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Quasiconvex relaxations based on interval arithmetic

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Abstract

Interval analysis provides a tool for (i) forward error analysis, (ii) estimating and controlling rounding and approximation errors automatically, and (iii) proving existence and uniqueness of solutions. In this context the terms self-validating methods, inclusion methods or verification methods are in use. In this paper, we present a new self-validating method for solving global constrained optimization problems. This method is based on the construction of quasiconvex lower bound and quasiconcave upper bound functions of a given function, the latter defined by an arithmetical expression. No further assumptions about the nonlinearities of the given function are necessary. These lower and upper bound functions are rigorous by using the tools of interval arithmetic. In its easiest form they are constructed by taking appropriate linear and/or quadratical estimators which yield quasiconvex/quasiconcave bound functions. We show how these bound functions can be used to define rigorous quasiconvex relaxations for constrained global optimization problems and nonlinear systems. These relaxations can be incorporated in a branch and bound framework yielding a self-validating method. © 2001 Elsevier Science Inc. All rights reserved.

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1. Introduction

Quasiconvex functions (see [3,35,36]) are of significant importance in optimization theory, engineering and management science. The reason is that

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quasiconvex functions arise in many applications and satisfy the underlying assumptions of important theorems. Quasiconvexity is defined as follows: a function $f : S \to \mathbb{R}$ which is defined on a convex set $S \subseteq \mathbb{R}^n$ is called *quasiconvex* if for all $x, y \in S$, $0 \leqslant \lambda \leqslant 1$, the inequality

$$f(\lambda x + (1 - \lambda)y) \leqslant \max\{f(x), f(y)\} \tag{1}$$

holds. Obviously, each convex function is quasiconvex. The function f is said to be *quasiconcave* if $-f$ is quasiconvex. A function which is both quasiconvex and quasiconcave is called quasilinear. If S is open, $f : S \to \mathbb{R}$ is differentiable on S, and for all $x, y \in S$ with $f'(x)^{\mathrm{T}}(x - y) \geqslant 0$ we have $f(y) \geqslant f(x)$, then f is said to be *pseudoconvex*. It can be shown that a pseudoconvex function is quasiconvex (see [4]).

Quasiconvex functions have among others the following useful properties: (i) each strict local minimum is a global minimum, (ii) the level sets are convex, and (iii) the necessary Kuhn–Tucker conditions for a nonlinear optimization problem are also sufficient provided that the objective and the constraints are defined by certain quasiconvex and quasiconcave functions. These properties of quasiconvex functions allow us to construct appropriate relaxations for optimization problems, and to develop methods for global optimization problems.

A *quasiconvex relaxation* of a global minimization problem P is a minimization problem $\tilde{\mathrm{P}}$ such that

(i) each feasible solution of P is feasible for $\tilde{\mathrm{P}}$;
(ii) the objective function of P is greater than or equal to the objective function of $\tilde{\mathrm{P}}$ for all feasible points of P;
(iii) the objective function of $\tilde{\mathrm{P}}$ is pseudoconvex, and the constraints of problem $\tilde{\mathrm{P}}$ are defined by quasilinear or quasiconvex functions.

From (i) and (ii) it follows that the global minimum value of the quasiconvex relaxation $\tilde{\mathrm{P}}$ provides a lower bound of the global minimum value of P. It follows (see [4]) from property (iii) that the Kuhn–Tucker conditions are sufficient for global minimum points. Hence, in order to calculate a global minimum value of a quasiconvex relaxation it is sufficient to compute a Kuhn–Tucker point of $\tilde{\mathrm{P}}$; then the objective value of this point is equal to the global minimum value of $\tilde{\mathrm{P}}$.

Methods using relaxations for special structured continuous global optimization problems were first introduced by Falk and Soland [11]. Their approach concerns separable nonconvex programming problems. Later, in the case of concave minimization, convex relaxations have been used by Bulatov [5], Bulatov and Kasinkaya [6], Emelichev and Kovalev [9], Falk and Hoffmann [10], and Horst [19]. For recent developments and improvements see [41], and the references cited therein.

Yamamura et al. [40] have solved separable nonlinear systems by using linear programming techniques inside a branch and bound framework. The linear programs solved there can be viewed as linear relaxations in a higher dimensional space. In order to solve more general nonlinear systems, Yamarura [39] has introduced an algorithm for representing nonseparable functions by separable functions.

The *major goal* of this paper is to show how quasiconvex lower bound and quasiconcave upper bound functions can be calculated for a given function by using the tools of interval arithmetic. We only assume that this function is given by an arithmetical expression, or a more general one as a program. Using these bound functions, we decribe the construction of quasiconvex relaxations for global constrained optimization problems and nonlinear systems, where the objective and the constraints are defined by arithmetical expressions. These relaxations are rigorous and can be generated very fast; in many cases only a few interval operations are necessary. Moreover, we describe a branch and bound algorithm which uses quasiconvex relaxations, and which solves global constrained optimization problems in a rigorous way.

The paper is organized as follows. In the following section the basic notations are given. In Section 3 it is shown how for a given function *f* convex lower bound and concave upper bound functions of order 0 can be constructed by using appropriate decompositions of *f*. Then in Section 4, based on a special linearization of *f*, we describe the construction of convex lower bound functions of the first order. By using appropriate quadratical estimators of *f*, we discuss quasiconvex lower bound functions of second order in Section 5. In Section 6 some basic techniques for decomposing functions are developed. Quasiconvex relaxations of global constrained optimization problems are presented in Section 7. A branch and bound framework using these relaxations is described in Section 8. Following, we give some hints how the branch and bound algorithm has to be implemented such that the computed results are guaranteed. Some numerical results are presented in Section 9. Finally, in Section 10 a short summary is given.

2. Notations

Throughout this paper we use the following notations. The absolute value and comparisons are used entrywise. By $\mathbb{R}^n$ we denote the set of real vectors with *n* components, and $\mathbb{R}^n_+$ denotes the first orthant of $\mathbb{R}^n$. An interval vector is defined by $X := [\underline{x}, \overline{x}] := \{x \in \mathbb{R}^n : \underline{x} \leqslant x \leqslant \overline{x}\}$, where $\underline{x}, \overline{x}$ are called the *lower bound* and *upper bound*, respectively. The set of interval vectors with *n* components is denoted by $\mathbb{IR}^n$. For any interval vector $X = [\underline{x}, \overline{x}] \in \mathbb{IR}^n$ the 2^n vertices $x(\sigma)$ can be described by

$$x(\sigma) = \underline{x} + \sum_{i=1}^{n} \sigma_i (\overline{x}_i - \underline{x}_i) e_i, \tag{2}$$

where $\sigma \in \{0, 1\}^n$ is an *n*-dimensional vector with components σ_i equal to 0 or 1, and e_i denotes the unit vector which is equal to the *i*th column of the $n \times n$ identity matrix. We simply denote the vector with all components equal to 0 by $0 \in \{0, 1\}^n$, and the vector with all components equal to 1 by $1 \in \{0, 1\}^n$; this will cause no confusion. It follows that $x(0) = \underline{x}$, $x(1) = \overline{x}$, and for fixed $\sigma \in \{0, 1\}^n$ formula (2) implies the following inequalities:

$$\text{if } \sigma_i = 0, \text{ then } x_i - x_i(\sigma) \geqslant 0 \quad \text{for all } x \in X,$$
$$\text{if } \sigma_i = 1, \text{ then } x_i - x_i(\sigma) \leqslant 0 \quad \text{for all } x \in X.$$

For a given real-valued function $f(x)$, the gradient and the Hessian is denoted by $f'(x)$ and $f''(x)$, respectively. Sometimes, a function depends on some parameters. In such situations the argument is separated from the parameters by a semicolon. For example, the function $f(x; X, \sigma)$ has the argument x and depends on the two parameters X and σ.

For $n \times n$ matrices A the (i, j)th coefficient, the ith row, and the jth column is denoted by A_{ij}, $A_{i:}$, $A_{:j}$, respectively.

Interval arithmetic (see, e.g., [2,27,29,30]) provides methods for calculating rigorous bounds of the solution for a given problem, and has been applied in the fields of numerical analysis, optimization, differential equations, and other disciplines. In this paper we assume that the reader is familiar with the basic concepts of interval arithmetic. Most of these methods basically use so-called *interval extensions* which were introduced by Moore [26]. They are defined in the following way:

Let $S \subseteq \mathbb{R}^n$, let IS denote the set of all interval vectors $X := [\underline{x}; \overline{x}]$ with $X \subseteq S$, and let $f : S \to \mathbb{R}$. A mapping $[\underline{f}, \overline{f}] : IS \to \mathbb{IR}$ with $[\underline{f}(X), \overline{f}(X)] := [\underline{f}, \overline{f}](X)$ is an *interval extension* of f, if for each interval vector $X \in IS$ the inequalities

$$\underline{f}(X) \leqslant f(x) \leqslant \overline{f}(X) \tag{3}$$

hold for all $x \in X$. In other words, interval extensions deliver an interval $[\underline{f}(X), \overline{f}(X)]$ which contains the range of f over X.

