = \emptyset \) then we can find the optimal solution from \( M \) since we know that for all \( j \in M \).
it holds that \( l_j < x_j < u_j \), i.e., we don’t have to consider the constraint (1c). Further, in Step 3.1 (and analogously for Step 3.2) when searching for \( j \in J^{k+1} \) such that \( \mu_j \in [\mu^*_j, \mu^*_{j}] \), we only have to consider \( j \in J^{k+1} \setminus U^k \), since we know that if \( j \in U^k \) then \( \hat{\mu}^k \leq \mu^*_j \). Note that for the case where \( \hat{\mu}^k = \mu^*_j \) the corresponding index \( j \) will continue to belong to \( J^{k+1} \). Finally we note that we don’t have to check if \( \mu_j \in [\mu^*_j, \mu^*_{j}] \) if \( \mu_l = -\infty \) and/or \( \overline{\mu} = \infty \).

**DIR5:**

**Initialization:**

Set \( k := 1, J^k := J, M^k = U^k = L^k := \emptyset, b^k := b, \mu = -\infty, \) and \( \overline{\mu} = \infty. \)

Calculate breakpoints \( \mu^l := (\mu^l_j)_{j \in J^k}, \mu^u := (\mu^u_j)_{j \in J^k} \) as in (5).

**Step 1** (solve relaxed dual problem):

Find the optimal dual variable \( \hat{\mu}^k \) of the relaxed problem (9).

**Step 2** (implicit evaluation):

Determine \( L(\hat{\mu}^k) \) and \( U(\hat{\mu}^k) \) from \( J^k \cup L^\_ \cup U^\_ \), compute \( \Delta^k = \alpha^k_+ - \beta^k_+ \) and \( \nabla^k = \beta^k_+ - \alpha^k_+ \).

If \( \Delta^k > \nabla^k \), then go to Step 3.1.

If \( \Delta^k < \nabla^k \), then go to Step 3.2.

If \( \Delta^k = \nabla^k \), then set \( x^*_j = l_j \) for \( j \in L(\hat{\mu}^k) \), \( x^*_j = u_j \) for \( j \in U(\hat{\mu}^k) \), \( x^*_j = x_j(\hat{\mu}^k) \) for \( j \in \{J^k \cup M^k \cup L^\_ \cup U^\_ \} \setminus \{L(\hat{\mu}^k) \cup U(\hat{\mu}^k)\} \), and stop.

**Step 3.1** (peg lower bounds):

Update lower bound, \( \mu := \hat{\mu}^k \), and resource \( b^{k+1} := b^k - \beta^k_+ \).

Set \( x^*_j := l_j \) for \( j \in L^k \), \( J^{k+1} := J^k \setminus L^k \) and \( L^{k+1} := L_k \setminus L^k \).

For \( j \in \{J^{k+1} \setminus U^k\} \): If \( \mu_j \leq \mu_j^l \) then \( J^{k+1} := J^{k+1} \setminus \{j\} \) and \( L^{k+1} := L^{k+1} \cup \{j\} \).

For \( j \in \{U^k \setminus U^k\} \): If \( \mu \leq \mu_j^l \) then \( U^k := U^k \setminus \{j\} \) and \( M^k := M^k \cup \{j\} \).

Set \( M^{k+1} := M^k \) and \( U^{k+1} := U^k \).

If \( J^{k+1} \cup L^{k+1} \cup U^{k+1} = \emptyset \) then find optimal solution and stop, else set \( k := k + 1 \) and go to Step 1.

**Step 3.2** (peg upper bounds):

Update upper bound, \( \mu := \hat{\mu}^k \), and resource \( b^{k+1} := b^k - \beta^k_+ \).

Set \( x^*_j := u_j \) for \( j \in U^k \), \( J^{k+1} := J^k \setminus U^k \) and \( U^{k+1} := U^k \setminus U^k \).

For \( j \in \{J^{k+1} \setminus L^k\} \): If \( \mu_j \leq \mu_j^l \) then \( J^{k+1} := J^{k+1} \setminus \{j\} \) and \( U^{k+1} := U^{k+1} \cup \{j\} \).

For \( j \in \{L^k \setminus L^k\} \): If \( \mu \leq \mu_j^l \) then \( L^k := L^k \setminus \{j\} \) and \( M^k := M^k \cup \{j\} \).

Set \( M^{k+1} := M^k \) and \( L^{k+1} := L^k \).

If \( J^{k+1} \cup L^{k+1} \cup U^{k+1} = \emptyset \) then find optimal solution and stop, else set \( k := k + 1 \) and go to Step 1.

**Remark 7.** Note that for DBR2 in Section 4.3.4 we determine whether we should continue with DIR or DER from \( |J^k| < 2|U(\hat{\mu}^k) \cup L(\hat{\mu}^k)\). This condition needs to be modified for the 3- and the 5-sets algorithms DBR3 and DBR5. This is done by substituting the condition mentioned by \( |J^k \cup M^k| < 2|U(\hat{\mu}^k) \cup L(\hat{\mu}^k)| \) and \( |J^k \cup M^k \cup L^\_ \cup U^\_| < 2|U^k(\hat{\mu}^k) \cup L^k(\hat{\mu}^k)| \) for 3- and 5-sets pegging, respectively.

