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Constraint aggregation for rigorous global optimization

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Abstract In rigorous constrained global optimization, upper bounds on the objective function help to reduce the search space. Obtaining a rigorous upper bound on the objective requires finding a narrow box around an approximately feasible solution, which then must be verified to contain a feasible point. Approximations are easily found by local optimization, but the verification often fails.

In this paper we show that even when the verification of an approximate feasible point fails, the information extracted from the results of the local optimization can still be used in many cases to reduce the search space. This is done by a rigorous filtering technique called constraint aggregation. It forms an aggregated redundant constraint, based on approximate Lagrange multipliers or on a vector valued measure of constraint violation. Using the optimality conditions, two-sided linear relaxations, the Gauss-Jordan algorithm and a directed modified Cholesky factorization, the information in the redundant constraint is turned into powerful bounds on the feasible set. Constraint aggregation is especially useful since it also works in a tiny neighborhood of the global optimizer, thereby reducing the cluster effect.

A simple introductory example demonstrates how our new method works. Extensive tests show the performance on a large benchmark.

Keywords constraint aggregation · global optimization · constraint satisfaction · filtering method · verified computing · interval analysis

Mathematics Subject Classification (2000) 90C26, 90C20, 90C46, 65K05

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1 Introduction

Global optimization is the task of finding the best admissible conditions to achieve an objective under given constraints, assuming that both are formulated in mathematical terms. Global optima can be found by a combination of a variety of filtering techniques usually embedded in a branch and bound scheme for complete search (see, e.g., the survey Neumaier [27]). If the results have to be rigorous, the calculations usually involve the use of interval arithmetic (see, e.g., Neumaier [25]).

Filtering (also called pruning) stands for reducing or discarding parts of the search space of an optimization problem. The classical filtering algorithms are based upon local consistencies [4] like 2B-consistency or Box-consistency (see, e.g., Benhamou et al. [2]), 3B-consistency (Lhomme [23]), HC4 (Benhamou et al. [1]), FBPD (Vu et al. [35]) and OCTUM (Chabert & Jaulin [3]). If applied to quadratic constraints, 2B-consistency or Box-consistency does not take advantage of the special properties of quadratic forms; therefore often results are poorer than desirable. 3B-consistency is more effective, but the practice shows that for quadratic problems they usually tend to be slow due to the exhaustive branching needed to achieve the required precision. Hull consistency techniques show promising results, but still do not optimally use the special structure of quadratic problems. For quadratic problems, improved filtering methods are discussed in Domes & Neumaier [7].

Higher order filtering methods usually include linear or convex relaxation. Rigorous linear over- and underestimators for general global nonlinear programming problems involving odd and even powers, reciprocals, exponentials, logarithms, square roots, and uncertain scalar multiples are discussed in Hongthong & Kearfott [15]. The relaxed linear program usually contains more variables and/or constraints than the original problem, but the constraints are much easier to exploit. A classical method by McCormick [24], extended by Sherali & Adams [34], called RLT (reformulation – linearization technique), is used by Lebbah et al. [22] in the QUAD algorithm.

The prize-winning (but nonrigorous) global optimization code BARON [28, 29] also uses linear relaxations. Another interesting approach was given by Kolev [21], and a selection of additional linear relaxation techniques can be found in Domes & Neumaier [8]. Higher degree relaxations and convex relaxations are also discussed in the literature; for example, affine and convex relaxations for non-convex multivariate polynomials in Garloff et al. [12].

Usually, filtering methods are very efficient at the beginning of a branch and bound procedure, but they tend to become inefficient close to the global solution, resulting in excessive branching until the required precision is achieved. This so-called cluster effect was first explained by Kaisheng & Kearfott [16]. Techniques designed to reduce or eliminate the cluster effect are discussed, e.g., by Schichl & Neumaier [31] and Goldsztejn et al. [13].

We introduce a new rigorous filtering technique called constraint aggregation. Based on an approximately feasible point, an aggregated redundant constraint is formed, using approximate Lagrange multipliers when the approximation is nearly feasible, or a vector valued measure of constraint violation when the approximation is sufficiently infeasible. Using appropriate symbolic reformulation, the optimality conditions, two-sided linear relaxations, the Gauss-Jordan algorithm and a directed mod-

ified Cholesky factorization, the information in the redundant constraint is turned into powerful bounds on the feasible set. Constraint aggregation is especially useful since it also works in a tiny neighborhood of the global optimizer, thereby reducing the cluster effect.

The following motivating example shows that constraint aggregation may drastically improve the enclosure of a feasible set. The example is only intended for demonstrating the new technique as simply as possible, not to show superiority to other filtering techniques. The theory developed in the present paper then explains the tricks behind this example – in fact variations of techniques used by Neumaier [26] to prove sufficient global optimality conditions for quadratic programs – into a general and powerful technique.

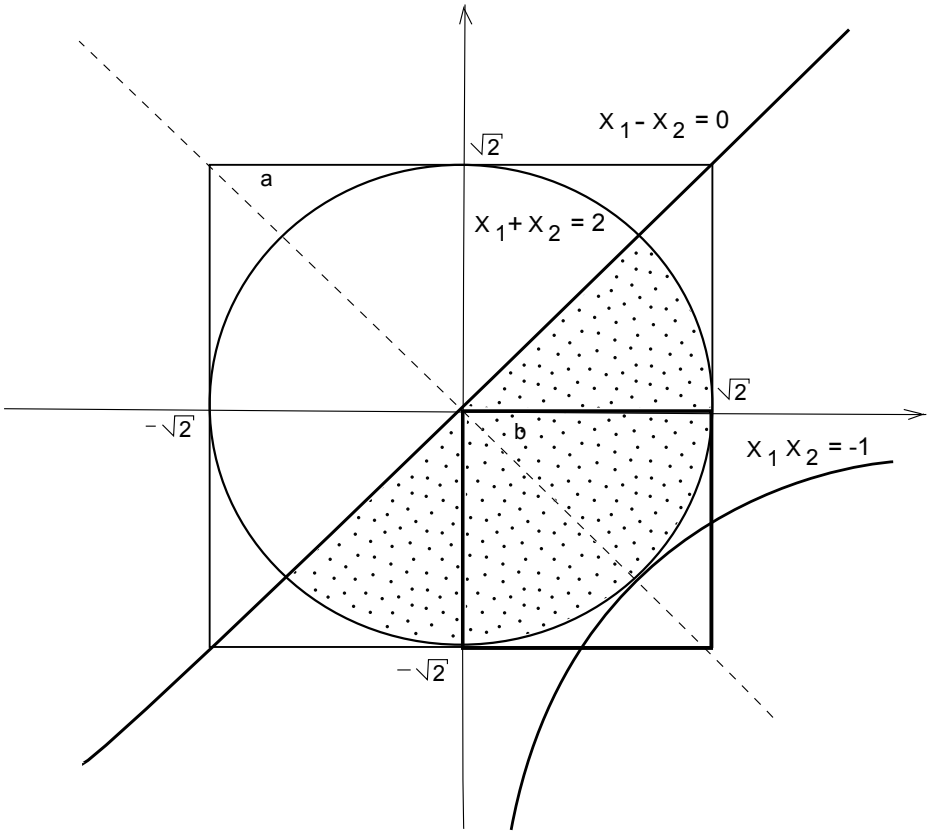

Fig. 1 Motivating example.

Example 1 Consider the simple two dimensional optimization problem

$$\begin{aligned} &\min\ x_1 x_2 \\ &\text{s.t.}\ \ x_1^2 + x_2^2 \le 2, \\ &\qquad x_1 - x_2 \ge 0. \end{aligned} \tag{1}$$

Suppose that a local optimizer found the optimal solution $x_1 = 1$, $x_2 = -1$ of (1), and the associated multipliers $\nu = 1$ (for the objective) and $y = (-0.5, 0)$ (for the constraints). The upper bound of the objective arising from the known point (namely the optimal solution) is $x_1 x_2 \leq -1$, resulting in the CSP

$$\begin{array}{ll} \text{find } (x_1, x_2) \\ \text{s.t.} & x_1 x_2 \leq -1, \\ & x_1^2 + x_2^2 \leq 2, \\ & x_1 - x_2 \geq 0 \end{array} \tag{2}$$

for potentially better points (see Figure 1). In the present case (as always when the local search happened to find the unique global minimizer), the CSP (2) has a feasible set consisting of a single point only: the minimizer.

Constraint propagation on the constraints of (2) results[1] in $x_1, x_2 \in [-\sqrt{2}, \sqrt{2}]$ only (see the box `a` in Figure 1). But if we aggregate the constraints using the multipliers $\nu = 1$ and $y = (-0.5, 0)$ we obtain

$$x_1 x_2 - (-0.5)(x_1^2 + x_2^2) + 0(x_1 - x_2) \leq 1(-1) - (-0.5)2 + 0, \tag{3}$$

hence $0.5(x_1 + x_2)^2 \leq 0$. The aggregated and simplified result is a strong new constraint since it implies $x_1 + x_2 = 0$. To make this an automatic consequence of constraint propagation we introduce the new variable z for $x_1 + x_2$ and transform this into the constraints

$$z = x_1 + x_2, \quad 0.5z^2 \leq 0. \tag{4}$$

Constraint propagation on (4) gives $z \in [0, 0]$. Therefore, the aggregated, transformed CSP may be written as

$$x_1 x_2 \leq -1, \quad x_1^2 + x_2^2 \leq 2, \quad x_1 - x_2 \geq 0, \quad z = x_1 + x_2, \quad 0.5z^2 \leq 0, \tag{5}$$

with the additional bounds $x_1, x_2 \in [-\sqrt{2}, \sqrt{2}]$. The interval hull of the linear subproblem

$$x_1 - x_2 \geq 0, \quad z = x_1 + x_2, \quad x_1, x_2 \in [-\sqrt{2}, \sqrt{2}], \quad z \in [0, 0], \tag{6}$$

obtainable constructively through linear bounding for the variables x_1 and x_2 (see Domes & Neumaier [8, p. 17]) is $x_1 \in [0, \sqrt{2}]$ and $x_2 \in [-\sqrt{2}, 0]$ (Figure 1, box `b`). With these improved bounds, constraint propagation on $x_1 x_2 \leq -1$ and $z = x_1 + x_2$ contracts the bounds to a single point, the optimal solution; cf. Figure 1.