The bounds $\underline{f}(X), \overline{f}(X)$ can be interpreted as constant functions, and constant functions are both convex and concave. Hence, interval extensions provide constant convex lower bound and constant concave upper bound functions of a given function.

3. Lower and upper bound functions of order 0

In general, the bounds $\underline{f}(X), \overline{f}(X)$ computed by using interval extensions overestimate the range of f over X, and this overestimation may be large due to the well-known problem of dependence (see, e.g., [29]). But even if these bounds do not overestimate the range of f, all information about the shape of f is lost when using interval extensions. This causes a main disadvantage of interval arithmetic. In order to approximate the shape of f in a better way, the first step is to choose an appropriate decomposition of f.

In the following we discuss a decomposition of f into three additive parts

$$f(x) = c(x) + e(x) + r(x). \tag{4}$$

For constructing a convex lower bound function $\underline{f}$ of f, we choose $c, e,$ and r as follows:

(i) function c is a convex part of f;

(ii) function e is a part of f which is not convex, but a convex underestimating function or a convex envelope $\underline{e}$ of e is known;

(iii) function r is defined as the difference $f - c - e$, and is estimated from below by the constant $\underline{r}(X)$ which is calculated by using an interval extension of r.

Because the sum of convex functions is convex, it follows that

$$\underline{f}(x; X) := c(x) + \underline{e}(x) + \underline{r}(X) \tag{5}$$

is a convex lower bound function of f.

A concave upper bound function is obtained in an analoguous way. We choose c, e, and r as follows:

(i) function c is a concave part of f;

(ii) function e is a part of f which is not concave but a concave overestimating function or a concave envelope $\overline{e}$ of e is known;

(iii) function r is defined as the difference $f - c - e$, and is estimated from above by the constant $\underline{r}(X)$ which is calculated by using an interval extension of r.

Obviously, it follows that the function

$$\overline{f}(x; X) := c(x) + \overline{e}(x) + \overline{r}(X) \tag{6}$$

is a concave upper bound function of f.

We call bound functions generated in this way of order 0, because first and second derivatives are not required. In general, there are various ways to construct bound functions of order 0. They depend on the chosen decomposition of f, the under- or overestimating function e, and the chosen interval extension for r. The following example illustrates this approach.

Example 3.1. Consider the function

$$f(x) = 2(x - 1.5)^2 + \ln(x + 0.25) + 0.1 \cdot \sin(4\pi x). \tag{7}$$

and the corresponding natural interval extension of f

$$2(X - 1.5)^2 + \ \mathrm{LN}(X + 0.25) + 0.1 \cdot \ \mathrm{SIN}(4\pi X), \tag{8}$$

where the real operations, real variables, and real standard functions ln and sin are replaced by the corresponding interval operations, interval variables, and interval standard functions LN and SIN, respectively.

The nonconvex function f is displayed in Fig. 1 (solid line) for the intervals $X = [0,\ 2]$ and $X = [0.9, 1.0]$. The natural interval extension computes for the interval $X = [0.2]$ the lower bound $\underline{f}(X) = -1.4862$, and for $X = [0.9, 1.0]$ the lower bound $\underline{f}(X) = 0.54465$.

For constructing a convex lower bound function we choose the decomposition (4) on $X = [\underline{x}, \overline{x}]$ in the following form. The convex part is defined as $c(x) := 2(x - 1.5)^2$. The function $e(x) := \ln(x + 0.25)$ is concave and can be bounded from below by the affine function $\underline{e}(x)$ satisfying $\underline{e}(\underline{x}) = \ln(\underline{x} + 0.25)$ and $\underline{e}(\overline{x}) = \ln(\overline{x} + 0.25)$. The remainder $r(x) := 0.1 \cdot \sin(4\pi x)$.

The natural interval evaluation $0.1 \cdot \ \mathrm{SIN}(4\pi X)$ gives the bounds $\underline{r}(X) = -0.1$, $\underline{r}(X) = 0.0951$ for the intervals $X = [0.2]$ and $X = [0.9, 1]$, respectively. The

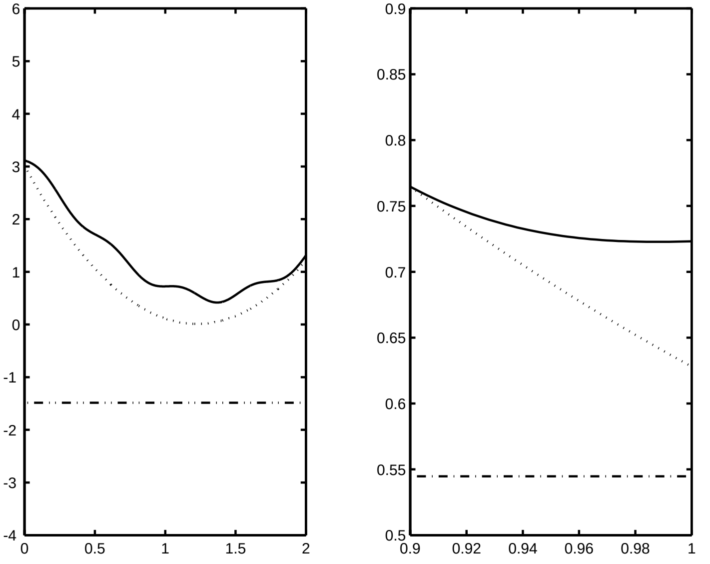

Fig. 1. Convex lower bound functions of order 0 (Example 3.1).

function *f* (solid), the constant lower bounds $\underline{f}(X)$ (dash–dotted), and the convex lower bound function $\underline{f}(x; X)$ (dotted) are displayed in Fig. 1 for the intervals $X = [0.2]$ and $X = [0.9, 1]$. For both intervals the convex lower bound function $\underline{f}(x; X)$ clearly improves the constant lower bound function $\underline{f}(X)$. Moreover, *f* is approximated rather close by $\underline{f}(x; X)$.

Improvements are typical for the aforementioned decompositions, because the additive convex or concave parts *c* of *f* are not changed or estimated. The quality of these bound functions is mainly influenced by the proximity of *f* and its convex or concave parts. In other words, these bound functions do not approximate *f* appropriately if the convex or concave parts are negligible, and the bounds for *e* and *r* are bad.

4. Lower and upper bound functions of first order

This section deals with the construction of convex lower and concave upper bound functions where first derivatives are required. This construction is based on the following theorem.

Theorem 4.1. *Given a continuously differentiable function* $f : S \to \mathbb{R}$ *with* $S \subseteq \mathbb{R}^n$, *and given an interval vector* $X \in \mathbb{IR}^n$ *with* $X \subseteq S$. *Suppose further that there exist two vectors* $\underline{d}, \overline{d} \in \mathbb{R}^n$ *such that the inequalities*

$$d \leqslant f'(x) \leqslant \overline{d} \tag{9}$$

hold for all $x \in X$. For a fixed vector $\sigma \in \{0,1\}^n$ let $x(\sigma) \in X, d(\sigma) \in D := [\underline{d}, \overline{d}]$ be the vertices of the interval vectors X, D, respectively. Then the linear functions

$$\underline{f}(x; X, \sigma) := d(\sigma)^{\mathrm{T}} \cdot x + \{f(x(\sigma)) - d(\sigma)^{\mathrm{T}} \cdot x(\sigma)\}, \tag{10}$$

$$\overline{f}(x; X, \sigma) := d(1-\sigma)^{\mathrm{T}} \cdot x + \{f(x(\sigma)) - d(1-\sigma)^{\mathrm{T}} \cdot x(\sigma)\} \tag{11}$$

satisfy for all $x \in X$ the inequalities

$$\underline{f}(x; X, \sigma) \leqslant f(x) \leqslant \overline{f}(x; X, \sigma), \tag{12}$$

and moreover

$$\underline{f}(x(\sigma); X, \sigma) = \overline{f}(x(\sigma); X, \sigma) = f(x(\sigma)). \tag{13}$$

This theorem is a special case of Theorem 1 in [22]. Following, we give a short proof to be independent from [22].

Proof. We prove only the assertions corresponding to the lower bound function. The remaining assertion can be proved in a similar way.