### 4.4 Optimality of the relaxation algorithms

For the inequality problem (1), optimality and validation for the pegging process for the primal relaxation algorithm PIR2 was established by Breitfauer and Shetty [BS02b, Propositions 1–9]. Let \( k^* \) be the iteration where the algorithm terminates. Then Breitfauer and Shetty state that the primal relaxation algorithm generates the following solution for problem (2):

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\[ \mu = \mu^k = -\phi'_j(x_j^k)/g_j(x_j^k), \quad j \in J^k, \]  
\[ \rho_j = \phi'_j(t_j^k) + \mu^k g'_j(x_j^k), \quad j \in L, \]  
\[ \rho_j = 0, \quad j \in J^k \cup U, \]  
\[ \lambda_j = -\phi'_j(u_j^k) - \mu^k g'_j(x_j^k), \quad j \in U, \]  
\[ \lambda_j = 0, \quad j \in J^k \cup U, \]

\[ x_j = l_j, \quad j \in L, \]  
\[ x_j = u_j, \quad j \in U, \]  
\[ x_j = x_j^k, \quad j \in J^k. \]

Brethauer and Shetty establish that this solution fulfills all KKT conditions, and therefore is optimal.

The optimality and convergence for the equality problem (2) can be established similarly to the proof for the inequality problem given in [BS02b] except for the proof for feasibility of the dual variables corresponding to the lower and upper bounds (Propositions 8 and 9 in [BS02b]). Additionally we do not have to prove that \( \mu^* \geq 0 \) (Proposition 4 in [BS02b]) for the equality problem. Therefore we give a complementary proof for the feasibility of the dual variables corresponding to the lower and upper bounds. For the equality problem (2) we have that \( g_j(x_j) = a_j x_j \) and in the proof we will assume that \( a_j > 0 \).

**Lemma 1.** Consider the equality problem (2) and algorithm PIR2 in Section 4.3.1.

(a) If \( \nabla^k > \Delta^k \) then \( \mu^k \geq \mu^k \).

(b) If \( \nabla^k < \Delta^k \) then \( \mu^k \leq \mu^k \).

**Proof.** The proof is similar to that of Proposition 7 in [BS02b].

**Proposition 6** (feasibility of dual variables corresponding to bounds). For problem (2), the solution (13) generated by PIR2 in Section 4.3.1 satisfies the feasibility of the dual variables \( (\rho_j, \lambda_j) \) corresponding to the lower and upper bounds.

**Proof.** (i) For \( j \in J^k \cup U \), we have from (13c) that \( \rho_j = 0 \).

(ii) For \( j \in L \), we have from (13c) that \( \rho_j = \phi'_j(l_j) + \mu^k a_j \). We know that all variables \( x_j \) with \( j \in L \) were pegged in the iterations \( k \) where \( \nabla^k > \Delta^k \). For these iterations \( k \) we have \( x_j^k < l_j \). Further, from the convexity of \( \phi_j \) and the assumption that \( a_j > 0 \), we have that \( \mu(x_j) = -\phi'_j(x_j)/a_j \) is decreasing in \( x_j \). Hence,

\[ \frac{\rho_j}{a_j} = \frac{\phi'_j(l_j)}{a_j} + \mu^k \geq \frac{\phi'_j(x_j^k)}{a_j} + \mu^k = -\mu^k + \mu^k \geq 0, \]  

where the last inequality follows from Lemma 1(a).

(iii) For \( j \in J^k \cup U \), we have from (13c) that \( \lambda_j = 0 \).

(iv) For \( j \in U \), we have from (13e) that \( \lambda_j = -\phi'_j(u_j) - \mu^k a_j u_j \). We know that all variables \( x_j \) with \( j \in U \) were pegged in the iterations where \( \nabla^k < \Delta^k \). For these iterations \( k \) we have \( x_j^k > u_j \). Further, from the convexity of \( \phi_j \) and the assumption that \( a_j > 0 \), we have that \( \mu(x_j) = -\phi'_j(x_j)/a_j \) is decreasing in \( x_j \). Hence,

\[ \frac{\lambda_j}{a_j} = \frac{-\phi'_j(u_j)}{g'_j(u_j)} - \mu^k \geq \frac{-\phi'_j(x_j^k)}{g'_j(x_j^k)} - \mu^k = \mu^k - \mu^k \geq 0, \]  

where the last inequality follows from Lemma 1(b).

The algorithms in Sections 4.3.2, 4.3.3, and 4.3.4 will also converge to the optimal solution since they are equivalent to PIR.

**Remark 8.** If we introduce the additional assumption that \( \phi_j \) and \( g_j \) are twice differentiable and that \( g'_j > 0 \), an alternative convergence result for the dual relaxation algorithm is found in [Ste01].
4.5 Time complexity

Consider algorithm PIR2 in Section 4.3.1. In Step 0 we need at most $2n$ comparisons to determine the primal variables and $C_0n$ operations, for a constant $C_0$, to determine if the solution is feasible or not. In Step 1, we solve the relaxed problem, which gives $C_1n$ operations for a constant $C_1$. In Step 2 we perform at most $2n$ comparisons to determine the lower and upper sets and we compute $\Delta^k$ and $\nabla^k$, which gives at most $C_2n$ operations for a constant $C_2$. Steps 3.1 and 3.2 give at most $2n + 1$ operations. Further, in the worst case the algorithm only pegs one primal variable in each iteration, which results in $n$ iterations. Hence, we conclude that the algorithm has a complexity of $O(n^2)$.

5 A quasi-Newton algorithm (NZ)

Nielsen and Zenios [NZ92, Section 1.4] develop a quasi-Newton method for finding the dual optimal solution $\mu^*$ of the problem (2). It is assumed that the objective term $\phi_j$ is strictly convex with a derivative $\phi'_j$ whose range is $\mathbb{R}$. They compare their numerical method with three linesearch methods [HKL80, CL81, Tse90]. Their results show that their numerical method always performs well compared with the other algorithms. They implement their algorithms on a massively parallel computer. This is not our intention. But since the algorithm seems to perform well on parallel computers it makes sense to evaluate it on non-parallel computers.