In floating point arithmetic, the same computations should have approximately the same results.

The paper is organized as follows. After providing basic notation and terminology in Section 2.1, 2.2, and 2.3 we discuss a method for computing Lagrange-multipliers in 2.4. Then we introduce uncertainties (Section 2.5) and use them in Section 2.6 to specify the problem class treated, namely the uncertain optimization problems. Then we conclude the preliminaries by discussing feasibility (Section 2.7), bounds on the objective and verification of feasible points in Section 2.8. The second part

[1] This is true for simple consistency algorithms such as 2B, HC4, Box consistency and the like. However, for this simple example, constraint propagation with 3B-consistency would (as our new technique) directly reduce the domains to the optimal point. This is a coincidence that is unlikely to happen with more complex quadratic constraints.

is concerned about the new method, in particular about filtering by constraint aggregation (Section 3.1), filtering a singly-quadratic constraint satisfaction problem (Section 3.2), and finding good aggregators (Section 4). The latter is related to computable certificates of infeasibility (Subsection 4.1). We conclude the paper by giving extensive numerical tests in Section 5.

2 Preliminaries

2.1 Matrix notation

$\mathbb{R}^{m\times n}$ denotes the vector space of all $m \times n$ matrices A with real entries A_{ik} ($i = 1,\dots,m,\ k = 1,\dots,n$), and $\mathbb{R}^n = \mathbb{R}^{n\times 1}$ denotes the vector space of all column vectors of length n. For vectors and matrices, the relations $=$, $\neq$, $<$, $>$, $\leq$, $\geq$ and the absolute value $|A|$ of a matrix A are interpreted component-wise.

The number of nonzero entries of a matrix A is denoted by $\mathrm{nnz}(A)$. The n-dimensional identity matrix is denoted by I and the n-dimensional zero matrix is denoted by 0. The transpose of a matrix A is denoted by A^T, and A^{-T} is short for $(A^T)^{-1}$. The ith row vector of a matrix A is denoted by $A_{i:}$ and the jth column vector by $A_{:j}$. For an $n\times n$ matrix A, $\mathrm{diag}(A)$ denotes the n-dimensional vector with $\mathrm{diag}(A)_i = A_{ii}$.

The number of elements of an index set N is denoted by $|N|$. The set $\neg N$ denotes the complement of N. Let $I \subseteq \{1,\dots,m\}$ and $J \subseteq \{1,\dots,n\}$ be index sets and let $n_I := |I|$, $n_J := |J|$. For an n-dimensional vector x, x_J denotes the n_J-dimensional vector built from the components of x selected by the index set J. For an $m \times n$ matrix A, the expression $A_{I:}$ denotes the $n_I \times n$ matrix built from the rows of A selected by the index sets I. Similarly, $A_{:J}$ denotes the $m \times n_J$ matrix built from the columns of A selected by the index sets J. Instead of using the index sets I and J we also write $A_{i:k,j:l}$ if $I = \{i, i+1,\dots,k\}$ and $J = \{j, j+1,\dots,l\}$.

2.2 Boxes

A **box** $\mathbf{x} = [\underline{x}, \overline{x}]$, i.e., the Cartesian product of the closed real intervals $\mathbf{x}_i := [\underline{x}_i, \overline{x}_i]$, represents a (bounded or unbounded) axiparallel box in $\mathbb{R}^n$. $\overline{\mathbb{IR}}^n$ denotes the set of all n-dimensional boxes. To take care of one-sided bounds on variables, the values $-\infty$ and ∞ are allowed as lower and upper bounds of a box, respectively. The condition $x \in \mathbf{x}$ is equivalent to the collection of simple bounds

$$\underline{x}_i \leq x_i \leq \overline{x}_i \quad (i = 1,\dots,n),$$

or, with inequalities on vectors and matrices interpreted component-wise, to the two-sided vector inequality $\underline{x} \leq x \leq \overline{x}$. Apart from two-sided constraints, this includes fixed variables $x_i = a$ in case $\mathbf{x}_i = [a, a]$, upper bounding $x_i \geq a$ if $\mathbf{x}_i = [a, \infty]$, lower bounding $x_i \leq a$ if $\mathbf{x}_i = [-\infty, a]$ and free variables if $\mathbf{x}_i = [-\infty, \infty]$.

For the notation in interval analysis we mostly follow [20]. The box

$$\square S := [\inf(S), \sup(S)]$$

is called the **interval hull** of a set S of points in $\mathbb{R}^n$. We also define the **minimal point**

$$\mu(\mathbf{r}) := \begin{cases} \underline{r} \text{ if } \underline{r} > 0, \\ \overline{r} \text{ if } \overline{r} < 0, \\ 0 \text{ otherwise}, \end{cases} \tag{7}$$

of an interval $\mathbf{r}$. The notation extends componentwise to boxes.

2.3 Optimization problems

With the notation introduced, the traditional continuous, single-objective **optimization problem** consisting of smooth equality and inequality constraints may be written in the compact interval form

$$\begin{array}{l} \min f(x) \\ \text{s.t. } F(x) \in \mathbf{F}, \quad x \in \mathbf{x}, \end{array} \tag{8}$$

where $f : \mathbf{x} \to \mathbb{R}$ and $F : \mathbf{x} \to \mathbb{R}^m$ are functions defined on the box $\mathbf{x}$, and $\mathbf{F} \in \overline{\mathbb{IR}}^m$ is a box defining two-sided constraints for the components of $F(x)$; again, equality constraints and one-sided inequality constraints are included. A point $x \in \mathbf{x}$ is called a **feasible point** of (8) if $F(x) \in \mathbf{F}$ is satisfied. If $F(x) \notin \mathbf{F}$ for all $x \in \mathbf{x}$ the constraints are called **inconsistent** and the problem is called **infeasible**.

For reasons of efficiency, we shall consider in place of (8) the slightly more complex formulation

$$\begin{array}{l} \min a^T F(x) \\ \text{s.t. } BF(x) \in \mathbf{b}, \, x \in \mathbf{x}, \end{array} \tag{9}$$

$F : \mathbf{x} \to \mathbb{R}^w$, and $a \in \mathbb{R}^w$, $\mathbf{b} \in \mathbb{R}^m$, $B \in \mathbb{R}^{m \times w}$. This is both a special case of (8) and a generalization of it, as the traditional formulation (8) is obtained from (9) if we take $w = m + 1$, $\binom{f}{F}$ in place of F, $u = 1$, $a = \binom{1}{0}$, $B = (0 \; I)$ and $\mathbf{b} = \mathbf{F}$. From the point of view of solvability, (8) and (9) are therefore equivalent, as one can redefine $\widetilde{f}(x) := a^T F(x)$ and $\widetilde{F}(x) := BF(x)$. However, from a computational point of view, the form (9) has advantages that typically lead to improved linear relaxations once $\binom{a^T}{B}$ has more than one entry in some column. As we shall see in Section 2.6, this form also allows a natural formulation of problems with uncertain coefficients.

If the objective function is missing or it is constant, then (8) and (9) take the form

$$\begin{array}{l} \text{find } x \in \mathbf{x} \\ \text{s.t. } F(x) \in \mathbf{F}, \end{array} \tag{10}$$

$$\begin{array}{l} \text{find } x \in \mathbf{x} \\ \text{s.t. } BF(x) \in \mathbf{b}, \end{array} \tag{11}$$

respectively, of a **constraint satisfaction problem** (**CSP**).

2.4 **Lagrange multipliers**

We now consider the first order optimality conditions for a minimizer $\widehat{x}$ of an optimization problem of the form (9), where $f(x)$ and $F(x)$ are continuously differentiable. Let

$$\begin{aligned} L^b &:= \{i \mid \underline{x}_i = \widehat{x}_i < \overline{x}_i\}, \\ U^b &:= \{i \mid \underline{x}_i < \widehat{x}_i = \overline{x}_i\}, \\ N^b &:= \{i \mid \underline{x}_i < \widehat{x}_i < \overline{x}_i\}, \end{aligned} \tag{12}$$

$$\begin{aligned} E^c &:= \{j \mid \underline{b}_j = \overline{b}_j\}, \\ L^c &:= \{j \mid \underline{b}_j = BF_j(\widehat{x}) < \overline{b}_j\}, \\ U^c &:= \{j \mid \underline{b}_j < BF_j(\widehat{x}) = \overline{b}_j\}, \end{aligned} \tag{13}$$

and write $\mathbf{y}$ and $\mathbf{z}$ for the interval vectors with components

$$\mathbf{y}_j := \begin{cases} [-\infty,\infty] & \text{if } j \in E^c, \\ [0,\infty] & \text{if } j \in L^c, \\ [-\infty,0] & \text{if } j \in U^c, \\ 0 & \text{otherwise.} \end{cases} \qquad \mathbf{z}_i := \begin{cases} [0,\infty] & \text{if } i \in L^b, \\ [-\infty,0] & \text{if } i \in U^b, \\ 0 & \text{if } i \in N^b, \end{cases} \tag{14}$$

The necessary optimality conditions say that there are multipliers $\nu \in \mathbb{R}$ and $y \in \mathbf{y}$, not both zero, such that

$$Z(\nu, x, y) := F'(x)^T(\nu a - B^T y) \in \mathbf{z}, \tag{15}$$

and the complementarity conditions

$$\max((BF_j(x) - \underline{b}_j)y_j, (BF_j(x) - \overline{b}_j)y_j) = 0 \tag{16}$$

hold for $j = 1, \ldots, m$.