By the mean-value theorem we have for all $x \in X$

$$f(x) = f(x(\sigma)) + f'(\xi)^{\mathrm{T}} \cdot (x - x(\sigma)),$$

where $\xi = \lambda x + (1-\lambda)x(\sigma)$ for some $\lambda \in [0,1]$. Then for $\sigma_i = 0$ $(i = 1, \ldots, n)$ the inequalities

$$f_i'(\xi) \geqslant d_i(\sigma), x_i - x_i(\sigma) \geqslant 0 \quad \text{for all } x \in X$$

hold, and for $\sigma_i = 1$ the inequalities

$$f_i'(\xi) \leqslant d_i(\sigma), x_i - x_i(\sigma) \leqslant 0 \quad \text{for all } x \in X$$

are valid. Therefore, by the mean-value theorem we get

$$\begin{aligned} f(x) &= f(x(\sigma)) + \sum_{i=1}^{n} f_i'(\xi) \cdot (x_i - x_i(\sigma)) \\ &\geqslant f(x(\sigma)) + \sum_{i=1}^{n} d_i(\sigma) \cdot (x_i - x_i(\sigma)) \\ &= f(x(\sigma)) + d(\sigma)^{\mathrm{T}} \cdot (x - x(\sigma)) \\ &= d(\sigma)^{\mathrm{T}} \cdot x + \{f(x(\sigma)) - d(\sigma)^{\mathrm{T}} \cdot x(\sigma)\}. \end{aligned}$$

Now using (10), we have $\underline{f}(x; X, \sigma) \leqslant f(x)$ for all $x \in X$, and $\underline{f}(x(\sigma); X, \sigma) = f(x(\sigma))$. □

With Theorem 4.1 it is possible to construct several affine lower bound functions. Bounds $\underline{d}, \overline{d}$ for the gradient $f'(x)$ over X can be calculated by using some interval extension of $f'(x)$. Moreover, calculating these bounds can be fully automatized, if automatic differentiation (see, e.g., [15]) is used. Then, a fixed vector $\sigma \in \{0, 1\}^n$ is chosen. Formula (10) yields an affine function $\underline{f}(x; X, \sigma)$. Inequality (12) implies that $\underline{f}(x; X, \sigma)$ is a lower bound function of f over X. Eq. (13) shows that this lower bound function coincides with the original function f in the vertex $x(\sigma)$.

Obviously, different vectors σ yield different affine lower bound functions. Because the maximum of affine lower bound functions is a convex lower bound function, improved convex lower bound functions can be obtained by using the maximum operator. Analoguosly, linear upper bound functions $\overline{f}(x; X, \sigma)$ can be constructed.

Example 4.1. We demonstrate this approach for the function of Example 3.1. Bounds for the derivative of f are computed by using the natural interval extension of the first derivative of f which is defined by the interval expression

$$4(X - 1.5) + \frac{1}{X + 0.25} + 0.1 \cdot 4\pi \cdot \mathrm{COS}(4\pi X). \tag{14}$$

This expression yields for the intervals $X = [0, 2]$ and $X = [0.9, 1.0]$ the bounds $D = [-6.8121, 7.2567]$ and $D = [-1.2116, 0.12621]$, respectively. The affine functions $\underline{f}(x; X, \sigma)$ which are defined by (10) are displayed for both intervals and for $\sigma = 0$ and $\sigma = 1$ as dash–dotted lines in Fig. 2.

For the small interval $X = [0.9, 1.0]$ these affine functions approximate f from below better than the convex lower bound functions of order 0 in Fig. 1. The contrary is true for the larger interval $X = [0, 2]$.

Bound functions which approximate the shape of f in a better way than these affine functions can be constructed by using the same decomposition technique as in the

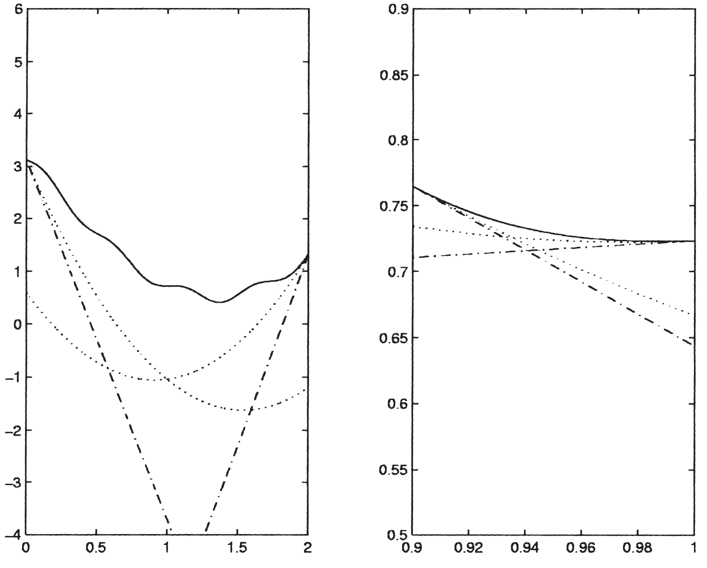

Fig. 2. Lower bound functions of first order (Example 4.1).

previous section. Theorem 4.1 can be applied to decompositions (4) by computing bounds for the derivative of r, that is $r'(x) \in D$ for all $x \in X$. Using (9) and (10) for the function r it follows that

$$\underline{f}(x; X, \sigma) := c(x) + \underline{e}(x) + d(\sigma)^{\mathrm{T}} \cdot x + \{r(x(\sigma)) - d(\sigma)^{\mathrm{T}} \cdot x(\sigma)\} \tag{15}$$

is a convex lower bound function of f.

For our function f in Example 3.1 we have chosen $c(x)$, $\underline{e}(x)$, and $r(x)$ as in the previous section. The convex lower bound functions $\underline{f}(x; X, \sigma)$ defined by (15) are displayed in Fig. 2 (dotted lines) for both intervals, and for $\sigma = 0$ and $\sigma = 1$. These functions clearly improve the corresponding affine lower bound functions.

By looking at the bound functions using decomposition techniques (dotted lines in Figs. 1 and 2), it follows that for the large interval $X = [0, 2]$ the lower bound functions of order 0 approximate the function f better than the lower bound functions of first order, but are worse for the smaller interval $X = [0.9, 1.0]$. In most of our experiments this behaviour is typical.

However, there are also many classes of functions where, independently of the diameter of X, the lower bound functions of first order yield the uniformly best possible convex lower bound functions, and thus always yield sharper results than those of order 0. Obviously, this is true for affine functions, because in this case Theorem 4.1 generates the original affine function itself.

It is also true for bilinear functions. In a large variety of engineering applications there occur nonlinear systems and constrained global optimization problems where many of the constraints are defined by bilinear functions. In [22] it is proved that for the bilinear function $f(x_1, x_2) := x_1 \cdot x_2$, Theorem 4.1 automatically generates the convex envelope, that is the uniformly best possible underestimating function: The function

$$\underline{f}(x) := \max\{\underline{f}(x; X, 0), \underline{f}(x, X, 1)\}, \tag{16}$$

where

$$\begin{aligned} \underline{f}(x; X, 0) &= \underline{x}_2 x_1 + \underline{x}_1 x_2 - \underline{x}_1 \underline{x}_2, \\ \underline{f}(x; X, 1) &= \overline{x}_2 x_1 + \overline{x}_1 x_2 - \overline{x}_1 \overline{x}_2, \end{aligned} \tag{17}$$

is the convex envelope of f on $X = [\underline{x}_1, \overline{x}_1] \times [\underline{x}_2, \overline{x}_2]$. A similar formula holds for the concave envelope. Originally, the convex envelope of a bilinear function is given in [1]. But it is interesting that this convex envelope is generated by applying Theorem 4.1.

Last we want to mention that Theorem 4.1 remains also valid if the bounds $[\underline{d}, \overline{d}]$ are replaced by corresponding bounds for slopes (see [17,25,32]). Therefore, Theorem 4.1 permits to construct also convex lower and concave upper bound functions for nondifferentiable functions. In this connection the reader is also referred to [18], where for the one-dimensional case a tolerance polyhedron is constructed which contains the range of a given function.

5. Lower and upper bound functions of second order

In this section we consider convex and quasiconvex lower bound functions which need second order information. First, we present a theorem concerning the convex case.

Theorem 5.1. *Let $f : S \to \mathbb{R}$ be a twice continuously differentiable function, where $S \subseteq \mathbb{R}^n$. Let $X \in \mathbb{IR}^n$ be an interval vector with $X \subseteq S$, and let $\sigma \in \{0, 1\}^n$. Suppose further that*

(1) *two real $n \times n$ matrices $\underline{H}, \overline{H}$ satisfy the inequalities*

$$\underline{H} \leqslant f''(x) \leqslant \overline{H} \quad \text{for all } x \in X, \tag{18}$$

(2) *the real $n \times n$ matrix $\underline{H}(\sigma)$ is defined by*

$$\underline{H}_{ij}(\sigma) := \begin{cases} \underline{H}_{ij} & \text{if } \sigma_i = \sigma_j, \\ \overline{H}_{ij} & \text{otherwise} \end{cases} \tag{19}$$

for $0 \leqslant i, j \leqslant n$,

(3) *an interval vector $Y := [\underline{y}; \overline{y}]$ is defined by*

$$Y := \tfrac{1}{2}\underline{H}(\sigma)(X - x(\sigma)), \tag{20}$$

where the operations are interval operations, and $x(\sigma)$ is the vertex of X corresponding to σ.