Let $f_j$, $j \in J$, be the inverse of $\phi'_j$ such that

$$\text{for } j \in J, \quad \phi_j(f_j(\mu)) = \mu, \quad \mu \in \mathbb{R}. \tag{16}$$

Similar to (5) we conclude that

$$x_j(\mu) = \max \{l_j, \min \{f_j(a_j\mu), u_j\}\}. \tag{17}$$

The heart of the algorithm is, like in the breakpoint algorithm, to find $\mu$ such that the primal constraint (1b) is fulfilled. In other words find $\mu$ such that

$$\Psi(\mu) := b - \sum_{j \in J} a_j x_j(\mu) = 0. \tag{18}$$

Nielsen and Zenios [NZ92, Section 1.4] define two functions $\Phi^+_j$ and $\Phi^-_j$:

$$\Phi^+_j(\mu) := \begin{cases} \min \{f_j(a_j\mu), u_j\}, & \text{if } a_j > 0, \\ \max \{l_j, f_j(a_j\mu)\}, & \text{if } a_j < 0 \end{cases}, \quad j \in J, \tag{19}$$

and

$$\Phi^-_j(\mu) := \begin{cases} \min \{f_j(a_j\mu), u_j\}, & \text{if } a_j < 0, \\ \max \{l_j, f_j(a_j\mu)\}, & \text{if } a_j > 0 \end{cases}, \quad j \in J. \tag{20}$$

Note that for $j \in J$, if $a_j > 0$ and $f_j$ is concave and increasing then $\Phi^+_j$ is concave and if $a_j > 0$ and $f_j$ is convex and decreasing then $\Phi^-_j$ is convex. Further, we define two sets of indices such that $J^+ := \{ j \in J \mid a_j > 0 \}$ and $J^- := \{ j \in J \mid a_j < 0 \}$. Define two approximation of $\Psi$ such that

$$\Psi^+(\mu) := b - \sum_{j \in J} a_j \Phi^+(\mu)$$

$$= b - \sum_{j \in J^+} a_j \min \{g(a_j\mu), u_j\} - \sum_{j \in J^-} \max \{l_j, g(a_j\mu)\}, \tag{21a}$$
Further, define $\mu^*$:

$$\Psi^-(\mu) := b - \sum_{j \in J} a_j \Phi^-(\mu) = b - \sum_{j \in J} a_j \min \{ g(a_j \mu), u_j \} - \sum_{j \in J^+} \max \{ l_j, g(a_j \mu) \}. \quad (22a)$$

Note that if $a_j > 0$ and $f_j$ is concave then $\Psi^+$ is convex and if $a_j > 0$ and $f_j$ is convex then $\Psi^-$ is concave. Define the sub- and superdifferentials of $\Psi^+$, respectively, $\Psi^-$, as

$$\partial \Psi^+(\mu) := \{ d \in \mathbb{R} \mid (\Psi^+(\mu') - \Psi^+(\mu)) \geq d(\mu' - \mu) \quad \forall \mu' \in \mathbb{R} \}, \quad (23a)$$

$$\partial \Psi^-(\mu) := \{ d \in \mathbb{R} \mid (\Psi^-(\mu') - \Psi^-(\mu)) \leq d(\mu' - \mu) \quad \forall \mu' \in \mathbb{R} \}. \quad (23b)$$

Further, define $\mu^*_{\epsilon}$ and $x^*_{\epsilon}$ as the approximate dual and primal solution such that $|\Psi(\mu^*_{\epsilon})| < \epsilon$ where $\epsilon > 0$. The algorithm (NZ) follows ([NZ92, Linesearch 4]):

**Initialization:** Set $\epsilon > 0$, $k = 0$, $\mu^0 \in \mathbb{R}$.

**Iterative algorithm:**

**Step 1** (compute step size):

- If $\Psi(\mu^k) > \epsilon$ then
  $$\Delta \mu^{k+1} := -\frac{\Psi(\mu^k)}{d^k} \text{ where } d^k \in \partial \Psi^+(\mu^k); \text{ go to Step 2},$$
- else if $\Psi(\mu^k) < -\epsilon$ then
  $$\Delta \mu^{k+1} := -\frac{\Psi(\mu^k)}{d^k} \text{ where } d^k \in \partial \Psi^-(\mu^k); \text{ go to Step 2},$$
- else
  $$\text{Set } \mu^*_{\epsilon} = \mu^k \text{ and determine } x^*_{\epsilon} \text{ from (17). Stop.}$$

**Step 2** (dual variable update):

- set $\mu^{k+1} := \mu^k + \Delta \mu^{k+1}$.

**Step 3:** Set $k := k + 1$ and go to Step 1.

The algorithm converges to a value $\mu^*_{\epsilon}$, such that $|\Psi(\mu^*_{\epsilon})| < \epsilon$ if the objective function components $\phi_j$ is such that the corresponding function $\Psi^+(\mu)$ is convex or if the corresponding function $\Psi^-(\mu)$ is concave [NZ92, Proposition 8]. For some problems, the inverse of the derivative might however result in imaginary values. One solution to this problem is to consider the equivalent maximization problem of (2), i.e., to maximize $x - \phi(x)$.