These conditions comprise the **Karush-John optimality conditions** for the problem (9); cf. the derivation and discussion of the history in Schichl & Neumaier [32].

If $\nu \neq 0$ we may rescale the multipliers to have $\nu = 1$, leading to the **Kuhn-Tucker optimality conditions**. We normalize instead by rescaling so that

$$\max(\nu, \|y\|_\infty) = 1,$$

which is possible even when $\nu = 0$, and leads to bounded multipliers. This is achieved by

$$\nu \leftarrow \frac{1}{\max(1, \|y\|_\infty)}, \qquad y \leftarrow \nu y. \tag{17}$$

The following result suggests a way to define Lagrange multipliers $y \in \mathbb{R}^m$ (for the constraints) and $\nu \in \mathbb{R}$ (for the objective) at an arbitrary point x (intended to be an approximate local minimizer).

Theorem 1 *If, for some $\widehat{x} \in \mathbb{R}^n$, the constrained optimization problem*

$$\begin{aligned} &\min\ g(y) := \|\mu(Z(1, \widehat{x}, y) - \mathbf{z})\|_2^2 \\ &\text{s.t.}\ \ y \in \mathbf{y} \end{aligned} \tag{18}$$

(with Z from (15) *and μ from* (7)*) has a solution $\widehat{y}$ with $g(\widehat{y}) = 0$ then $(\widehat{x}, \widehat{y})$ satisfies the Kuhn-Tucker conditions for* (9)*, and* (17) *defines the associated normalized multipliers satisfying the Karush-John conditions.*

Proof From $g(\widehat{y}) = 0$ it follows that $\mu(Z(1,\widehat{x},y) - \mathbf{z}) = 0$ implying $Z(1,\widehat{x},y) \in \mathbf{z}$, and therefore (15) is satisfied. Since $\widehat{y} \in \mathbf{y}$, the definition (14) of $\mathbf{y}$ implies that the complementary conditions (16)

$$\max(c_1, c_2) = 0, \quad c_1 := \ (BF_j(\widehat{x}) - \underline{b}_j)\widehat{y}_j, \quad c_2 := (BF_j(\widehat{x}) - \overline{b}_j)\widehat{y}_j),$$

are satisfied:
If $BF_j(\widehat{x}) = \underline{b}_j < \overline{b}_j$ then $\widehat{y}_j \geq 0$ therefore $c_1 = 0$ and $c_2 \leq 0$.
If $BF_j(\widehat{x}) = \overline{b}_j > \underline{b}_j$ then $\widehat{y}_j \leq 0$ therefore $c_1 \leq 0$ and $c_2 = 0$.
If $BF_j(\widehat{x}) = \underline{b}_j = \overline{b}_j$ then $\widehat{y}_j$ is arbitrary and $c_1 = 0$, $c_2 = 0$.
If $\underline{b}_j < BF_j(\widehat{x}) < \overline{b}_j$ then $\widehat{y}_j = 0$ therefore $c_1 = 0$ and $c_2 = 0$.
In each case, $\max(c_1, c_2) = 0$. Therefore the Kuhn-Tucker conditions are satisfied and $\widehat{x}$ must be a critical point of (9). □

Note that if $\widehat{x}$ is a Kuhn–Tucker point, then the (possibly underdetermined) system of equations

$$F'(\widehat{x})^T_{N^b:} B^T_{:V} y_V = F'_{N^b}(\widehat{x})^T a, \quad y_{\neg V} = 0, \quad V = E^c \cup L^c \cup U^c, \tag{19}$$

must have a solution $\widehat{y}$. If, in addition to this, $\widehat{y} \in \mathbf{y}$, and the inequalities

$$Z(1,\widehat{x},\widehat{y})_i \geq 0 \text{ for } i \in L^b, \quad Z(1,\widehat{x},\widehat{y})_i \leq 0 \text{ for } i \in U^b, \tag{20}$$

are satisfied, then $\widehat{y}$ is a Lagrange multiplier corresponding to $\hat{x}$, and (17) defines the associated normalized multipliers. If it works, this method gives a cheaper alternative for computing $\widehat{y}$; otherwise the more expensive constrained non-linear optimization problem (18) must be solved.

Algorithm 1: Computing the Lagrange multipliers

Input: A point $\widehat{x} \in \mathbb{R}^n$ approximately satisfying the bound constraint $x \in \mathbf{x}$ of (9) and a small tolerance $\delta \ll 1$ (e.g., $\delta := 10^{-9}$).
Output: The Lagrange multipliers: $\widehat{\nu}$ for the objective and $\widehat{y}$ for the constraints.

Compute $\delta^b_i = \min(\delta, \text{wid}(\mathbf{x}_i)/10)$ for $i = 1, \ldots, m$;
if $\widehat{x}_i < \min(\underline{x}_i + \delta^b_i, \overline{x}_i)$ **then** $\widehat{x}_i \leftarrow \underline{x}_i$;
if $\max(\underline{x}_i, \overline{x}_i - \delta^b_i) < \widehat{x}_i$ **then** $\widehat{x}_i \leftarrow \overline{x}_i$;
Form the index sets L^b, U^b, and N^b as defined in (12);
Compute $\delta^c_j = \min(\delta, \text{wid}(\mathbf{b}_j)/10)$ for $j = 1, \ldots, m$;
Form the index sets from (13) by

$$\begin{aligned} E^c &:= \{j \mid \overline{b}_j - \underline{b}_j \leq \delta\}, \quad L^c := \{j \notin E^c \mid BF_j(\widehat{x}) \leq \min(\underline{b}_j + \delta^c_j, \overline{b}_j)\}, \\ U^c &:= \{j \notin E^c \mid BF_j(\widehat{x}) \geq \max(\underline{b}_j, \overline{b}_j - \delta^c_j)\}. \end{aligned} \tag{21}$$

Construct the boxes $\mathbf{z}$ and $\mathbf{y}$ as given by (14);
Solve the linear system of equations (19) in order to obtain $\widehat{y}$;
if $\widehat{y} \notin \mathbf{y}$ *or one of the conditions* (20) *is not satisfied* **then**
  Solve the problem (18) by using a bound constrained solver;
  if *the solver found the solution* $\widetilde{y}$ *with* $g(\widetilde{y}) = 0$ **then** set $\widehat{y} \leftarrow \widetilde{y}$;
  else $\widehat{x}$ cannot satisfy the Kuhn-Tucker conditions, therefore signal failure;
end
Compute and return $\widehat{\nu}$ and $\widehat{y}$ according to (17);

In floating point arithmetic, the equalities and inequalities from above are often not satisfied exactly but only by a small tolerance δ. Algorithm 1 describes the solution process suitable for numerical computations.

2.5 Uncertain vectors and matrices

To rigorously account for inaccuracies in computed entries of a matrix, we use interval matrices, standing for uncertain real matrices whose coefficients are between given lower and upper bounds. Note that all boxes may be considered as interval vectors, i.,e., column vectors ($n \times 1$ matrices) with uncertain components, whose values are known only to lie withing given intervals. The midpoint, width and the radius of an interval matrix $\mathbf{A}$ are the scalar matrices defined by

$$\mathrm{mid}(\mathbf{A}) := (\overline{A} + \underline{A})/2, \quad \mathrm{wid}(\mathbf{A}) := \overline{A} - \underline{A}, \quad \mathrm{rad}(\mathbf{A}) := \mathrm{wid}(\mathbf{A})/2,$$

respectively. An interval, interval vector, or interval matrix is called **thin** or **degenerate** if its width is zero, and **thick** if its width is positive. A real matrix A is identified with the thin interval matrix with $\underline{A} = \overline{A} = A$.

The expression $\mathbf{A} := [\underline{A}, \overline{A}] \in \overline{\mathbb{IR}}^{m\times n}$ denotes an $m \times n$ interval matrix with lower bound $\underline{A}$ and upper bound $\overline{A}$. $\mathbf{A} \in \overline{\mathbb{IR}}^{n\times n}$ is symmetric if $\mathbf{A}_{ik} = \mathbf{A}_{ki}$ for all $i, k \in \{1, \ldots, n\}$. Given an expression $p(x)$ in $x = (x_1, \ldots, x_n)^T$ such that the evaluation at any $x \in \mathbf{x}$ is a real number, there are a number of methods for defining an **interval enclosure** of $p(x)$, i.e., a box $p(\mathbf{x})$ such that $p(x) \in p(\mathbf{x})$ holds for all $x \in \mathbf{x}$. The simplest is the interval evaluation, where one substitutes $\mathbf{x}_i$ for each occurrence of x_i in $p(x)$. More sophisticated (and often, but not always, better) possibilities include centered forms (for details, see, e.g., [25]).

2.6 Uncertain optimization problems

Traditionally, the coefficients of $f(x)$ and $F(x)$ are taken to be exactly known. To be able to rigorously account for uncertainties due to one of the following sources:

- measurements of limited accuracy,
- conversion errors from an original representation to our normal form,
- rounding errors when creating new constraints by relaxation techniques,

we allow the coefficients to vary in narrow intervals. All uncertainties can be conveniently expressed if we formulate an arbitrary optimization problem with uncertain coefficients as an instance of the following **uncertain optimization problem** (**UOP**)

$$\begin{array}{ll} \min & a^T F(x) \\ \text{s.t.} & BF(x) \in \mathbf{b},\ x \in \mathbf{x}, \\ \text{for some } a \in \mathbf{a},\ B \in \mathbf{B}. & \end{array} \tag{22}$$

Here $F : \mathbf{x} \to \mathbb{R}^w$ is defined on the box $\mathbf{x} \in \overline{\mathbb{IR}}^n$, and $a \in \mathbf{a} \in \mathbb{IR}^w$, $\mathbf{b} \in \overline{\mathbb{IR}}^m$, $B \in \mathbf{B} \in \mathbb{IR}^{m\times w}$. The entries of a and B are *not* variables but uncertain constants, whose precise values within the bounds $a \in \mathbf{a}$ and $B \in \mathbf{B}$ are not known. Thus whether a particular vector x is a solution of the UOP may depend on which $a \in \mathbf{a}$ and

$B \in \mathbf{B}$ is the true value. This ambiguity makes working with uncertain constraints nontrivial. It requires great care in the derivation of methods to ensure the validity of an enclosure no matter which value $a \in \mathbf{a}$ and $B \in \mathbf{B}$ is the true value.