Then the following results hold:

(a) *The quadratic function*

$$\begin{aligned} \underline{f}(x; X, \sigma) := {} & f(x(\sigma)) + f'(x(\sigma))^{\mathrm{T}}(x - x(\sigma)) \\ & + \tfrac{1}{2}(x - x(\sigma))^{\mathrm{T}}\underline{H}(\sigma)(x - x(\sigma)) \end{aligned} \tag{21}$$

is a lower bound function of f with $\underline{f}(x(\sigma); X, \sigma) = f(x(\sigma))$.

(b) *If $\underline{H}(\sigma)$ is positive semidefinite, then $\underline{f}(x; X, \sigma)$ is a convex lower bound function of f on X.*

(c) *The function*

$$\begin{aligned} \underline{g}(x; X, \sigma) := {} & f(x(\sigma)) + f'(x(\sigma))^{\mathrm{T}}(x - x(\sigma)) \\ & + \sum_{i=1}^{m} \max\{q_i^1(x), q_i^2(x)\}, \end{aligned} \tag{22}$$

where

$$q_i^1(x) := \underline{y}_i(x_i - x_i(\sigma)) + \tfrac{1}{2}(\underline{x}_i - x_i(\sigma))\underline{H}_{i:}(\sigma)(x - x(\sigma)) - (\underline{x}_i - x_i(\sigma))\underline{y}_i,$$
$$q_i^2(x) := \overline{y}_i(x_i - x_i(\sigma)) + \tfrac{1}{2}(\overline{x}_i - x_i(\sigma))\underline{H}_{i:}(\sigma)(x - x(\sigma)) - (\overline{x}_i - x_i(\sigma))\overline{y}_i,$$

is a convex lower bound function of f with $\underline{g}(x(\sigma); X, \sigma) = f(x(\sigma))$.

Proof. (a) The Taylor expansion of *f* with respect to $x(\sigma)$ gives for $x \in X$

$$\begin{aligned} f(x) = {} & f(x(\sigma)) + f'(x(\sigma))^{\mathrm{T}}(x - x(\sigma)) \\ & + \tfrac{1}{2}(x - x(\sigma))^{\mathrm{T}} f''(\zeta)(x - x(\sigma)), \end{aligned} \tag{23}$$

where $\zeta = \lambda x + (1 - \lambda)x(\sigma)$ for some $\lambda \in [0, 1]$.

If $\sigma_i = \sigma_j = 0$, or if $\sigma_i = \sigma_j = 1$, then using formula (2) it follows that

$$(x_i - x_i(\sigma)) \cdot (x_j - x_j(\sigma)) \geqslant 0,$$

and $\sigma_i \neq \sigma_j$ implies

$$(x_i - x_i(\sigma)) - (x_j \cdot x_j(\sigma)) \leqslant 0.$$

Hence, definition (19) yields

$$(x_i - x_i(\sigma))(f''(\zeta))_{ij}(x_j - x_j(\sigma)) \geqslant (x_i - x_i(\sigma)) \cdot \underline{H}_{ij}(\sigma)(x_j - x_j(\sigma))$$

for all $i, j = 1, \ldots, n$, and therefore

$$(x - x(\sigma))^{\mathrm{T}} f''(\zeta)(x - x(\sigma)) \geqslant (x - x(\sigma))^{\mathrm{T}} \cdot \underline{H}(\sigma)(x - x(\sigma)) \tag{24}$$

for all $x \in X$. Using (21), (23) and (24), it follows that $\underline{f}(x; X, \sigma) \leqslant f(x)$ for all $x \in X$, and $\underline{f}(x(\sigma); X, \sigma) = f(x(\sigma))$.

(b) This follows from the well-known fact that $\underline{f}(x; X, \sigma)$ is convex iff the Hessian $\underline{H}(\sigma)$ is positive semidefinite.

(c) From definition (20) it follows that *Y* is the interval hull of

$$\{z = \tfrac{1}{2}\underline{H}(\sigma) \cdot (x - x(\sigma)) : x \in X\}.$$

Hence, for each $x \in X$ there exists a $y \in Y$ such that

$$y = \tfrac{1}{2}\underline{H}(\sigma) \cdot (x - x(\sigma)),$$

and the quadratic function (21) can be written as a bilinear form

$$b(x) := f(x(\sigma)) + f'(x(\sigma))^{\mathrm{T}}(x - x(\sigma)) + \sum_{i=1}^{n} y_i \cdot (x_i - x_i(\sigma)).$$

Using (16) and (17) it follows that the convex envelope of the bilinear functions $y_i \cdot (x_i - x_i(\sigma))$ is

$$\max\{\alpha_i^1(x, y), \alpha_i^2(x, y)\}, \tag{25}$$

where

$$\alpha_i^1(x,y) := \underline{y}_i(x_i - x_i(\sigma)) + (\underline{x}_i - x_i(\sigma)) \cdot y_i - (\underline{x}_i - x_i(\sigma)) \cdot \underline{y}_i,$$
$$\alpha_i^2(x,y) := \overline{y}_i(x_i - x_i(\sigma)) + (\overline{x}_i - x_i(\sigma)) \cdot y_i - (\overline{x}_i - x_i(\sigma)) \cdot \overline{y}_i.$$

Substituting $y_i = \frac{1}{2}\underline{H}_{i:}(\sigma)(x - x(\sigma))$ in (25) proves assertion (c). □

Next, we state a theorem concerning differentiable pseudoconvex lower bound functions on $\mathbb{R}^n{}_+$.

Theorem 5.2. *With the assumptions of Theorem* 5.1 *let* $S \subseteq \mathbb{R}^n{}_+$, *and suppose further that*
(i) $\underline{H}(\sigma)$ *has exactly one negative eigenvalue*, $\underline{H}(\sigma) \leqslant 0$, *and* $f'(x(\sigma)) \leqslant 0$;
(ii) *there exists a vector* $s \in \mathbb{R}^n$ *such that*

$$\underline{H}(\sigma) \cdot s = -f'(x(\sigma)); \; \textit{and} \; f'(x(\sigma))^{\mathrm{T}} \cdot s \geqslant 0. \tag{26}$$

Then the quadratic function $\underline{f}(x; X, \sigma)$ *defined by* (21) *is quasiconvex on* $\mathbb{R}^n{}_+$ *and pseudoconvex on the interior of* $\mathbb{R}^n{}_+$.

Proof. Using Theorem 5.1 of [36], it follows that the quadratic function $\underline{f}(x; X, \sigma)$ is pseudoconvex on the interior of $\mathbb{R}^n{}_+$. Corollary 2.1 in [36] implies that $\underline{f}(x; X, \sigma)$ is quasiconvex on $\mathbb{R}^n_+$. □

Since global optimization problems and nonlinear systems with simple lower bounds $\underline{x} \in \mathbb{R}^n$ can be transformed into the positive orthant by using the transformation $y := x - \underline{x}$, the assumption $S \subseteq \mathbb{R}^n_+$ is not restrictive. There are several possibilities for checking conditions (i) and (ii) of Theorem 5.2. For example, Cottle's algorithm [7] can be used to check whether $\underline{H}(\sigma)$ has exactly one negative eigenvalue and that condition (26) holds.

We mention that it is easy to formulate theorems similar to Theorems 5.2 and 5.1, which allow us to construct quasiconcave upper bound functions.

In this section and the previous two we developed several bound functions. We do not present a detailed convergence analysis. But it is straightforward to prove that these bound functions converge for all $x \in X$ to the original function if the width of X converges to 0, provided the used interval extensions are convergent to its corresponding range functions. The bound functions of Sections 4 and 5 are constructed by using the Taylor expansion which determines the order of convergence.

6. Decomposition techniques

For many functions it is difficult to prove quasiconvexity or quasiconcavity, or to bound these functions appropriately by quasiconvex or quasiconcave functions. But frequently these functions can be decomposed into parts which have certain convexity and sign properties. The following theorem presents some basic rules for constructing quasiconvex lower bound functions of appropriately decomposed functions.