**Remark 9.** In practice we will choose $\epsilon > 0$ and the algorithm will in most cases stop such that $|\Psi(\mu^k)| > 0$. Hence we will end up with an approximate solution of the optimal dual variable $\mu^*_{\epsilon}$. The map from the dual space to the primal might not be linear. Hence the primal error might be larger than we expect, i.e., $|x^*_{\epsilon} - x^*| >> |\mu^*_{\epsilon} - \mu^*|$.

However, there are methods for generating primal optimal solutions from any Lagrangian dual vector (see for example [LMOP08]). Another plausible method to find the optimal solution from the approximate solution $\mu^*_{\epsilon}$ is to use a breakpoint or a relaxation algorithm, starting from $\mu^*_{\epsilon}$.

## 6 Method of algorithm evaluation

This section serves to provide an overview of the procedure for the numerical study. In Section 6.1 we define problem instances for the numerical study. Some theory on how the problem instances can be designed follows in Section 6.2. In Section 6.3 we give a brief overview of performance profiles ([DM02]) which are used for the evaluation of the numerical study. Finally, in Section 6.4, we describe the computational environment.
6.1 Problem set

For the numerical study we consider five common special cases of problem (2); it also covers the inequality problem (1) when $\mu > 0$. Only finite values of the lower an upper bounds (2c) are considered, i.e., for $j \in J$, $l_j > -\infty$ and $u_j < \infty$. The five problem cases are briefly specified next:

**Quadratic problem** The convex separable quadratic problem is the special case of (2), where

$$
\phi_j(x_j) = \frac{w_j}{2} x_j^2 - c_j x_j \quad \text{for} \quad j \in J,
$$

(24)

where $w_j, c_j > 0$, $j \in J$. Numerical studies of algorithms for problem (24) are widely explored; e.g., see [NZ92, Kiw07, Kiw08a, Kiw08b]. In our numerical study the parameters are randomized such that $a_j \in [1, 30]$, $w_j \in [1, 20]$, $c_j \in [1, 25]$, $l_j \in [0, 3]$ and $u_j \in (3, 11]$.

**Stratified sampling** If we have a large population and would like to perform a statistical research among the population, it is practically infeasible to examine every single individual in the population. Instead we can stratify the population into $n$ strata. An example of a stratum might be people of a certain age. Let $M$ be the number of individuals in the entire population and $M_j$ the number of individuals in strata $j$. If we want to minimize the variance of the entire population we need to allocate the number of samples $x_j$ from each strata from:

$$
\phi_j(x_j) = \omega_j \frac{(M - x_j) \rho_j^2}{(M - 1) x_j} \quad \text{for} \quad j \in J,
$$

(25)

where $\omega_j = M_j / M$ and $\rho_j$ is an estimate of the variance for strata $j$. From $b$ in the resource constraint we specify the total sample size. In our numerical study the parameters are randomized such that $a_j \in [1, 30]$, $m_j \in [5, 30]$, $c_j \in [1, 4]$, $l_j \in [1, 3]$ and $u_j \in (3, 15]$.

**Sampling** According to [BRS99], often the objective terms for sampling problems can be written as

$$
\phi_j(x_j) = c_j / x_j \quad \text{for} \quad j \in J.
$$

(26)

In our numerical study the parameters are randomized such that $a_j \in [1, 4]$, $c_j \in [5, 30]$, $l_j \in [0, 3]$ and $u_j \in (3, 6]$.

**The theory of search** In the theory of search problem it is determined how a resource $b$ of time should be spent to find an object among $n$ subdivisions of an area with the largest probability. It is assumed that we know the probability $m_j$ for an object to be found in subdivision $j$. The objective component $\phi_j$ describes the probability of finding the object in subdivision $j$ and takes the form:

$$
\phi_j(x_j) = m_j (e^{-b_j x_j} - 1) \quad \text{for} \quad j \in J.
$$

(27)

This problem is widely explored by Koopman [Koo53, Koo99] and the problem is possible to apply to a large variation of search problems, e.g., searching for refugees fleeing from Cuba [Sto81]. In our numerical study the parameters are randomized in the following intervals: $m_j \in [0.5, -8]$, $b_j \in [0.1, 3]$, $a_j \in [1, 3]$, $l_j \in [0, 0.1]$ and $u_j \in (0.1, 5]$.

**Negative entropy function** The negative entropy function mentioned in [NZ92]:

$$
\phi_j(x_j) = x_j \log \left( \frac{x_j}{a_j} \right) - 1 \quad \text{for} \quad j \in J.
$$

(28)

In our numerical study the parameters are randomized such that $c_j \in [50, 250]$, $l_j \in [20, 100]$ and $u_j \in (30, 210]$. 

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6.2 Design of problem instances

Similarly to the numerical study in [KL98], we divide our set of test problem instances into groups containing different portions of the activities within the lower and upper bounds at the optimal solution. Let $H := \{ j \in J \mid l_j < x_j^* < u_j \}$. Then, the percentage is determined as $|H|/n$. To motivate this approach, we refer to the variance of CPU times for different portions of active activities in [KL98]. Further, similar to the numerical study in [Kiw07], we consider different problem sizes $n$ since the theoretical CPU time for different algorithms vary between $O(n)$ and $O(n^2)$.

For the problem set, we pseudo randomize the parameters $l_j$, $u_j$ and all the parameters associated with $\phi_j$ and $g_j$. In the numerical study we use a linear resource constraint such that $g_j(x_j) = a_j x_j$, where $a_j > 0$ for all $j \in J$. This simplifies the design of the problem set, since $\phi_j$ is convex and $l_j < u_j$ for all $j \in J$. We have that

$$x_j^* = \begin{cases} 
  x_j^*, & \text{if } \mu^* = -\phi'_j(x_j^*)/a_j, \\
  l_j, & \text{if } \mu^* \geq -\phi'_j(l_j)/a_j \geq -\phi'_j(u_j)/a_j, \\
  u_j, & \text{if } \mu^* \leq -\phi'_j(u_j)/a_j \leq -\phi'_j(l_j)/a_j.
\end{cases} \tag{29}$$

By using the properties of (29) we can determine $H$ such that $|H|/n = y$ for any $y \in [0, 1]$.