If $\mathbf{a}$ and $\mathbf{B}$ are thin, (22) reduces to the **exact optimization problem** (**EOP**) (9).

If $\mathbf{a} = 0$ then (22) becomes the **uncertain constraint satisfaction problem** (**UCSP**)

$$\begin{array}{ll} \text{find} & x \in \mathbf{x} \\ \text{s.t.} & BF(x) \in \mathbf{b} \\ \text{for some } a \in \mathbf{a},\ B \in \mathbf{B}. & \end{array} \tag{23}$$

If, in addition, $\mathbf{a}$ and $\mathbf{B}$ contain only a single matrix, (22) reduces to the **exact constraint satisfaction problem** (ECSP) (11).

Any optimization problem with uncertain coefficients can be brought into the UOP form (22) by introducing new variables for every subexpression composed of a product with an uncertain coefficient or a linear combination in which a coefficient is uncertain. The transformation to this form will be done automatically in the upcoming version of GloptLab (Domes [5]).

As an example we consider the nonlinear, exact optimization problem

$$\begin{array}{l} \min\ x_1 + x_2 \\ \text{s.t.}\ \ x_1 + e^{0.1x_1 + 0.2x_2^2} \leq 1,\ x_1 \in [-1,1],\ x_2 \in [-2,0]. \end{array} \tag{24}$$

Since not all decimal numbers occurring in the problem are exactly representable as floating-point numbers, (24) must be represented internally as an UOP by introducing the intermediate variable $x_3 = 0.1x_1 + 0.2x_2^2$. Thus we have

$$\begin{array}{l} \min\ x_1 + x_2 \\ \text{s.t.}\ \ 0.1x_1 - x_3 + 0.2x_2^2 = 0,\ \ x_1 + e^{x_3} \leq 1, \\ \qquad x_1 \in [-1,1],\ \ x_2 \in [-2,0],\ \ x_3 \in [-\infty,\infty], \end{array}$$

ending up in

$$\begin{array}{l} \min\ a^T F(x) \\ \text{s.t.}\ \ BF(x) \in \mathbf{b},\ \ x \in \mathbf{x}, \end{array} \tag{25}$$

where

$$F(x) := (x_1,\ x_2,\ x_3,\ x_2^2,\ e^{x_3})^T,$$

$$a^T := (1\ 1\ 0\ 0\ 0), \quad B := \begin{pmatrix} 0.1 & 0 & -1 & 0.2 & 0 \\ 1 & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$\mathbf{x} := ([-1,1]\ [-2,0]\ [-\infty,\infty])^T, \quad \mathbf{b} := \begin{pmatrix} [0,0] \\ [-\infty,1] \end{pmatrix}.$$

In binary floating point arithmetic, the coefficient 0.1 cannot be represented. To ensure that the problem can be solved rigorously even in floating point arithmetic, we rewrite the unrepresentable exact problem (25) as the representable uncertain problem

$$\begin{array}{ll} \min & a^T F(x) \\ \text{s.t.} & BF(x) \in \mathbf{b}, \quad x \in \mathbf{x}, \\ \text{for some } B \in \mathbf{B}, & \end{array} \tag{26}$$

where a, $\mathbf{x}$ and $F(x)$ are as before, and

$$\mathbf{B} := \begin{pmatrix} [\nabla 0.1, \Delta 0.1] & [0,0] & [-1,-1] & [\nabla 0.2, \Delta 0.2] & [0,0] \\ [1,1] & [0,0] & [0,0] & [0,0] & [1,1] \end{pmatrix},$$

where ∇x denotes the largest vector of floating point numbers with $\nabla x \leq x$, and Δx denotes the smallest vector of floating point number with $\Delta x \geq x$.

2.7 **Feasibility**

The traditional definition of feasibility for an optimization problem does not make sense for the uncertain constraint satisfaction problem (22). For example, in case of the UOP

$$\begin{array}{ll} \min & x_1 + x_2 \\ \text{s.t.} & x_1 + a x_2 = 1, \quad x_1 \in [0,2], \quad x_2 \in [0,2] \\ \text{for some } a \in \mathbf{a} := [0.79, 0.81], & \end{array} \tag{27}$$

no single point can be feasible since it cannot satisfy (27) for all $a \in \mathbf{a}$. But the problem should not be classified as infeasible since, e.g., $x_1 = 1 - a$, $x_2 = 1$ should be considered as a coefficient-dependent solution. Since a is uncertain, this "solution" comprises the set $\{x \in \mathbb{R}^2 \mid x_1 \in [0.19, 0.21],\ x_2 = 1\}$. Therefore we must generalize the definition:

A set $Z \subseteq \mathbf{x}$ is called **feasible** for the uncertain optimization problem (22) if for all $B \in \mathbf{B}$ there is an $x \in Z$ with $BF(x) \in \mathbf{F}$, **infeasible** if $BF(x) \notin \mathbf{F}$ for all $B \in B$ and $x \in Z$, and **partially feasible** otherwise. The problem (8) is called feasible (infeasible) if $\mathbf{x}$ is feasible (infeasible). The **feasible set** of (22) is the set

$$\widehat{Z} := \{x \in \mathbf{x} \mid BF(x) \in \mathbf{b} \text{ for some } B \in \mathbf{B}\}$$

of all feasible or partially feasible points of (22).

The definition implies that if the set Z is feasible then all sets $Z' \subseteq \mathbf{x}$ containing Z are also feasible. In particular, the definition applies to boxes $Z = \mathbf{z}$, and a feasible set exists iff the box $\mathbf{x}$ is feasible, i.e., iff the problem itself is feasible. The solution set is nonempty iff $\mathbf{x}$ is feasible or partially feasible.

For example in the case of (27), the box $\mathbf{z}_1 := ([1.2, 1.27]\ [0,0])^T$ is feasible, the box $\mathbf{z}_2 := ([0.9, 0.95]\ [0,0])^T$ is infeasible and the box $\mathbf{z}_3 := ([1.25, 1.25]\ [0,0])^T$ is partially feasible. The problem (27) is feasible since $\mathbf{z}_1$ is feasible, $\mathbf{z}_1 \subset \mathbf{x}$ and thus the box $\mathbf{x}$ is feasible.

Given the uncertain optimization (22) or constraint satisfaction problem (23), we use the minimal point (7) to define the vector-valued **feasibility measure**

$$d(x) := \mu(\mathbf{B}F(x) - \mathbf{b}) \tag{28}$$

of a point $x \in \mathbb{R}^n$. For a given positive definite, diagonal scaling matrix D, the number $\|d(x)\|_D^2$ is called the **feasibility distance** of x for the problem (22).

A point x is called δ**-feasible** if $x \in \mathbf{x}$ and $\|d(x)\|_D^2 \leq \delta$, where $\delta > 0$ is a **feasibility tolerance**. In particular, feasible points are δ-feasible for every $\delta > 0$, and in an UCSP, a point is 0-feasible iff it is feasible for some choice of the uncertainties.

2.8 **Bounds on the objective and verification of feasible points**

To take account of the best known upper and lower bound in the objective function of an UOP we define

$$\begin{array}{ll} \min & a^T F(x) \in \mathbf{r} \\ \text{s.t.} & BF(x) \in \mathbf{b},\ x \in \mathbf{x}, \\ \text{for some } a \in \mathbf{a},\ B \in \mathbf{B}, \end{array} \tag{29}$$

as shorthand for

$$\begin{array}{ll} \min & a^T F(x) \\ \text{s.t.} & a^T F(x) \in \mathbf{r},\ BF(x) \in \mathbf{b},\ x \in \mathbf{x}, \\ \text{for some } a \in \mathbf{a},\ B \in \mathbf{B}, \end{array}$$

and similarly

$$\begin{array}{l} \min\ a^T F(x) \in \mathbf{r} \\ \text{s.t.}\ \ BF(x) \in \mathbf{b},\ x \in \mathbf{x}, \end{array} \tag{30}$$

as shorthand for

$$\begin{array}{l} \min\ a^T F(x) \\ \text{s.t.}\ \ a^T F(x) \in \mathbf{r},\ BF(x) \in \mathbf{b},\ x \in \mathbf{x}. \end{array}$$

Finding a good upper bound on the optimal objective function value is essential for efficiently solving global optimization problems. Using an upper bound from a feasible (and ideally nearly optimal) point eliminates most of the search space – leaving a CSP with a tiny feasible region only – and therefore usually saves a large amount of time by speeding up the branch and bound process.

To find a rigorously valid upper bound requires the verification of feasible points. Verification techniques usually consist of finding a narrow box centered at a given approximately feasible point, for which it was verified that it contains a feasible point. An upper bound on the function value over this box, computed by interval evaluation, then gives a rigorous upper bound on the objective function value. Of course, there may be no close feasible point, in which case a verification attempt will return without a result.

Various verification techniques are discussed by Hansen [14, Section 12] and Kearfott [17–19]; they where summarized and improved by Domes & Neumaier [11]. These verification techniques do not require to have an approximate local solution of the UOP (22) or the EOP (9); in principle, an arbitrary approximately feasible point suffices. But although finding a local optimizer takes more time, it is usually preferable over just finding an arbitrary approximately feasible point.