Theorem 6.1. *Let $f, g : X \to \mathbb{R}$ be given where $X \subseteq \mathbb{R}^n$ is convex, and let $\underline{f}, \overline{f}, \underline{g}, \overline{g} : X \to \mathbb{R}$ be convex lower and concave upper bound functions on X for f and g, respectively. Then*:
1. *$\underline{f} + \underline{g}$ is a convex lower bound function of the sum $f + g$ on X.*
2. *$\underline{f} - \overline{g}$ is a convex lower bound function of the difference $f - g$ on X.*
3. *If f is nonpositive and g is nonnegative on X, then $\underline{f} \cdot \overline{g}$ is a quasiconvex lower bound function of the product $f \cdot g$ on X.*
4. *If $\underline{f}$ and $\underline{g}$ are positive and $1/\underline{f}$ or $1/\underline{g}$ is concave on X, then $\underline{f} \cdot \underline{g}$ is a quasiconvex lower bound function of the product $f \cdot g$ on X.*
5. *If $\overline{f}$ and $\overline{g}$ are negative and $1/\overline{f}$ or $1/\overline{g}$ is convex on X, then $\overline{f} \cdot \overline{g}$ is a quasiconvex lower bound function of the product $f \cdot g$ on X.*
6. *If $\underline{f}$ is nonnegative and g is positive on X, then $\underline{f}/\overline{g}$ is a quasiconvex lower bound function of the ratio f/g on X.*
7. *If f is nonpositive and $\underline{g}$ is positive on X, then $\underline{f}/\underline{g}$ is a quasiconvex lower bound function of the ratio f/g on X.*
8. *If f is positive on X, then $1/\overline{f}$ is a convex lower bound function of the reciprocal $1/f$ on X.*

Proof. Because the sum of two convex functions is convex, assertions 1 and 2 follow.

3. For $x \in X$ it is $\underline{f}(x) \leqslant f(x) \leqslant 0$ and $0 \leqslant g(x) \leqslant \overline{g}(x)$, and therefore $\underline{f}(x) \cdot \overline{g}(x) \leqslant f(x) \cdot \overline{g}(x) \leqslant f(x) \cdot g(x)$. Hence, $\underline{f} \cdot \overline{g}$ is a lower bound function of $f \cdot g$ on X. Because $-\underline{f}$ and $\overline{g}$ are nonnegative and concave, Table 5.1 in [4] yields the quasiconcavity of $-\underline{f} \cdot \overline{g}$, and therefore the quasiconvexity of $\underline{f} \cdot \overline{g}$.

4. The positivity of $\underline{f}$ and $\underline{g}$ implies that $\underline{f} \cdot \underline{g}$ is a lower bound function of $f \cdot g$. Since $1/\underline{f}$ or $1/\underline{g}$ is concave, Table 5.1 in [4] yields the quasiconvexity of the product $\underline{f} \cdot \underline{g}$.

5. The assumption is equivalent to $-\overline{f}$ and $-\overline{g}$ are positive, and $-1/\overline{f}$ or $-1/\overline{g}$ is concave on X. Table 5.1 in [4] yields the quasiconvexity of the product $-\overline{f} \cdot (-\overline{g})$. Observing that $-\overline{f}(x) \leqslant -f(x)$, $-\overline{g}(x) \leqslant -g(x)$ implies that $-\overline{f} \cdot (-\overline{g})$ is a quasiconvex lower bound function of $-f \cdot (-g)$.

6. For $x \in X$ the inequalities $0 < g(x) \leqslant \overline{g}(x)$, $0 \leqslant \underline{f}(x)$ imply $\underline{f}(x)/\overline{g}(x) \leqslant \underline{f}(x)/g(x) \leqslant f(x)/g(x)$, demonstrating that $\underline{f}/\overline{g}$ is a lower bound function of f/g. The quasiconvexity follows from Table 5.4 in [4] by using the convexity of $\underline{f}$ and the concavity of $\overline{g}$.

7. The assumptions imply that $\underline{f}(x) \leqslant f(x) \leqslant 0$ and $0 < 1/g(x) \leqslant 1/\underline{g}(x)$ for $x \in X$. Hence $\underline{f}(x)/\underline{g}(x) \leqslant f(x)/g(x) \leqslant f(x)/g(x)$ for all $x \in X$.

Since $-\underline{f}$ is nonnegative and concave and $\underline{g}$ is positive and convex, Table 5.4 in [4] yields the quasiconcavity of $-\underline{f}/\overline{g}$. Therefore, $\underline{f}/\overline{g}$ is quasiconvex.

Property 8 follows from the fact that the reciprocal function of a positive concave function is convex. □

We remark that in Section 3 the decomposition of a function into additive parts is a simple application of assertion 1 of this theorem. The other assertions of Theorem 6.1 allow us additionally to consider decompositions with respect to the other real operations. In the case where one of the parts is an affine function, stronger statements can be proved.

Theorem 6.2. *Let $X \subseteq \mathbb{R}^n$ be convex, and suppose that $f : X \to \mathbb{R}$ with convex lower and concave upper bound functions $\underline{f}$ and $\overline{f}$, respectively. Let $g : \mathbb{R}^n \to \mathbb{R}$ be an affine function. Then*:

1. *If f is nonpositive and g is nonnegative on X, then $\underline{f} \cdot g$ is a quasiconvex lower bound function of $f \cdot g$ on X.*
2. *If f is nonnegative and g is nonpositive on X, then $\overline{f} \cdot g$ is a quasiconvex lower bound function of $f \cdot g$ on X.*
3. *If $\underline{f}$ is positive, $1/\underline{f}$ is concave, and g is nonnegative on X, then $\underline{f} \cdot g$ is a quasiconvex lower bound function of $f \cdot g$ on X.*
4. *If $\overline{f}$ is negative, $1/\overline{f}$ is convex, and g is nonpositive on X, then $\overline{f} \cdot g$ is a quasiconvex lower bound function of $f \cdot g$ on X.*

Proof. 1. The inequalities $\underline{f}(x) \leqslant f(x)$ and $g(x) \geqslant 0$ yield the lower bound function $\underline{f}(x) \cdot g(x) \leqslant f(x) \cdot g(x)$. Using Table 5.2 in [4] proves the first assertion. Analoguously, the remaining assertions can be proved. □

A similar theorem can be proved for the ratio of two functions. The following theorem considers the composition.

Theorem 6.3. *Let $X \subseteq \mathbb{R}^n$ be convex, and let $g_i : X \to \mathbb{R}$ for $i = 1, \ldots, m$ with convex lower and concave upper bound functions $\underline{g}_i, \overline{g}_i : X \to \mathbb{R}$, respectively. Let $I \subseteq \{1, \ldots, m\}$, $J := \{1, \ldots, m\} - I$, and let $\hat{g}_i := \underline{g}_i$ for $i \in I$ and $\hat{g}_j := \overline{g}_j$ for $j \in J$. Suppose further that $f : Y \to R$ is a quasiconvex function, where $Y \subseteq \mathbb{R}^m$ is convex and contains the range of $g := (g_1, \ldots, g_m)$ and $\hat{g} := (\hat{g}_1, \ldots, \hat{g}_m)$ over X. If f is nondecreasing in the variables y_i with $i \in I$ and nonincreasing in the variables y_j with $j \in J$, then $f(\hat{g}(x))$ is a quasiconvex lower bound function of the composition $f(g(x))$ over X.*

Proof. We assume $I = \{1, \ldots, l\}$, $J = \{l+1, \ldots, m\}$. Because $\underline{g}_i(x) \leqslant g_i(x)$ and $\overline{g}_i(x) \geqslant g_i(x)$, the monotonicity properties of f imply

$$f(\hat{g}(x)) = f(\underline{g}_1(x), \ldots, \underline{g}_l(x), \overline{g}_{l+1}(x), \ldots, \overline{g}_m(x)) \leqslant f(g(x)),$$

i.e., $f(\hat{g})$ is a lower bound function of the composition $f(g)$.

Let $x^1, x^2 \in X$ and $0 \leqslant \lambda \leqslant 1$. Then the convexity and concavity of the components of $\hat{g}$ together with the monotonicity of f imply that

$$\begin{aligned} &f(\hat{g}(\lambda x^1 + (1-\lambda)x^2)) \\ &\quad \leqslant f(\lambda g_1(x^1) + (1-\lambda)g_1(x^2), \ldots, \lambda g_m(x^1) + (1-\lambda)g_m(x^2)). \end{aligned}$$

Since f is quasiconvex, this inequality implies

$$f(\hat{g}(\lambda x^1 + (1-\lambda)x^2) \leqslant \max\{f(g(x^1)), f(g(x^2))\},$$

yielding the quasiconvexity of $f(\hat{g}(x))$ on X. □

It should be noticed that $f(\hat{g}(x))$ is a convex lower bound function of the composition $f(g(x))$, provided f is convex. This follows immediately from the previous proof.

For differentiable functions the quasiconvexity in the above theorems can be replaced by pseudoconvexity (see [4]). Similar theorems can be proved for quasiconcave upper bound functions of sums, differences, products, ratios and compositions. Moreover, several other special rules can be derived by using the theory in [4]. But this is out of the scope of this paper.