6.3 Performance profiles

Dolan and Moré [DM02] propose a performance profile for the evaluation of optimization software. The method is briefly summarized as follows: Assume that we have a set $A$ of algorithms that consist of $n_a$ algorithms and a problem set $P$ that consists of $n_p$ problem instances. Let $t_{p,a}$ denote the time it takes for algorithm $a \in A$ to solve problem $p \in P$. A performance ratio $r_{p,a}$ is introduced:

$$r_{p,a}(t_{p,a}) := \frac{t_{p,a}}{\min\{t_{p,l} \mid l \in A\}}. \tag{30}$$

For a problem $p$, the performance ratio is a measure of how fast algorithm $a$ is relative to the fastest algorithm solving problem $p$. Fix a constant $r_M$ such that $r_M \geq r_{p,a}$ for all $p \in P$, $a \in A$ and let $r_M = r_{p,a}$ if algorithm $a$ fails to solve problem $p$. Further, we introduce the distribution

$$\rho_a(\tau) = \frac{1}{n_p} |\{p \in P \mid r_{p,a} \leq \tau\}|, \tag{31}$$

for each algorithm, where $|\cdot|$ denote the cardinality of a set and $\tau \in [1, r_M]$. For algorithm $a$, the distribution $\rho_a$ describes the percentage of problem instances that are solved at least as fast as $\tau$ times the fastest algorithm for problem $p$. Note that $\rho_a(1)$ is the percentage for algorithm $a$ being the fastest. Moreover, $\lim_{\tau \to r_M} \rho_a(\tau)$ is the probability that algorithm $a$ will solve a problem $p$ in $P$. If we have a large problem set $P$ then $\rho_a(\tau)$ will not be affected much by a small change in $P$ ([DM02, Theorem 1]).

6.4 Program language, computer and code

The algorithms are implemented in Fortran 95, compiled with gfortran under mac OS X 10.8.2 (2.5 GHz Intel Core i5, 4 GB 1600 MHz DDR3).

7 Computational experiments

In this section we present the results from numerical experiments of the problems defined in Section 6.1. If nothing else is mentioned, 100 problem instances of each problem is evaluated for each problem size. Further, the problem instances are designed such that different values of $|H|/n$ are considered, see Section 6.2.
The development of numerical experiments for the problem (1) is illustrated in Table 1, where we cite the size of the largest test problem reported during each decade; the table is an extension of Table 2 in [Pat08].

<table>
<thead>
<tr>
<th>Decade</th>
<th>50s</th>
<th>60s</th>
<th>70s</th>
<th>80s</th>
<th>90s</th>
<th>00s</th>
<th>10s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Breakpoint algorithm</td>
<td>2</td>
<td>60</td>
<td>12</td>
<td>200</td>
<td>10^4</td>
<td>2 · 10^6</td>
<td>30 · 10^6</td>
</tr>
<tr>
<td>Relaxation algorithm</td>
<td>–</td>
<td>–</td>
<td>200</td>
<td>200</td>
<td>10^4</td>
<td>2 · 10^6</td>
<td>110 · 10^6</td>
</tr>
</tbody>
</table>

In Section 7.1 we present performance profiles for the relaxation algorithms defined in Section 4. In Section 7.2 we evaluate the pegging process for both the breakpoint and the relaxation algorithm defined in Section 3. In Section 7.3, the best performing relaxation algorithm and breakpoint algorithm are compared with the quasi-Newton algorithm in Section 5. In Section 7.4 we give a critical review of the numerical study. Finally, in Section 8, we make some overall conclusions.

In the following Figures 2–4 we show performance profiles, as defined in Section 6.3, for three competing sets of algorithms. To summarize the appearance of these plots, for each plot and corresponding competing set of algorithms, the graph for one algorithm shows the portion (between 0 and 1 on the y-axis) of the problem instances considered that are solved within \( \tau \) (on the x-axis) times the fastest algorithm in the test for problem \( p \). In particular, the value of \( \rho_a(1) \) is the portion of the problems in which algorithm \( a \) is the fastest, and \( \lim_{\tau \to \infty} \rho_a(\tau) \) is the probability that algorithm \( a \) will solve a problem \( p \) in \( P \). (The latter information is particularly illustrative and relevant for Figure 4.)

### 7.1 Evaluation of the relaxation algorithm

We evaluate the different paths in Figure 1. First, recall that PIR2 determines the primal variables while DIR2 determines the dual variable. As can be seen in the leftmost performance profile in Figure 2, DIR2 is the fastest in 67.8% of the problem instances solved. The result is what we can expect from theory, since DIR2 does not need as many operations in Step 1; see Sections 4.3.1 and 4.3.2. PIR2 is faster in 32.2% of the problems solved; the latter cases stem mainly from to the negative entropy problem (28) but also from the theory of search problem (27) and the stratified sampling problem (25) when \( n \) and \( |H|/n \) is small. The reason for PIR2 to be faster in almost all cases for the negative entropy problem is due to the computationally simple expression of the primal variables \( x_k^j(\mu^k) = \frac{a}{\sum_{j\in j_k} c_j} \) while the dual variable is evaluated from \( \mu^k = \log \sum_{j\in j_k} c_j - \log b \). Also the computations of the breakpoints might be a larger part of the total time when the equations for the primal/dual variables are simple.