3 Constraint aggregation

In this section we generalize the ideas of Example 1, and present novel and efficient filtering method called constraint aggregation. The method proceeds in the following way:

- We start with the uncertain constraint satisfaction problem (23) or the uncertain optimization problem (29).

- Similar to (3) of Example 1, the first step of the method is to generate a linear combination of constraints (including constraints on the objective), called the aggregated constraint. The resulting new constraint satisfaction problem (which includes the original constraints and the new aggregated constraint) can be used to contract the starting box by means of arbitrary filtering methods. This step is discussed in Subsection 3.1.
- In case the original problem only contains linear and quadratic constraints (an arbitrary number of them), the aggregated constraint is also quadratic. By linearly relaxing the original constraints a singly quadratic constraint satisfaction problem is obtained. This subproblem can be efficiently solved by the method presented in Subsection 3.2, which generalizes the idea presented in Example 1.
- Finally, the aggregator, i.e., the vector of coefficients of the linear combination, can in favorable cases be determined such that the resulting constraint intersects the box in a point or even not at all. Choosing the aggregator is the topic of Section 4.
- If the whole box was reduced the method can be repeated with a new aggregated constraint, until no further improvement is possible.

As demonstrated by our later numerical results, the resulting aggregation filtering method often leads to far better improvements than traditional filtering based on a quadratic constraint and bound constraints only.

We concentrate on quadratic problems; algebraic problems can be transformed to quadratic ones by introducing intermediate variables (as it is done, e.g., in GLOPTLAB [5]). If quadratic underestimation techniques such as those discussed in SCHICHL & MARKÓT [30, page 13] are used, all results can even be extended to work for general nonlinear programs.

3.1 **Filtering by constraint aggregation**

An **aggregator** of the uncertain constraint satisfaction problem (23) is a nonzero vector $y \in \mathbb{R}^m$. The corresponding **constraint aggregation** of (23) is the uncertain constraint

$$u^T F(x) \in \mathbf{v} := y^T \mathbf{b} \text{ for some } u \in \mathbf{u} := \mathbf{B}^T y. \tag{31}$$

Let $Ex \le d$ a linear relaxation of the constraints of (23) over the box $\mathbf{x}$ and let $\mathcal{P}$ be a pruning method. The vector y is a **certificate of infeasibility** if $\mathcal{P}$ is applied to the constraint (31), the polyhedron defined by $Ex \in \mathbf{d}$, and the bound constraints $x \in \mathbf{x}$ result in the elimination of $\mathbf{x}$.

Using centered form the two-sided inequality (31) with interval coefficients can be transformed into a single scalar inequality

$$s(x) \le \gamma, \quad s(x) := \widehat{u}^T F(x), \quad \gamma := \sup\{\overline{v} - (u - \widehat{u})^T F(x) \mid u \in \mathbf{u}, x \in \mathbf{x}\}. \tag{32}$$

(A lower bound on $s(x)$ could also be considered, but by construction of the aggregator, usually only the upper bound will have a significant effect.) Note that if $\mathbf{B}$ is the identity matrix then $\gamma = \overline{v}$. Now (31) together with $Ex \in \mathbf{d}$ and $x \in \mathbf{x}$ defines a singly-nonlinear constraint satisfaction problem as in (35).

If a valid bound on the objective of an uncertain optimization problem is known, the problem can be represented as in (29). An **aggregator** of the uncertain optimization problem (29) is a pair (ν, y) with $\nu \in \mathbb{R}$, $y \in \mathbb{R}^m$. The corresponding

constraint aggregation of (29) is the uncertain constraint

$$wf(x) + u^T F(x) \in \mathbf{v} := \nu\mathbf{r} + y^T\mathbf{b} \text{ for some } w \in \mathbf{w} := \mathbf{a}^T\nu, \quad u \in \mathbf{u} := \mathbf{B}^T y, \quad (33)$$

and (32) changes to

$$\begin{array}{l} s(x) \le \gamma, \quad s(x) := \widehat{w} f(x) + \widehat{u}^T F(x), \\ \gamma := \sup\{\overline{v} - (w - \widehat{w}) f(x) - (u - \widehat{u})^T F(x) \mid w \in \mathbf{w}, u \in \mathbf{u}, x \in \mathbf{x}\}. \end{array} \quad (34)$$

Using rigorous filtering methods (e.g., constraint propagation [7] or linear relaxations [8]) on (34) may yield tighter bounds $x \in \widehat{\mathbf{x}} \subseteq \mathbf{x}$. Since each solution of the original problem is also a solution of (34) and $\widehat{\mathbf{x}}$ was obtained by rigorous methods, $x \in \widehat{\mathbf{x}}$ can be used as improved bound constraints without losing feasible points. This gives a cheap filtering method that reuses the information obtained from the local search procedure.

If the above method result in a 'significant' bound improvement the point $\widetilde{x}$ may lie outside the new box $\widehat{\mathbf{x}}$. In this case it may be worth starting a new local search in order to find a feasible point or to further improve the bounds. In this case the point $\widetilde{x}$ could be projected into the new box and taken as the starting point of the local search.

3.2 Filtering a singly-quadratic constraint satisfaction problem

We now introduce a new method for enclosing the feasible set of constraint satisfaction problems with linear constraints and a single quadratic constraint. In particular, it can be applied to an aggregated constraint if it is quadratic (or, if not, to a quadratic relaxation of it). In this case, the linear constraints will be those of a linear relaxation of all constraints.

We consider the uncertain **singly-quadratic constraint satisfaction problem** (**SQCSP**)

$$\begin{array}{ll} \text{find} & x \in \mathbf{x} \\ \text{s.t.} & c^T x + \frac{1}{2} x^T G x \le \gamma, \\ & Ex \in \mathbf{d} \\ \text{for some } G \in \mathbf{G}, & E \in \mathbf{E}, \quad c \in \mathbf{c}, \end{array} \quad (35)$$

where $\mathbf{x} \in \mathbb{IR}^n$ is a bounded box, $\mathbf{G} \in \mathbb{IR}^{n\times n}$ is symmetric, $\mathbf{E} \in \mathbb{IR}^{m\times n}$, $\mathbf{c} \in \mathbb{IR}^n$, and $\mathbf{d} \in \mathbb{IR}^m$. Intersecting $\mathbf{d}$ with $E\mathbf{x}$ if necessary, we may assume without loss of generality that $\mathbf{d} \subseteq E\mathbf{x}$ is bounded, too.

We compute an approximate local minimizer $\widetilde{x}$ of the quadratic program

$$\begin{array}{l} \min c^T x + \frac{1}{2} x^T G x \\ \text{s.t.} \quad Ex = d, \quad x \in \mathbf{x}, \end{array} \quad (36)$$

where G, E, c, and d are approximate midpoints of $\mathbf{G}$, $\mathbf{E}$, $\mathbf{c}$, and $\mathbf{d}$. If γ is close to or less than the associated objective function value, one expects that the feasible domain of (35) is tiny or empty. Our goal is to transform the problem into an uncertain CSP where the single quadratic constraint becomes separable, in such a way that it becomes obvious that under the stated conditions constraint propagation will reduce the box to a narrow or empty domain.

To handle the equality constraint, we construct a rigorous null space representation as follows. We use $\widetilde{x}$ to find an estimate N of the set of indices of variables that are free at the exact minimizer of (36). We fix the variables estimated active (with indices in the complement $\neg N$) at the values determined by $\widetilde{x}$, and consider the remaining uncertain linear system

$$E_{:N}x_N = e \quad \text{for some } E \in \mathbf{E},\ e \in \mathbf{e} := \mathbf{d} - \mathbf{E}_{:\neg N}\widetilde{x}_{\neg N}.$$

Later we require $|N| \geq m$ which is only possible if the index set $\neg N$ of estimated active variables has a size at most $n-m$. Since the minimizer $\widetilde{x}$ and therefore which bound constraints are active is only approximative, we can build the index set of the active variables

$$N^0 := \{i \mid \widetilde{x}_i \leq \underline{x}_i \text{ or } \widetilde{x}_i \geq \overline{x}_i\},$$

and the index set $N^1 \subseteq \neg N^0$ of the most approximately active variables such that $|N^1| \leq n - m - |N^0|$. Then we define $\neg N := N^0 \cup N^1$ which satisfies $|\neg N| \leq n - m$ and therefore we have $|N| \geq m$. We then redefine $\widetilde{x}$ exactly with respect to these active bound constraints.

The Gauss-Jordan algorithm from Domes & Neumaier [8, Section 4] is applied to an approximate midpoint of $\mathbf{E}_{:N}$, with scaling factors

$$\delta = \sqrt{\varepsilon}, \quad U = \operatorname{diag}(u), \text{ and } V = \operatorname{diag}(v) \tag{37}$$

determined such that the equations matching the constraints with tighter bounds are preferred as pivot rows, and columns of E matching the variables with tighter bounds are preferred as pivot columns. Here ε denotes the machine precision and

$$u = (\overline{e} - \underline{e}) + \delta|\mathbf{e} - \mathbf{E}_{:N}\mathbf{x}_N|, \quad w := \max\{-\underline{x}_i,\ \overline{x}_j \mid i,j \in N\},$$
$$\mathbf{w} = \mathbf{x}_N \cap [-w,w]^{|N|}, \quad v = (\overline{w} - \underline{w})/\max\{\overline{w}_k - \underline{w}_k \mid k = 1,\ldots,|N|\}.$$

This produces an index list $P \subseteq N$ of size $p := |P|$ and a matrix $C \in \mathbb{R}^{p\times m}$ such that

$$CE_{:P} \approx I \in \mathbb{R}^{p\times p}.$$

By construction, $E_{:P}$ is likely to be invertible, and we compute enclosures $\mathbf{X}$, $\mathbf{S}$ of

$$X := E_{:P}^{-1} \in \mathbb{R}^{p\times p}, \quad S := XE_{:Q} \in \mathbb{R}^{p\times(n-p)},$$

where $Q := \{1,\ldots,n\} \setminus P$ is the complementary index list of size $|Q| = n - p$. This may be done, e.g., by computing

$$\mathbf{X} := (C\mathbf{E}_{:P})^G C, \quad \mathbf{S} := \mathbf{X}\mathbf{E}_{:Q}, \tag{38}$$

where $\mathbf{A}^G\mathbf{B}$ is the interval matrix obtained by applying interval Gauss elimination (see, e.g., Neumaier [25, pp. 152-166]) to the uncertain linear equation $AX = B$ for some $A \in \mathbf{A}$ and some $B \in \mathbf{B}$. Note that in the present case, the coefficient matrix is nearly the identity, so that interval Gauss elimination should not suffer from excessive overestimation. If interval Gauss elimination fails, the problem is considered degenerate, and no relaxation is computed.