7. Quasiconvex relaxations

Next we show how the bound functions which are described in the previous sections can be used to construct quasiconvex relaxations of the constrained global optimization problem

$$\min_{x \in F} f(x) \tag{27}$$

with the set of *feasible solutions*

$$F := F(X) := \left\{ x \in S : \quad \begin{array}{l} g_i(x) \leqslant 0 \text{ for } i = 1, \ldots, m \\ h_j(x) = 0 \text{ for } j = 1, \ldots, l \\ x \in X \end{array} \right\}, \tag{28}$$

where $S \subseteq \mathbb{R}^n$, $X := [\underline{x}, \overline{x}] \in \mathbb{IR}^n$ with $X \subseteq S$, and f, g_i, h_j are real-valued functions defined on S. We denote the global minimum value (if it exists) by f^* and the set of global minimum points by F^*.

The basic idea of relaxations for problem (27), (28) is to relax all equality and inequality constraints which do not satisfy certain desired properties. Relaxing a constraint means either to omit this constraint or to replace it by some constraints which (i) have these desired properties, and (ii) do not cut off feasible solutions.

The construction of quasiconvex relaxations for problem (27), (28) is based on the following simple observation: Let $\underline{g}_{ik}(x; X)$ with $k = 1, \ldots, k_i$ be quasiconvex lower bound functions of the function g_i. Then

$$\{x \in X\colon g_i(x) \leqslant 0\} \subseteq \{x \in X\colon \underline{g}_{ik}(x; X) \leqslant 0\} \quad \text{for } k = 1, \ldots, k_i,$$

and $\{x \in X : \underline{g}_{ik}(x;X) \leqslant 0\}$ are convex sets for every k. Hence, replacing in the set of feasible solutions F the ith inequality by some quasiconvex inequalities $\underline{g}_{ik}(x;X) \leqslant 0$, the resulting set of solutions contains F, and has at least k_i quasiconvex inequalities.

We now proceed as follows. The relaxation is presently defined by all quasiconvex inequalities and all quasilinear equations of F. The remaining inequalities $\{x \in X : g_i(x) \leqslant 0\}$ which are not quasiconvex are replaced by some quasiconvex inequalities $\{x \in X : \underline{g}_{ik}(x;X) \leqslant 0\}$. The remaining equations $\{x \in X : h_j(x) = 0\}$ which are not quasilinear are written as two inequalities $\{x \in X : h_j(x) \leqslant 0\}$, $\{x \in X : -h_j(x) \leqslant 0\}$, and these two inequalities are treated in the same way as the inequalities above. It follows that this process leads to a relaxed solution set $R = R(X)$, which contains $F = F(X)$ and consists only of quasiconvex inequalities and quasilinear equations. The objective function $\underline{f}(x;X)$ of our quasiconvex relaxation is defined as a pseudoconvex lower bound function of the objective f over X.

For such a quasiconvex relaxation

$$\min_{x \in R} \underline{f}(x;X) \tag{29}$$

it is well known (cf. [3]) that the Kuhn–Tucker points are the global minimum points. There are very efficient methods (for example interior-point methods or SQP-methods) for calculating Kuhn–Tucker points. Hence, a lower bound of the global minimum value for problem (27), (28) can be computed efficiently.

Many algorithms for solving problem (27), (28) with interval arithmetic (see, e.g., [17,23,31]) can be viewed as specialized branch and bound schemes using an interval relaxation, where all constraints of this problem are omitted with exception of the simple bounds X. Then a lower bound of the global minimum value is calculated using an interval extension of the objective evaluated over the box X. By using these interval relaxations all informations and dependencies coming from the constraints disappear. However, all these methods use additionally acceleration algorithms like Interval-Newton methods, monotonicity tests, convexity tests, etc.

Example 7.1. We illustrate the construction of relaxations for an example such that some of the previous results can be used. We discuss the problem of variable dimension n:

$$\begin{aligned}
\text{minimize} \quad & f(x) := -\frac{\ln((5+x_1)^2 + \sum_{i=1}^n x_i)}{1 + \sum_{i=1}^n x_i^2} \\
\text{subject to} \quad & h_1(x) := \sum_{i=1}^n i \cdot x_i - n = 0, \\
& g_1(x) := \sum_{i=1}^n x_i^2 - 0.5\pi^2 \leqslant 0, \\
& g_2(x) := -\left(\tfrac{1}{2}x_1^2 + \tfrac{1}{2}x_2^2 + x_3^2 + 2x_1x_2 + 4x_1x_3 + 2x_2x_3\right) \leqslant 0,
\end{aligned}$$

$$g_3(x) := -x_1^2 - 6x_1x_2 - 2x_2^2 + \cos(x_1) + \pi \leqslant 0,$$
$$x_i \in X_i := [0.5] \text{ for } i = 1, \ldots, n. \tag{30}$$

For $x \geqslant 0$ the numerator of *f* is nonpositive and convex, and the denominator of *f* is positive and convex. Theorem 6.1 assertion 7 yields the quasiconvexity of *f*. The differentiability implies the pseudoconvexity of *f*. The equation $h_1(x) = 0$ is linear, and the inequality $g_1(x) \leqslant 0$ is convex.

A short computation shows that

$$g_2(x) = (x_1, x_2, x_3) \cdot H \cdot \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \text{ with } H = -\begin{pmatrix} 0.5 & 1 & 2 \\ 1 & 0.5 & 1 \\ 2 & 1 & 1 \end{pmatrix}. \tag{31}$$

For this quadratic function we choose $\sigma = 0$. Then, $x(\sigma) = 0$, $\underline{H}(\sigma) = \underline{H} = \overline{H} = H \leqslant 0$, $g_2'(x(\sigma)) = 0$, and $\underline{H}(\sigma)$ has exactly one negative eigenvalue -3.4429. For the vector $s := 0$, condition (ii) of Theorem 5.2 is fulfilled. Hence, g_2 is a quasiconvex function on $\mathbb{R}^n{}_+$.

The third constraint function $g_3(x)$ can be bounded from below by using the lower bound function

$$\underline{g}_3(x) := -x_1^2 - 6x_1x_2 - 2x_2^2 + \underline{e}(X), \tag{32}$$

where $\underline{e}(X) := \inf\{\mathrm{COS}(X_1) + \pi\}$ is computed using interval arithmetic. This yields

$$\underline{g}_3(x) = (x_1, x_2) \cdot H \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \underline{e}(X),\ H = \begin{pmatrix} -1 & -3 \\ -3 & -2 \end{pmatrix}, \tag{33}$$

For $\sigma = 0$ we get $x(\sigma) = 0$, $\underline{H}(\sigma) = \underline{H} = \overline{H} = H \leqslant 0$, $\underline{g}_3'(x(\sigma)) = 0$, $\underline{H}(\sigma)$ has exactly one negative eigenvalue -4.5414, and $s := 0$ satisfies condition (ii) of Theorem 5.2. Hence, $\underline{g}_3$ is also quasiconvex on $\mathbb{R}^n{}_+$. Using the construction rules above, we get the quasiconvex relaxation

$$\min_{x \in R} f(x),\ R := \{x \in X : h_1(x) = 0,\ g_1(x) \leqslant 0,\ g_2(x) \leqslant 0,\ \underline{g}_3(x) \leqslant 0\}, \tag{34}$$

where the pseudoconvex objective f and the constraints $h_1(x) = 0$, $g_1(x) \leqslant 0$, $g_2(x) \leqslant 0$ are unchanged.

The numerical experiments of the following section show that for dimension $n = 50$ the global minimum value is $f^* = -1.8424$ (in the following we display only five decimal digits). Using the above quasiconvex relaxation, the MATLAB-routine *fmincon* (an implementation of the SQP-method) has computed a Kuhn–Tucker point yielding the lower bound -2.2757 for the box X with $X_i = [0,\ 5]$ for $i = 1, \ldots, n$. Using the natural interval extension of the objective (that is we use the aforementioned interval relaxation), we get for this box the lower bound -5.8579. In contrast to the natural interval extension, the lower bound calculated with the SQP-method is rather close.

Obviously, the quasiconvex relaxation (34) converges to the original problem (30) iff the constraint function $\underline{g}_3$ converges to g_3. From definition (32) it follows that this convergence occurs if the width of X_1 converges to 0. Therefore, if we use in a branch and bound method this quasiconvex relaxation to obtain lower bounds, only the first coordinate of box X has to be bisected such that the lower bounds converge to the global minimum value of the original problem. This advantage of quasiconvex relaxations (only few coordinates of box X have to be bisected in many cases) can significantly reduce the computational costs.

Similar to global optimization, it is possible to construct relaxations for calculating all zeros of a nonlinear system of equations $f(x) = 0$, where $x \in \mathbb{R}^n$, and the components f_i, $i = 1, \ldots, n$, of f are real-valued functions defined on $\mathbb{R}^n$. For a given box $X \in \mathbb{IR}^n$, we define a relaxed set R as a system of equations and inequalities consisting of

(i) all quasilinear equations,
(ii) all inequalities which arise if each nonquasilinear equation $f_i(x) = 0$ is replaced by at least two inequalities $\underline{f}_i(x; X) \leqslant 0$, and $\overline{f}_i(x; X) \geqslant 0$.