We recall that DER2 applies explicit evaluation, DIR2 applies implicit evaluation and DBR2 applies the theoretically most profitable evaluation. The results are in favour of DBR2 and DIR2; see the rightmost performance profile in Figure 2. DBR2 is fastest in 70.6%, DIR2 is fastest in 25.9% and DER2 is fastest in 4.7% of the problems solved. (Note that 70.6% + 25.9% + 4.7% = 100.2%; in some cases two algorithms are equally fast.)

Figure 2 also shows that the performance of DIR2 and DBR2 are quite similar. For just a few cases DIR2 is more than 1.30 times slower than the fastest algorithm while for as few cases DBR2 is only 1.2 times slower than the fastest algorithm. On average DBR2 performs somewhat better than DIR2.

**Conclusion** For the problem set considered, it is more profitable to evaluate the dual variable even if we have to compute all the breakpoints at the beginning of the algorithm. Hence for the problem set considered DIR2 seems to outperform PIR2.
For the problem set considered, the results show that in most cases it is more profitable to evaluate a solution \( x^k \) implicitly. The small difference between the performance of DBR2 and DIR2 implies that in most cases \( |J^k| > 2|L(\mu^k) \cup U(\mu^k)| \). We conclude that DBR2 performs slightly better than DIR2 which agrees with the theory in Section 4.3.4.

### 7.2 Evaluation of the pegging process

We compare the three pegging approaches for the breakpoint and relaxation algorithms described in Sections 3.3–3.5 and 4.3.5, respectively. For the breakpoint algorithm median search is implemented similarly to [PTVF92, Section 8.5].

The performance profiles in Figure 3 show that 5-sets pegging is nearly always the fastest (MB5 in 95% and DBR5 in 94% of the problem instances solved). Additionally, when 5-sets pegging is not fastest it is never more than 10% slower than the fastest algorithm. It is obvious that for the few cases when 2-sets pegging performs best are when few optimal primal variables equals the lower or upper bounds (\( |H|/n \) is small). This follows from the fact that 2-sets pegging does not check if the variables belong to the additional sets that are used in 3- and 5-sets pegging.

**Conclusion**  In general 5-sets pegging is the most profitable.

**Remark 10.** Numerical experiments for a breakpoint algorithm applying bisectional search of a sorted sequence of breakpoints, using quicksort as in [Knu98, Section 5.2.2], was also performed. The algorithm was on average 1.5 times slower than MB2. Also the algorithm in [Zip80], where the upper bounds are relaxed, was evaluated. The algorithm performed poorly, on average 2.9 times as slow as the breakpoint algorithm applying sorting.

### 7.3 A comparison between relaxation, breakpoint, and quasi-Newton methods

In this section we compare the best performing relaxation algorithm (DBR5), the best performing breakpoint algorithm (MB5), and the numerical quasi-Newton method (NZ) in Section 5. For NZ we use the stopping criterion \( \frac{\sum_{i \in J} x_i^2}{b} - 1 \) < 0.01 which is weaker than the stopping criterion in [NZ92] (< 10^{-4}). This will of course give us
an approximate optimal solution only. The initial value of the dual variable $\mu$ is set to the mean of the breakpoints $\mu^0 = (\sum_{j \in J} \phi_j(l_j)/a_j + \sum_{j \in J} \phi_j(u_j)/a_j)/(2n)$. If the algorithm does not converge within 100 CPU seconds, we start over with the mean of the breakpoints corresponding to the lower breakpoints $\mu^0 = (\sum_{j \in J} \phi_j(l_j)/a_j)/n$. Similarly, if the algorithm does not converge within 100 CPU seconds then we start over with the mean of the breakpoints corresponding to the upper breakpoints: $\mu^0 = (\sum_{j \in J} \phi_j(u_j)/a_j)/n$. If the algorithm does not terminate within 300 CPU seconds then we terminate the algorithm and consider the problem as unsolved.

The reader may have noticed that the breakpoint algorithms in Sections 3.3–3.5 are given without the use of the sets for the pegging process ($L, U, M, L-, U+$) while the relaxation algorithms in Section 4.3.1–4.3.5 are given with the use of these sets. Of course the notation using these sets, as for the relaxation algorithms, are theoretically more elegant. However, our implementations of the algorithms in Fortran 95 showed that for breakpoint algorithms it was in general more profitable to not use the pegging sets.

Figure 4 shows the performance profile for the algorithms. In general, we can see a significant advantage of using DBR5 since it is fastest for $99.0\%$ of the problem instances solved. Moreover, when DBR5 is not the fastest algorithm it is almost as fast as the fastest. From the figure we also see that MB5 is more than 2.7 times slower than the fastest algorithm in $50\%$ of the problem instances solved.

The Newton method terminated the fastest for only $1\%$ of the test problems, which probably is due to good initial values. Also we should have in mind that NZ terminates with an approximate solution only. The Newton method performs relatively well for the quadratic problem (24), the theory of search problem (27), and the negative entropy problem (28) when $|H|/n > 0.8$. It is not very successful for the stratified sampling problem (25) and the sampling problem (26). We can see from the performance profile that in $28\%$ of the problem instances tested, NZ is more than 5.5 times slower than DBR5 (the fastest algorithm). In $5.3\%$ ($158/3000$) of the problem instances the algorithm does not solve the problem; these problem instances mainly stem from the stratified sampling problem (25) and the sampling problem (26) when $|H|/n < 0.3$.