The columns of the matrix $Z \in \mathbb{R}^{n\times(n-p)}$ defined by $Z_{P:} = -S$ and $Z_{Q:} = I$ form a basis of the null space of the matrix E; indeed, we have

$$XEZ = XE_{:P}(-S) + XE_{:Q}I = -S + S = 0,$$

hence $EZ = 0$. Assuming for the moment that the P indices are sorted before the Q indices, we have $Z = \binom{-S}{I}$, and the reduced Hessian $G_{\text{red}} \in \mathbb{R}^{(n-p)\times(n-p)}$ takes the form

$$G_{\text{red}} := Z^T G Z = (-S^T \; I) \begin{pmatrix} G_{PP} & G_{PQ} \\ G_{QP} & G_{QQ} \end{pmatrix} \begin{pmatrix} -S \\ I \end{pmatrix}.$$

It can be easily seen that the resulting equation

$$G_{\text{red}} = S^T G_{PP} S - S^T G_{PQ} - G_{QP} S + G_{QQ}$$

remains valid even when the indices are not sorted. From a directed modified Cholesky factorization (cf. Domes & Neumaier [9]) of the enclosure

$$\mathbf{G}_{\text{red}} = \mathbf{S}^T(\mathbf{G}_{PP}\mathbf{S} - \mathbf{G}_{PQ}) - \mathbf{G}_{QP}\mathbf{S} + \mathbf{G}_{QQ} \tag{39}$$

of G_{red} with $M := \{i \mid Q_i \in N\}$ and $\zeta = 10^{-6}$, we may obtain a nonsingular matrix $R \in \mathbb{R}^{(n-p)\times(n-p)}$ and a diagonal matrix $D \in \mathbb{R}^{(n-p)\times(n-p)}$ such that the residual matrix

$$\Delta := \mathbf{G}_{\text{red}} + D - R^T R \tag{40}$$

is positive semidefinite and tiny. Note that the bracketing in (39) improves the enclosure, which can be improved further by intersecting $\mathbf{G}_{\text{red}}$ with its transpose, which is valid since G_{red} is symmetric.

With the approximate solution $\widetilde{x}$ found by a local solver, we form

$$\widetilde{d} := Ex - E\widetilde{x} \in \widetilde{\mathbf{d}} := \mathbf{d} - \mathbf{E}\widetilde{x} \approx 0. \tag{41}$$

For any feasible x, the correction vector

$$s := x - \widetilde{x}$$

satisfies

$$Es = \widetilde{d} \in \widetilde{\mathbf{d}}, \quad s \in \mathbf{s} := \mathbf{x} - \widetilde{x}. \tag{42}$$

Moreover, since $s_P + Ss_Q = X(E_{:P}s_P + E_{:Q}s_Q) = XEs = X\widetilde{d}$, we have

$$(Zs_Q)_P = Z_{P:}s_Q = -Ss_Q = s_P - X\widetilde{d}, \quad (Zs_Q)_Q = Z_{Q:}s_Q = s_Q,$$

hence

$$r := s - Zs_Q \in \mathbf{r} \approx 0,$$

where

$$\mathbf{r}_P := \mathbf{X}\widetilde{\mathbf{d}}, \quad \mathbf{r}_Q := [0,0]. \tag{43}$$

Thus $x = \widetilde{x} + s = x' + Zs_Q$, where

$$x' = \widetilde{x} + r \in \mathbf{x}' := \widetilde{x} + \mathbf{r}, \tag{44}$$

and

$$\begin{aligned} \widetilde{\sigma} &:= 2c^T x + x^T G x - (2c^T x' + x'^T G x') \\ &= 2g^T Z s_Q + (Zs_Q)^T G Z s_Q \\ &= h^T s_Q + s_Q^T G_{\text{red}} s_Q, \end{aligned}$$

where

$$g := c + Gx' \in \mathbf{g} := \mathbf{c} + \mathbf{G}\mathbf{x}', \tag{45}$$

$$h := 2Z^T g = 2(g_Q - S^T g'_P) \in \mathbf{h} := 2(\mathbf{g}_Q - \mathbf{S}^T \mathbf{g}_P). \tag{46}$$

Since

$$s_Q^T G_{\mathrm{red}} s_Q + s_Q^T (R^T R - D) s_Q + s_Q^T \Delta s_Q \geq (Rs_Q)^T (Rs_Q) - s_Q^T D s_Q,$$

we may introduce

$$z := Rs_Q \in \mathbf{z} := R\mathbf{s}_Q, \tag{47}$$

and find the separable quadratic relaxation

$$z^T z - s_Q^T D s_Q + h^T s_Q \leq \sigma := \sup\Big(2\gamma - (\mathbf{c} + \mathbf{g})^T \mathbf{x}'\Big), \tag{48}$$

where σ bounds $\widetilde{\sigma}$, and the linear constraints

$$Es \in \widetilde{d}, \quad s_P + Ss_Q \in \mathbf{r}_P, \quad Rs_Q - z = 0, \quad s \in \mathbf{s}, \quad z \in \mathbf{z}. \tag{49}$$

With an approximate constraint multiplier y for (35) at $\widetilde{x}$ (computed by Algorithm 1, or simply $y = 0$), we may introduce

$$h' := 2(g - E^T y) \in \mathbf{h}' := 2(\mathbf{g} - \mathbf{E}^T y), \tag{50}$$

and rewrite the linear term $h^T s_Q$ in (48) as

$$h^T s_Q = 2g^T Z s_Q = (h'^T + y^T E) Z s_Q = h'^T Z s_Q = h'^T (s - r)$$

since $EZ = 0$. This gives the alternative separable quadratic relaxation

$$z^T z - s_Q^T D s_Q + h'^T s \leq \sigma' := \sigma + \sup(\mathbf{h}'^T \mathbf{r}). \tag{51}$$

Therefore s and z are solutions of the uncertain quadratic constraint satisfaction problem

$$\begin{array}{ll} \text{find} & s \in \mathbf{s},\ z \in \mathbf{z}, \\ \text{s.t.} & z^T z - s_Q^T D s_Q + h^T s_Q \leq \sigma, \\ & z^T z - s_Q^T D s_Q + h'^T s \leq \sigma', \\ & Es \in \widetilde{\mathbf{d}}, \quad (CE)s \in C\widetilde{\mathbf{d}}, \\ & s_P + Ss_Q \in \mathbf{r}_P, \quad Rs_Q - z = 0, \\ \text{for some} & E \in \mathbf{E}, \quad h \in \mathbf{h}, \quad h' \in \mathbf{h}', \quad S \in \mathbf{S}, \end{array} \tag{52}$$

depending on the $n + (n - p)$ variables x and z and consisting of two separable quadratic inequality constraints and $m+p+(n-p) = m+n$ linear equality constraints.

Note that (as as discussed in Domes & Neumaier [8, Section 3]) adding the redundant constraint $(CE)s \in C\widetilde{\mathbf{d}}$ in (52) sometimes significantly improves the quality of the enclosure, though the main effect of the filtering by aggregation is due to the other constraints.

A constraint propagator that optimally handles single linear and separable quadratic constraints (see Domes & Neumaier [7]) produces an improved enclosure $\mathbf{s}^{\mathrm{new}}$ for s or proves that (52) and therefore (35) is infeasible. In the first case one recovers an improved enclosure $\mathbf{x}^{\mathrm{new}} := \widetilde{x} + \mathbf{s}^{\mathrm{new}}$ of solution set of (35).

Algorithm 2 turns the above considerations into a precise prescription.

Algorithm 2: Quadratic Filtering (QuadFil)

Input: An SQCSP given by (35), the local solver precision $\delta \ll 1$ and an arbitrary starting point $x^0 \in \mathbf{x}$.
Output: A reduced box $\mathbf{x}^{\text{new}} \subseteq \mathbf{x}$ (or the empty set), containing all solutions of (35).