Here $\underline{f}_i$, $\overline{f}_i$ denote a quasiconvex lower bound and a quasiconcave upper bound function of f_i on X, respectively.

Obviously, R is a convex set which contains all zeros of f in X. Therefore, if $0 \notin R$, then X contains no zeros of f. Since R is a convex set, the test, whether 0 is contained in R or not, can be computationally solved by using one of the feasibility methods which are well-known in optimization (see, e.g., [12]). This test can be incorporated in branch and bound schemes for determining all zeros of f in a given region X.

8. A branch and bound method

Many deterministic algorithms for solving continuous global optimization problems and combinatorial optimization problems are based on a branch and bound framework (see, e.g., [12,17,20,21,23,31] and references cited therein).

The basic idea of branch and bound methods is (i) to partition the set of feasible solutions, (ii) to compute upper and lower bounds of the global minimum value for the partitioned subproblems, and (iii) to discard subproblems which are infeasible, or which cannot contain global minimum points of the original problem. Branch and bound algorithms differ in a number of items, for example how the bounds are calculated, in their partition rules, infeasibility tests, acceleration strategies, etc. Convergence of special branch and bound algorithms can be proved, provided mild conditions on the partitioning and bounding are valid (see [21]).

In the following algorithm for solving problem (27), (28) we use quasiconvex relaxations for computing lower bounds of the global minimum value, and a box reduction strategy based on interval arithmetic. The basic steps are as follows:

(1) *Initialization*: Set a tolerance ϵ, set the lower and upper bounds of the global minimum value $\underline{f}^* := -\infty$, $\overline{f}^* := \infty$, set the simple bounds $X^0 := [\underline{x}; \overline{x}]$ of problem

(27), (28), and initialize a list $L := \{(\underline{f}^*, X^0)\}$ which contains the lower bounds for the minimum value of the subproblems together with the simple bounds.

(2) *Choosing a subproblem*: If the list L of subproblems is empty, then the set of feasible solutions is empty and the algorithm is terminated. Otherwise choose a subproblem $(\underline{f}^*, X^0)$ from list L, and discard it from list L.

(3) *Computing the upper bound*: Choose a starting point $x_0 \in X^0$, and apply an optimization routine for problem (27) with the simple bounds X^0.
If the optimization routine calculates a Kuhn–Tucker point $\tilde{x}$, and $f(\tilde{x}) < \overline{f}^*$, then the overall upper bound $\overline{f}^* := f(\tilde{x})$ is updated, and $\tilde{x}$ is stored in a list A which contains all calculated Kuhn–Tucker points of problem (27).

(4) *Computing the lower bound*: Apply an optimization routine for computing a Kuhn–Tucker point $\underline{\tilde{x}}$ of the quasiconvex relaxation (29) with respect to the simple bounds X^0.
If the set of feasible solutions $R(X^0)$ of the relaxed problem is empty, then goto step (2), that is the current subproblem is discarded.
If the calculated Kuhn–Tucker point satisfies $f(\underline{\tilde{x}}) > \overline{f}^*$, then our current subproblem cannot contain a global minimum point of the original problem (27). Goto step (2), that is the current subproblem is discarded.
If $f(\underline{\tilde{x}}) \leqslant \overline{f}^*$, then the overall lower bound $\underline{f}^*$ is updated as the minimum of $f(\underline{\tilde{x}})$ and the lower bounds of the subproblems stored in list L.

(5) *Box contraction*: In this step we try to contract the bounds X^0 of our current subproblem such that no global minimum point of the original problem (27) is lost (see the remark below).

(6) *Branching*: For the current box of simple bounds X^0 an index $j \in J$ is selected, where J is a subset of $\{1, \ldots, n\}$ which is related to the given quasiconvex relaxation (see below). Then X_j is bisected yielding two new boxes X^1, X^2. The new subproblems $(f(\underline{\tilde{x}}), X^1)$ and $(f(\underline{\tilde{x}}), X^2)$ are stored on list L.

(7) *Termination*: If $(\overline{f}^* - \underline{f}^*) > \epsilon$, then goto step (2). Otherwise, *ϵ-convergence* is fulfilled, and the Kuhn–Tucker point on list A with smallest objective value satisfies $\overline{f}^* = f(\underline{\tilde{x}}) \geqslant \underline{f}^*$.

Some remarks to this algorithm. Step (4) requires to decide whether the set of feasible solutions of the relaxed problem is empty or not. This can be checked in the usual way by using one of the feasibility tests.

The efficiency of our branch and bound method is affected by the quality how close the relaxation approximates the corresponding subproblem. We get a close approximation of our quasiconvex relaxation, provided the generated bound functions are close approximations of the corresponding original functions. The diameters of the simple bounds of the subproblems mainly influence this approximation quality. Therefore, many techniques for contracting the simple bounds X^0 without cutting off global minimum points have been developed.

In order to contract the simple bounds X^0 in step (5), we prefer a nonlinear version of the interval Gauss–Seidel method. This technique was introduced by

Neumaier [28], and is based on the Gauss–Seidel method for linear interval equations (see also [8,23,29]). The advantage is that in many cases only a few operations are necessary to contract the simple bounds and to accelerate the branch and bound method.

For other contraction strategies which do not use interval arithmetic the reader is referred to [16,34,37,41].

As in our example of the previous section, we bisect in step (6) only those coordinates of box X^0 which are necessary for the convergence of the quasiconvex relaxation to the original problem. The indices of these coordinates are stored in J, and the indices are chosen such that the width of X_j converges to 0 for each $j \in J$. If F is nonempty, then a global minimum point exists, and after a finite number of bisections list A will be nonempty and termination (7) occurs. If F is empty, then after finitely many bisections all relaxed subproblems are empty, and list L will be empty; that is, the algorithm terminates in step (2) with the result that F is empty.

From the previous section it follows that for linear, convex and quasiconvex global optimization problems the original problem coincides with its quasiconvex relaxation. Hence, in steps (3) and (4) the same Kuhn–Tucker points are calculated, and our algorithm terminates during the first iteration in step (7) with $\overline{f}^* = \underline{f}^* = f^*$. Therefore, the global optimization problem is solved with about the same computational work which is needed for calculating a Kuhn–Tucker point. This termination property also indicates that almost quasiconvex optimization problems may be solved efficiently. We remark that the classical interval branch and bound methods have severe difficulties in solving constrained global optimization problems, and they do not terminate in a reasonable time even for linear programming problems of small size. In this connection Kearfott [23, p. 170] and Van Hentenryck et al. [38, p. 157] have remarked that only a few numerical results for global constrained optimization problems are known.

Due to rounding and cancellation errors the above branch and bound algorithm may compute wrong approximations of the global minimum points and the lower and upper bounds of the global minimum value. But with the tools of interval arithmetic it is possible to compute rigorous results, if one considers the following details in an implementation. First, the bound functions described in the previous sections are rigorous, if the interval extensions for computing the corresponding ranges are rigorous. If Theorem 5.2 is applied, then additionally one has to check conditions (i) and (ii). This check can be done by using self-validating methods for symmetric eigenvalue problems and for linear systems.

Secondly, in step (3) a verified feasible solution of problem (27), (28) must be computed, and in step (4) a verified solution of the Kuhn–Tucker conditions for the relaxed problem (29) must be computed. For both problems interval algorithms for nonlinear systems can be used. The verification of the Kuhn–Tucker conditions requires enclosures of the second derivatives of the objective function and the constraints.

Third, during the box contraction process no global minimum points are permitted to be lost. The contraction strategies based on interval arithmetic have this property.

At the moment the results computed by our code are not fully guaranteed. Because our programming environment does not allow us to compute automatically enclosures of second derivatives, we cannot verify the Kuhn–Tucker conditions. But in our future work we want to implement a completely self-validating algorithm. Some preliminary experiments demonstrate that the computational work of such a self-validating code should not exceed twice of the computational time of our present code.

9. Numerical results

Following, five examples are discussed. The first two problems are constructed in such a way that (i) they support and make clear the earlier analysis and discussion on quasiconvexity, and that (ii) the behaviour of quasiconvex relaxations for varying dimension can be illustrated. The following two examples are the seemingly most difficult examples in the benchmarks of NUMERICA [38], which is a recently developed commercial software package for solving constrained global optimization problems and nonlinear systems, and which has solved several applications and problems very successfully. The last example is a practical application. All numerical experiments were executed on a PC with a 400 MHz processor. Our algorithm is written in MATLAB using the toolbox INTLAB [33] which supports the computation with interval quantities.