By comparing the performance profiles in Figure 4, we can see that they are very similar. In other words, relative to each other, the performance of the algorithms seems to be similar for different problem sizes $n$.

Considering the breakpoint algorithm MB5, Figure 5 shows that the CPU time increases when the number of optimal primal variables strictly within the bounds $|H|/n$ grows for the problems in the problem set. Concerning the relaxation algorithm DBR5 the result shows no significant dependence of $|H|/n$, neither does NZ.

Figure 3: The leftmost figure shows the performance profile for MB2, MB3 and MB5 and the rightmost for DBR2, DBR3 and DBR5. The numerical experiment was done according to the description in Section 6.2 for $n = 50 \cdot 10^3; 100 \cdot 10^3; 200 \cdot 10^3; 500 \cdot 10^3; 10^6; 2 \cdot 10^6$ and for the problems in Section 6.1. The algorithms were implemented uniformly.
Figure 4: Performance profile for DBR5, MB5 and NZ. (Left) The numerical experiment was done according to the description in Section 6.2 for $n = 50 \cdot 10^3, 100 \cdot 10^3, 200 \cdot 10^3, 500 \cdot 10^3, 10^6, \text{ and } 2 \cdot 10^6$ for the problems in Section 6.1. (Right) The numerical experiment was done according to the description in Section 6.2 but with 10 problem instances and for $n = 4 \cdot 10^6, 6 \cdot 10^6, 8 \cdot 10^6, 10 \cdot 10^6, 15 \cdot 10^6, 20 \cdot 10^6, 25 \cdot 10^6, \text{ and } 30 \cdot 10^6$ for the problems in Section 6.1.

Figure 5: The average CPU time for $n = 10^6$ is plotted as a function of the average portion of the optimal variables that obtain a value between the lower and upper bounds.

In Figure 6, we can see that the CPU time for MB5 and DBR5 is linear for $n \in [50 \cdot 10^3, 2 \cdot 10^6]$ respectively $n \in [50 \cdot 10^3, 30 \cdot 10^6]$. This is impressive, since DBR5 has a worst-case time complexity of $O(n^2)$. For problem sizes a bit larger than $30 \cdot 10^6$ variables the CPU time tends to increase faster. However, additional computations on a more powerful computer have shown that, for the relaxation algorithm, the quadratic problem has a linear time complexity up to $n = 90 \cdot 10^6$, the sampling problem up to $n = 100 \cdot 10^6$, the theory of search problem up to $n = 70 \cdot 10^6$ and the negative entropy problem up to $n = 110 \cdot 10^6$. Hence we would also like to stress that the linearity probably is constrained by the memory of the computer rather than the algebra in the algorithm.

Tables 2–6 show the mean CPU time in seconds, for solving the problems in the problem set for DBR5, NZ and MB5. The tables show the great advantage of using DBR5.
FIGURE 6: The average CPU time is plotted as a function of the size of the problem $n$ for DBR5 and MB5. The values in the left figure are the mean of 100 problem instances solved and the values in the right figure are the mean of 10 problem instances solved.

TABLE 2: The average CPU times algorithms MB5, DBR5 and NZ for solving the quadratic problem (24). Each value is the mean of 100 randomized computations and the CPU times are given in seconds.

<table>
<thead>
<tr>
<th>$n$</th>
<th>50,000</th>
<th>100,000</th>
<th>200,000</th>
<th>500,000</th>
<th>1,000,000</th>
<th>2,000,000</th>
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<tbody>
<tr>
<td>DBR5</td>
<td>0.0031</td>
<td>0.0065</td>
<td>0.0136</td>
<td>0.0346</td>
<td>0.0702</td>
<td>0.1438</td>
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<tr>
<td>NZ</td>
<td>0.0083</td>
<td>0.0179</td>
<td>0.0378</td>
<td>0.1018</td>
<td>0.1923</td>
<td>0.3822</td>
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<tr>
<td>MB5</td>
<td>0.0097</td>
<td>0.0205</td>
<td>0.0428</td>
<td>0.1144</td>
<td>0.2346</td>
<td>0.4807</td>
</tr>
</tbody>
</table>

TABLE 3: The average CPU times algorithms MB5, DBR5 and NZ for solving the stratified sampling problem (25). Each value is the mean of 100 randomized computations and the CPU times are given in seconds. For NZ only the cases when NZ found the optimal solution have been considered.

<table>
<thead>
<tr>
<th>$n$</th>
<th>50,000</th>
<th>100,000</th>
<th>200,000</th>
<th>500,000</th>
<th>1,000,000</th>
<th>2,000,000</th>
</tr>
</thead>
<tbody>
<tr>
<td>DBR5</td>
<td>0.0040</td>
<td>0.0082</td>
<td>0.0167</td>
<td>0.0436</td>
<td>0.0875</td>
<td>0.1773</td>
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<tr>
<td>NZ</td>
<td>0.0379</td>
<td>0.0952</td>
<td>0.1529</td>
<td>0.3560</td>
<td>0.9026</td>
<td>1.8299</td>
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<tr>
<td>MB5</td>
<td>0.0098</td>
<td>0.0214</td>
<td>0.0438</td>
<td>0.1178</td>
<td>0.2390</td>
<td>0.4981</td>
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TABLE 4: The average CPU times algorithms MB, DBR5 and NZ for solving the sampling problem (26). Each value is the mean of 100 randomized computations and the CPU times are given in seconds. For NZ only the cases when NZ found the optimal solution have been considered.