Solve the quadratic program (36) by an approximate local solver starting from the point x^0, to precision δ, and obtain the optimizer $\widetilde{x} \in \mathbb{R}^n$;
if $\widetilde{x}_i < \min(\underline{x}_i + \delta, \overline{x}_i)$ **then** $\widetilde{x}_i \leftarrow \underline{x}_i$;
if $\max(\underline{x}_i, \overline{x}_i - \delta) < \widetilde{x}_i$ **then** $\widetilde{x}_i \leftarrow \overline{x}_i$;
Form the index set $N := \{i \mid \underline{x}_i < \widetilde{x}_i < \overline{x}_i\}$ and compute $\mathbf{e} := \mathbf{d} - \mathbf{E}_{:\neg N}\widetilde{x}_{\neg N}$;
Use the Gauss-Jordan algorithm for $\text{mid}(\mathbf{E}_{:N})$, with scaling factors U, V and δ determined as in (37). This results in the index list $P \subseteq N$ and the matrix C;
Use the interval Gauss elimination on the interval system of equations $(C\mathbf{E}_{:P})X = C$ to find the solution set $\mathbf{X} \in \mathbb{IR}^{p \times p}$;
Compute $Q := \{1, \ldots, n\} \setminus P$ and $\mathbf{S} := \mathbf{X}\mathbf{E}_{:Q}$;
Partition G and compute the enclosure $\mathbf{G}_{\text{red}}$ for the reduced Hessian as given by (39);
Improve the enclosure $\mathbf{G}_{\text{red}}$ by computing $\mathbf{G}_{\text{red}} \leftarrow \mathbf{G}_{\text{red}} \cap \mathbf{G}_{\text{red}}^T$;
Use the directed modified Cholesky factorization (Domes & Neumaier [9, Algorithm ModDirChol]) with $M := \{i \mid Q_i \in N\}$ and $\zeta = 10^{-6}$ to find matrices R and D such that the residual matrix defined by (40) is positive semidefinite for all $G_{\text{red}} \in \mathbf{G}_{\text{red}}$;
if *the directed modified Cholesky factorization failed* **then return** signaling failure;
else
    Compute $\widetilde{\mathbf{d}}$ by (41), $\mathbf{s}$ by (42), $\mathbf{r}$ by (43), $\mathbf{x}'$ by (44), $\mathbf{g}$ by (45), $\mathbf{h}$ by (46), $\mathbf{z}$ by (47) and σ by (48);
    Find the approximate constraint multiplier y for (35) at $\widetilde{x}$ by using Algorithm 1 and compute $\mathbf{h}'$ by (50) and σ' by (51);
    Create the uncertain quadratic constraint satisfaction problem (52);
    Use a rigorous filtering method (e.g., quadratic separable constraint propagation) on (52) in order to obtain tighter bounds $\mathbf{s}^{\text{new}}$ and $\mathbf{z}^{\text{new}}$ for the variables s and z;
    if $\mathbf{s}^{\text{new}}$ *or* $\mathbf{z}^{\text{new}}$ *is empty* **then** return that $\mathbf{x}$ contains no solution of (35);
    else return the box $\mathbf{x}^{\text{new}} := \widetilde{x} + \mathbf{s}^{\text{new}}$;
end

4 Choosing the aggregator

It remains to discuss the choice of aggregators. Clearly, an arbitrary choice is unlikely to be beneficial; for example if we take as aggregator a $(0, 1)$ unit vector, we just recover the original constraints, without any advantage.

In this section, we discuss two sensible choices. The first choice is based on the solution of an auxiliary least squares problem and gives under suitable conditions an aggregator that provides a certificate of infeasibility, reducing the box defining the bound constraints to the empty set. The second choice utilizes the Lagrange multipliers of an approximately optimal point.

4.1 Certificates of infeasibility

If for the uncertain optimization or constraint satisfaction problem (22) a local search yields no (weakly) feasible point but an infeasible $\widetilde{x} \in \mathbf{x}$, the nonzero, signed feasibility measure vector (28) can be used as an aggregator.

The following theorem gives sufficient conditions under which the appropriate aggregator may serve as a certificate of infeasibility, proving that the aggregated

constraint is trivially infeasible. If these conditions are not satisfied by a limited margin only, one may expect that the aggregated constraint, while usually not sufficient to prove infeasibility, will still be strong enough to reduce the box when the reduction technique described above is applied.

Theorem 2 *Let F be continuously differentiable, and let D be a scaling matrix. Let $\widehat{x}$ be a stationary point of*

$$\begin{array}{l} \min\ f(x) := \frac{1}{2}||\mu(BF(x) - \mathbf{b})||_D^2, \\ \text{s.t.}\ \ x \in \mathbf{x} \end{array} \tag{53}$$

and let

$$y := D\mu(BF(\widehat{x}) - \mathbf{b}), \quad u := B^T y. \tag{54}$$

Then

(i) $f(x)$ is continuously differentiable with

$$\frac{\partial f(x)}{\partial x_k} = F'(x)^T B^T D d(x), \tag{55}$$

and $g := F'(\widehat{x})^T u$ satisfies

$$\begin{cases} g_i \geq 0 & \text{if } \underline{x}_i = \widehat{x}_i < \overline{x}_i, \\ g_i \leq 0 & \text{if } \underline{x}_i < \widehat{x}_i = \overline{x}_i, \\ g_i = 0 & \text{if } \underline{x}_i < \widehat{x}_i < \overline{x}_i. \end{cases} \tag{56}$$

(ii) If $y \neq 0$ the inequality

$$u^T F(x) \in y^T \mathbf{b} < u^T F(\widehat{x}) \tag{57}$$

holds for all feasible x.

(iii) If $y = 0$ then $\widehat{x}$ is feasible.

(iv) If $y \neq 0$ and $u = 0$ then there is no feasible point.

(v) If $y \neq 0$ and F is linear then y is a certificate of infeasibility.

Proof (iii) D is nonsingular and $y = 0$; therefore $\mu(BF(\widehat{x}) - \mathbf{b}) = 0$, giving

$$0 \in BF(\widehat{x}) - \mathbf{b} \implies BF(\widehat{x}) \in \mathbf{b}.$$

Since $\widehat{x} \in \mathbf{x}$ by construction $\widehat{x}$ must be feasible.

(i) Write $d(x) := \mu(BF(x) - \mathbf{b})$. Then

$$\frac{\partial d_i(x)}{\partial x_k} = \begin{cases} (BF'(x))_{ik} & \text{if } d_i(x) \neq 0, \\ 0 & \text{otherwise,} \end{cases}$$

is a continuous partial derivate except when $(BF(x))_i \in \{\underline{b}_i, \overline{b}_i\}$. Since

$$f(x) = \frac{1}{2}||d(x)||_D^2 = \frac{1}{2} d(x)^T D d(x)$$

vanishes at each point of discontinuity, the derivative

$$\frac{\partial f(x)}{\partial x_k} = \frac{\partial d(x)^T}{\partial x_k} D d(x) = \sum_i D_{ii} \frac{\partial d_i(x)}{\partial x_k} d_i$$

is continuous. (55) follows from

$$\begin{aligned}\frac{\partial f(x)}{\partial x_k} &= \sum_i \frac{\partial d_i(x)}{\partial x_k} D_{ii} d_i(x) = \sum_i [BF'(x)]_{ik} D_{ii} d_i(x) \\ &= [BF'(x)]_{:k}^T Dd(x) = [F'(x)^T B^T Dd(x)]_{:k}.\end{aligned}$$

Since $y = Dd(\widehat{x})$ and $u = B^T y$, we have

$$\frac{\partial f(\widehat{x})}{\partial x} = F'(\widehat{x})^T B^T Dd(\widehat{x}) = F'(\widehat{x})^T u = g. \tag{58}$$

The first order necessary conditions for optimality now give

$$\begin{aligned}\frac{\partial f(\widehat{x})}{\partial x_k} &\geq 0 \quad \text{if } \underline{x}_i = \widehat{x}_i < \overline{x}_i, \\ \frac{\partial f(\widehat{x})}{\partial x_k} &\leq 0 \quad \text{if } \underline{x}_i < \widehat{x}_i = \overline{x}_i, \\ \frac{\partial f(\widehat{x})}{\partial x_k} &= 0 \quad \text{if } \underline{x}_i < \widehat{x}_i < \overline{x}_i,\end{aligned}$$

and using (58), we find (56).

(ii) Let $y \neq 0$. Then the constraints can be aggregated, resulting in $u^T F(x) \in y^T \mathbf{b}$. By construction of y we have

$$\begin{aligned}(BF(\widehat{x}))_i &> \overline{b}_i \quad \text{if } y_i > 0, \\ (BF(\widehat{x}))_i &< \underline{b}_i \quad \text{if } y_i < 0, \\ (BF(\widehat{x}))_i &\in \mathbf{b}_i \quad \text{if } y_i = 0.\end{aligned}$$

From this it follows that $y_i(BF(\widehat{x}))_i \geq \sup(y_i \mathbf{b}_i)$, with equality only if $y_i = 0$. We conclude that

$$u^T F(\widehat{x}) = y^T BF(\widehat{x}) = \sum y_i (BF(\widehat{x}))_i \geq \sup \sum y_i \mathbf{b}_i = \sup(y^T \mathbf{b}), \tag{59}$$

with equality only if all $y_i = 0$. However $y = 0$ leads to a contradiction. Therefore (59) holds with strict inequality, proving (ii).

(iv) is an immediate consequence of (ii).

(v) If F is linear then $F(x) = F_0 + F_0' x$, $F'(x) = F_0'$, and $g = F'(\widehat{x})^T u = (F_0')^T u$, leading to

$$\begin{aligned}u^T(F(\widehat{x}) - F(x)) &= u^T(F_0 + F_0'\widehat{x} - (F_0 + F_0' x)) = u^T F_0'(\widehat{x} - x) \\ &= g^T(\widehat{x} - x) = \textstyle\sum_i g_i(\widehat{x}_i - x_i).\end{aligned} \tag{60}$$

By (56),

$$\begin{aligned}\widehat{x}_i = \underline{x}_i &\quad\Longrightarrow\quad \widehat{x}_i - x_i = \underline{x}_i - x_i \leq 0, \quad g_i \geq 0, \\ \widehat{x}_i = \overline{x}_i &\quad\Longrightarrow\quad \widehat{x}_i - x_i = x_i - \overline{x}_i \geq 0, \quad g_i \leq 0, \\ \widehat{x}_i \in \iint \mathbf{x}_i &\quad\Longrightarrow\quad g_i = 0, \\ \widehat{x}_i = \underline{x}_i = \overline{x}_i &\quad\Longrightarrow\quad \widehat{x}_i - x_i = 0.\end{aligned}$$

In all cases, $g_i(\widehat{x}_i - x_i) \leq 0$, and by (60) we conclude that $u^T(F(\widehat{x}) - F(x)) \leq 0$. On the other hand, (57) gives the inequality $0 \leq u^T(F(\widehat{x}) - F(x))$ for all feasible x, with equality only if $y = 0$. Therefore $y = 0$ for all feasible x. □

4.2 **Aggregation heuristics**

Theorem 2 suggests that we use the feasibility violation vector as an aggregator. Indeed, we found it suitable in the case when a box is unlikely to contain a nearly feasible point. On the other hand, if we know a nearly feasible point, the feasibility violation vector typically consists of noise only, and we need a different aggregator. The introductory example suggests that we use in this case a Lagrange multiplier. Uncertainties can be ignored in the computation of the multipliers, thus we use approximate midpoints to define the problem passed to Algorithm 1.