<table>
<thead>
<tr>
<th>$n$</th>
<th>50,000</th>
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<tbody>
<tr>
<td>DBR5</td>
<td>0.0032</td>
<td>0.0069</td>
<td>0.0146</td>
<td>0.0375</td>
<td>0.0788</td>
<td>0.1597</td>
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<tr>
<td>NZ</td>
<td>0.1069</td>
<td>0.2403</td>
<td>0.5670</td>
<td>1.4319</td>
<td>3.8036</td>
<td>6.3949</td>
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<tr>
<td>MB5</td>
<td>0.0089</td>
<td>0.0192</td>
<td>0.0397</td>
<td>0.1066</td>
<td>0.2213</td>
<td>0.4522</td>
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</table>
Table 5: The average CPU times algorithms MB5, DBR5 and NZ for solving the theory of search problem (27). Each value is the mean of 100 randomized computations and the CPU times are given in seconds.

<table>
<thead>
<tr>
<th>n</th>
<th>50,000</th>
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<tbody>
<tr>
<td>DBR5</td>
<td>0.0063</td>
<td>0.0132</td>
<td>0.0259</td>
<td>0.0679</td>
<td>0.1382</td>
<td>0.2778</td>
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<tr>
<td>NZ</td>
<td>0.0187</td>
<td>0.0434</td>
<td>0.0940</td>
<td>0.2669</td>
<td>0.4511</td>
<td>0.9258</td>
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<tr>
<td>MB5</td>
<td>0.0127</td>
<td>0.0273</td>
<td>0.0549</td>
<td>0.1454</td>
<td>0.2983</td>
<td>0.6090</td>
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</table>

Table 6: The average CPU times algorithms MB5, DBR5 and NZ for solving the negative entropy problem (28). Each value is the mean of 100 randomized computations and the CPU times are given in seconds.

<table>
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<tr>
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<th>500,000</th>
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</thead>
<tbody>
<tr>
<td>DBR5</td>
<td>0.0036</td>
<td>0.0074</td>
<td>0.0157</td>
<td>0.0406</td>
<td>0.0837</td>
<td>0.1698</td>
</tr>
<tr>
<td>NZ</td>
<td>0.0071</td>
<td>0.0171</td>
<td>0.0310</td>
<td>0.0819</td>
<td>0.1709</td>
<td>0.3191</td>
</tr>
<tr>
<td>MB5</td>
<td>0.0096</td>
<td>0.0206</td>
<td>0.0427</td>
<td>0.1131</td>
<td>0.2326</td>
<td>0.4774</td>
</tr>
</tbody>
</table>

Summary  Even if NZ only finds an approximate solution and even if the stop criterion is weak, NZ is outperformed by DBR5. Hence, we see no reason to evaluate methods for finding the exact optimal solution $x^*$ from the approximate solution $x\_\varepsilon$ generated by NZ. In many cases, NZ fails to solve the stratified sampling problem (25) and the sampling problem (26). This is probably due to the stiffness of the problems.

MB5 performs very well for problems where $|H|/n$ is small. This is due to the pegging process: since we peg a large part of $x_k^k \in J^k$ in each iteration, the problem is reduced in the next iteration. This follows from the reduction of breakpoints by half in each iteration; note that this does not hold for the relaxation algorithm. This might be the reason for MB5:s dependency of $|H|/n$. However, DBR5 performs best for almost all of the problem instances solved and it is worth noting that DBR5 never performs poorly.

7.4 A critical review

When we set up the initial values for NZ, we tried different initial values and concluded that the one used was the most profitable on average. However, especially if we customize initial values for each problem, there may still be potential improvements available.

Considering the results in Section 7.1, we consider the dual algorithm (DIR2) to outperform the primal algorithm (PIR2) since it performs better in general. Then we continued to evaluate several modification of the dual algorithm while similar modifications of the primal relaxation algorithm were not evaluated, i.e., we don’t evaluate blended evaluation or 3- and 5-sets pegging for the primal algorithm. However since the plausible modification of the primal algorithm would take the same form as for the modification of the dual algorithm it is assumed that a modified dual algorithms will outperform a similar modified primal algorithm.

8 Conclusion

We have complemented the survey in [Pat08] on the resource allocation problem at hand, and introduced, and critically evaluated, new implementations of breakpoint and relaxation algorithms for its solution.

The results show that our new implementations (DIR2 and DBR2) of the relaxation algorithm outperform the earlier algorithms (PIR2 and DER2). Hence we should evaluate the dual variable for the relaxation algorithm,
i.e., DIR2 outperforms PIR2. Moreover, it is more profitable in theory, as well as in practice, to apply blended evaluation, i.e., DBR2 outperforms DER2 and DIR2. Our results, as well as the results in [RJL92, KL98, Kiw08b], imply that the relaxation algorithm is to prefer when a closed form of the dual variable $\mu$ can be found.

We introduced 3- and 5-sets pegging for the relaxation algorithm and showed that it is most profitable to apply 5-sets pegging, which also holds for the breakpoint algorithm.

For the problems considered, MB5 and DBR5 have a practical time complexity of $O(n)$ also for very large values of $n$. We also showed that the relaxation algorithm DBR5 performs better than both the Newton-like algorithm NZ and the breakpoint algorithm MB5. Potential future improvements include the implementation of a pegging method for a Newton-like algorithm and/or a hybrid of the different algorithms (NZ, DBR5 and MB5), and, hence, it would be of interest to compare the best algorithms from our study to these.

The findings made herein can most certainly be profitably utilized also in the efficient solution of the more complex versions of the resource allocation problem discussed, for example, in the books [Mje83, IK88, Lus12].

References


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<tr>
<th>Reference</th>
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