Algorithm 3: Aggregator chooser (AggrCh)

Input: An uncertain optimization problem given by (29), the point $x \in \mathbf{x}$ and the feasibility tolerance $\delta \geq 0$.
Output: An objective and constraints aggregator (ν, y) as well as the aggregator type `aggrt` $\in$ { `feas`, `mult`}.

1 Compute the feasibility violation vector $y := \mu(\mathbf{B}F(x) - \mathbf{b})$ and the objective violation $\nu := \mu(\mathbf{a}^T f(x) - \mathbf{r})$;
2 **if** $\|(\nu, y)\|_D^2 \leq \delta$ **then**
3 Recompute (ν, y) by applying Algorithm 1 to x and the midpoint approximation of (29). Also put `aggrt=mult`;
4 **else** put `aggrt=feas`;
5 **return** (ν, y) and `aggrt`;

5 Numerical results

In this section we present numerical results for the new constraint aggregation method on a large set of test problems. Our tests simulate the situation in a branch and bound scheme when a narrow box containing the global solution is processed. This case is especially interesting since this is the point where the traditional filtering methods usually lose their efficiency, resulting in excessive splitting due to the cluster effect.

5.1 **Testing procedure**

We selected from the Coconut Environment Testset ([33]) all constrained quadratic optimization problems with no more than 300 variables and no more than 300 constraints, resulting in 135 problems. The Test Environment [6] provides for each problem an approximate (global) solution x^*, the best approximation among those found by a number of solvers applied to the problem.

We performed two kinds of tests, one to test the contraction properties when a box contains the global minimizer, and one to test the elimination properties when a box is close to the global minimizer but does not contain it. Both cases are important to assess the degree to which the cluster effect can be reduced by our new method.

The first test therefore tests the case of aggregation by multiplier, given an approximate minimizer x^* (which we take as the best point provided by the Test

Environment). For each problem, we construct a box with tiny `start_box_radius` r around x^* and intersect it with the original bound constraints to get the test box $\mathbf{x}^*$. We impose on the objective function the upper bound

$$f(x) \leq \overline{f} := f(x^*) + f_\epsilon, \quad f_\epsilon := \max(e_a, e_r|f(x^*)|),$$

where $0 < e_a \ll 1$ is an absolute, and $0 < e_r \ll 1$ a relative error factor. Since x^* (and thus $f(x^*)$) is only an approximately feasible solution these factors have to be chosen carefully; choosing them too small may result in an infeasible problem and choosing them too large may prevent the contraction of $\mathbf{x}^*$ (see Figure 2). In this test we first choose them as $e_a = e_r = 0$ then increase them (to $e_a = e_r = 10^{-14}$ and then by successive multiplication with 10) until the problem becomes feasible for the constructed box $\mathbf{x}^*$. The f_ϵ used for each problem can be found in the `objsh` column of the detailed results table. Using the objective upper bounds each test problem can be written in the form of (29) with $\mathbf{r} := [-\infty, \overline{f}]$ and $\mathbf{x} := \mathbf{x}^*$.

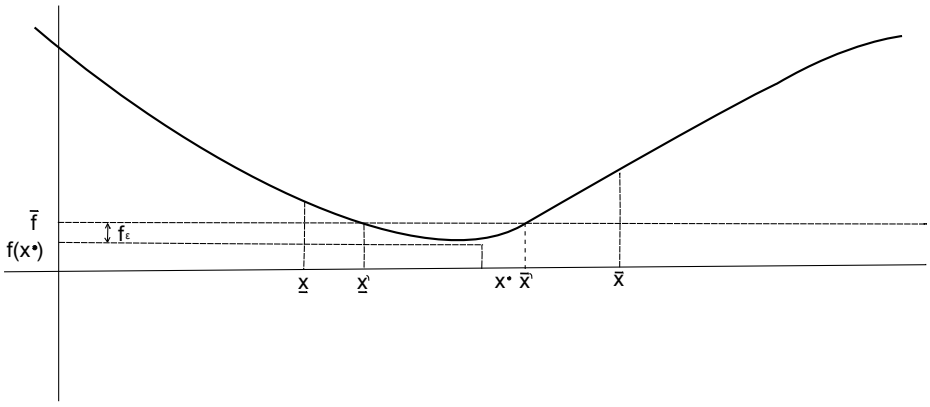

Fig. 2 Choosing a suitable objective upper bound explained on a simple one dimensional problem. The approximate objective value $f(x^*)$ at the approximate minimizer x^* has to be adjusted by f_ϵ. If the adjustment is not big enough $\overline{f}$ would be below the global minimum and the problem becomes infeasible, if it is too big it is not possible to significantly contract the box $\mathbf{x} := [\overline{x}, \underline{x}]$. With the adjustment shown in the plot the box $\mathbf{x}$ can be contracted at most to the box $\mathbf{x}' := [\overline{x}', \underline{x}']$.

To show that the new method has powerful contraction properties even after state of the art filtering techniques are applied, constraint propagation and linear relaxations are used to the solve (29). The constraint propagation method (which is especially powerful for quadratic problems) was taken from [7] and the linear relaxations from [8] and [22]. This should eliminate the dominant effects of a contraction obtained by traditional zero and first order filtering methods. This also includes 2B-consistency, Box-consistency and 3B-consistency which for quadratic problems are reported to be inferior to the linear relaxations applied here (see [22, Section 6]).

The next step is using a local solver to find an approximately feasible point $\widehat{x} \in x^*$. If $\widehat{x}$ is not δ-feasible, the nonzero, signed feasibility distance vector (28) is

used to aggregate as in (32). If $\widehat{x}$ is δ-feasible, a local search is started from $\widehat{x}$ to obtain a local minimum of (29) and $\widehat{x}$ is replaced by the local minimum found. In this case, the multipliers (ν, y) at the local minimum were used to aggregate as in (34). On the aggregated system constraint propagation [7] is used. This step is referred as the constraint aggregation (`AG`). Then the constraints are linearly relaxed around $\widehat{x}$ inside the box $\mathbf{x}^*$, and the new system is solved by linear constraint propagation (`LR`). Finally the quadratic filtering Algorithm 2 (`QF`) is applied.

In the second test we assess the quality of aggregation by feasibility violation, applied to boxes that are very close to the solution but contain no feasible point. For each problem we consider the small box $\mathbf{x}'$ around the solution obtained in the first test and construct $2n$ (n = problem dimension) boxes

$$\mathbf{x}^{(k)} \text{ with } \mathbf{x}_i^{(k)} := \begin{cases} [\underline{x}'_i - \kappa - 2r, \underline{x}'_i - \kappa] & \text{if } k \le n \text{ and } k = i \\ [\overline{x}'_i + \kappa, \overline{x}'_i + \kappa + 2r] & \text{if } k > n \text{ and } k - n = i \\ \mathbf{x}'_i & \text{otherwise,} \end{cases}$$

where κ is a small `infeasible_box_shift`, and r is again the `start_box_radius`. Then we apply `AG`, `LR`, and `QF` to each box, and count how often they prove that the box contains no feasible point. We define the **elimination factor** `elim`$:= e/n$, where e denotes the number of eliminated boxes.

5.2 **Test results**

We applied the above test procedures to our 135 quadratic optimization problems. For 6 of them – due to the poor reference solutions – we could not create an initial box containing any feasible points. For these 6 problems, we also skipped the second test. For the rest of the problems we obtained promising results, which can be found online at:

`http://www.mat.univie.ac.at/~dferi/research/AggregateTests.pdf`,

while the following table gives the summary of them.

Test Result Summary (135 problems)	`AG`	`LR`	`QF`
First step; arithmetic mean cube-ratio	0.43	0.9	0.32
First step; arithmetic mean max-width-ratio	0.67	0.98	0.57
First step; geometric mean cube-ratio	0.2	-	0.32
First step; geometric mean max-width-ratio	0.11	0.63	0.14
First step; one component width reduced below $1{\cdot}10^{-8}$	21	3	14
First step; all component widths reduced below $1{\cdot}10^{-8}$	9	1	8
Additional steps; arithmetic mean cube-ratio	0.99	1	0.98
Additional steps; arithmetic mean max-width-ratio	1	1	1
Infeasible problems	6		
Elimination test success ratio; arithmetic mean	0.82		
Elimination test success ratio; geometric mean	0.79		

The summary table shows that the method – and especially the aggregation (`AG`) and the quadratic filter (`QF`) part – strongly contracts most boxes containing the

solution. Performing more than one step of the method does not improve the quality anymore. Since the boxes to be contracted and the objective upper bound used depend on the approximate reference solution used (which sometimes was not very accurate), we did not expect contraction to a single point; however for 18 problems, all component widths were reduced below $1 \cdot 10^{-8}$.

The elimination test shows that for each problem, most of the $2n$ boxes created near to the solution were eliminated, hence proved to contain no feasible point. Since the tests focus on the most difficult problem of filtering boxes very close to the global solution, this shows that our method is indeed a powerful tool for eliminating the cluster effect.

The performance of the new techniques within a framework for global optimization depends on how these techniques are combined with other, traditional methods. We intend to report on this in a separate paper [10] describing the Java implementation JGloptLab of our earlier GloptLab constraint satisfaction package [5].

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