Example 9.1. First, we illustrate the numerical behaviour of our branch and bound algorithm for the constrained global optimization problem which is defined in Example 7.1. We have solved this problem with NUMERICA [38], just to get an impression about the tractablility.

The numerical results of NUMERICA for our example are displayed in Table 1.

The lower and upper bounds $\underline{f}^*, \overline{f}^*$ of the global minimum value f^* are very close, but the time is growing exponentially with dimension n. For dimension $n = 17$ NUMERICA needs almost one day, and for $n > 30$ NUMERICA would not compute reasonable bounds $\underline{f}^*, \overline{f}^*$ in an appropriate time. Moreover, the number of splits (splittings into subproblems during the branch and bound process) grows exponentially. Summarizing, this example seems to be a hard one.

For our branch and bound algorithm we have chosen the relaxed problem (34) and $J := \{1\}$. Then (see Example 7.1) the constraints of this problem are equal to or

Table 1
Results of NUMERICA for Example 9.1

n	$\left[\underline{f}^*, \overline{f}^*\right]$	Splits	Time/s
5	[−1.71 690 290, −1.71 690 288]	222	25
11	[−1.73 942 247, −1.73 942 243]	5381	2371
17	[−1.77 241 420, −1.77 241 417]	52,093	86,123

Table 2
Results of our algorithm for Example 9.1

n	$\left[\underline{f}^*, \overline{f}^*\right]$	Splits	Time/s
5	[−1.71 697 410, −1.71 689 781]	83	51
11	[−1.73 948 743, −1.73 941 734]	91	102
17	[-1.77 248 308, −1.77 240 890]	93	228
50	[−1.84 244 447, −1.84 235 747]	91	879
100	[−1.86 829 917, −1.86 816 530]	93	3976

converge to the constraints of problem (30) provided the width of X_1 converges to 0. The numerical results for some different dimensions n are displayed in Table 2.

By comparing Tables 1 and 2 it can be seen that in contrast to the results of NUMERICA, here the number of splits is almost constant for all dimensions. This demonstrates that the chosen problem is not very complicated. In the case $n = 5$ NUMERICA is faster than our algorithm, but this behaviour changes for larger dimensions. NUMERICA's results are more accurate. NUMERICA uses the interval Newton method as a technique to compute very accurate bounds. This technique requires enclosures of Hessians for the objective and the constraints. If information about the derivatives of second order are not used, then the precision of the bounds may be not very accurate and a cluster problem may occur. For a theoretical treatment of such cluster problems, see [24]. At the moment our programming environment does not allow us to compute automatically enclosures of second derivatives. But in the future we intend to incorporate interval Newton's method in our code. However, the precision of our present code is satisfactory from a practical point of view.

Example 9.2. The following example of variable dimension n is constructed in such a way that the set of feasible solutions is not connected, and the objective function is not pseudoconvex:

$$
\begin{aligned}
\text{minimize}\quad & f(x) := \tfrac{1}{2}(x_2 - x_1^2)^2 + (1 - x_1)^2 + \sum_{i=1}^{n}(x_i - 1)^2 \\
\text{subject to}\quad & h_1(x) := x_1 \cdot x_2 - 0.1 = 0, \\
& g_1(x) := \sum_{i=1}^{n} x_i^2 - 1 \leqslant 0, \\
& x_i \in X_i := [-1, 1], \quad i = 1, \ldots, n.
\end{aligned}
\tag{35}
$$

Results of NUMERICA for this example are displayed in Table 3.

In order to construct a relaxation, we use for the objective function the decomposition $f(x) = c(x) + e(x) + r(x)$, where

Table 3
Results of NUMERICA for Example 9.2

n	$[\underline{f}^*, \overline{f}^*]$	Splits	Time/s
10	[5.06 511 561, 5.06 511 576]	899	65
12	[6.48 337 242, 6.48 337 259]	4572	861
14	[7.95 417 880, 7.95 417 886]	26,903	6052
16	[9.46 556 251, 9.46 556 271]	148,233	86,102

$$
\begin{aligned}
c(x) &:= \tfrac{1}{2}x_1^4 + \tfrac{1}{2}x_2^2 + (1 - x_1)^2 + \sum_{i=1}^{2n}(x_i - 1)^2,\\
e(x) &:= 0,\\
r(x) &:= -x_1^2 x_2.
\end{aligned}
$$

Then c is a convex function. We set $\underline{e}(x) := 0$, $\sigma := 0$, and we use formula (15) to get a convex lower bound function.

Because $r'(x) = -(2x_1x_2, x_1^2)^{\mathrm{T}}$, it follows that for

$$
[\underline{d}, \overline{d}] := -\begin{pmatrix} 2[\underline{x}_1, \overline{x}_1] \cdot [\underline{x}_2, \overline{x}_2] \\ [\underline{x}_1, \overline{x}_1]^2 \end{pmatrix}
$$

the inequalities $\underline{d} \leqslant r'(x) \leqslant \overline{d}$ hold for all $x \in X := [\underline{x}, \overline{x}]$.

Therefore,

$$
\underline{f}(x, X, 0) = c(x) + \underline{d}_1 x_1 + \underline{d}_2 x_2 + \{-\underline{x}_1^2 \underline{x}_2 - \underline{d}_1 \underline{x}_1 - \underline{d}_2 \underline{x}_2\}
$$

is a convex lower bound function of the objective function.

First, we add to the relaxation the convex constraint $g_1(x) \leqslant 0$ and the simple bounds of the original problem. The bilinear function $-x_1x_2 + 0.1$ is quasiconvex for nonnegative variables x_1, x_2. In order to bound the equation $\{x \in \mathbb{R}^n : h_1(x) = 0\}$ from one side, we add to our relaxation the quasiconvex inequality

$$
-x_1x_2 + 0.1 \leqslant 0 \quad \text{if } \; x_1 \geqslant 0, x_2 \geqslant 0. \tag{36}
$$

Moreover, using formulae (16) and (17) we bound this bilinear equation additionally by the corresponding convex and concave envelopes. A short calculation shows that the constraints of this relaxation are given by

$$
\begin{aligned}
&\underline{x}_2 x_1 + \underline{x}_1 x_2 - \underline{x}_1 \underline{x}_2 - 0.1 \leqslant 0,\\
&\overline{x}_2 x_1 + \overline{x}_1 x_2 - \overline{x}_1 \overline{x}_2 - 0.1 \leqslant 0,\\
&\overline{x}_2 x_1 + \underline{x}_1 x_2 - \underline{x}_1 \overline{x}_2 - 0.1 \geqslant 0,\\
&\underline{x}_2 x_1 + \overline{x}_1 x_2 - \overline{x}_1 \underline{x}_2 - 0.1 \geqslant 0,\\
&-x_1x_2 + 0.1 \leqslant 0, \text{ if } x_1 \geqslant 0, x_2 \geqslant 0,\\
&\sum_{i=1}^{n} x_1^2 - 1 \leqslant 0, x_i \in X_i := [-1, 1], \quad i = 1, \ldots, n.
\end{aligned} \tag{37}
$$

Table 4
Numerical results of our method for Example 9.2

n	$\left[\underline{f}^*, \overline{f}^*\right]$	Splits	Time/s
10	[5.06 509 838, 5.06 512 073]	31	73
12	[6.48 334 993, 6.48 337 850]	31	71
14	[7.95 410 774, 7.95 418 662]	27	85
16	[9.46 551 215, 9.46 557 043]	29	127
50	[37.8 024 490, 37.8 028 132]	31	1332
100	[82.4 977 028, 82.4 983 736]	32	18,072

Obviously, this relaxation converges to the original problem provided the widths of the components X_1 and X_2 converge to 0. Hence, we define $J := \{1, 2\}$. Using this relaxation together with our simple branch and bound scheme yields the numerical results which are displayed in Table 4.

For our method the number of splits is slightly decreasing for growing dimensions. The reason for this behaviour is that for growing dimension only variables are added which appear in convex or quasiconvex terms of the original problem. Hence, this relaxation approximates the original problem very well for growing dimension.

Example 9.3. In the following, we discuss briefly the example of largest dimension in the benchmarks of NUMERICA [38, pp. 158, 201]. There, it is reported, that 701 s and 3983 splittings are required for solving this problem. On our PC, NUMERICA needs 930 s and 3983 splits. In this example, all variables which do not appear in convex terms appear in bilinear terms. These bilinear terms are bounded as in the previous example yielding a quasiconvex relaxation.

Using this relaxation in our branch and bound method, we get after 35 splits the enclosure

$$[\underline{f}^*, \overline{f}^*] = [24.3046,\ 24.3063]$$

The computing time is 44 s.

Example 9.4. The following example (see h93.mth in [38]) is the most difficult and most time-consuming constrained optimization problem of the benchmarks in NUMERICA. There, it is reported that 69759 s and 459163 splits are required. On our PC, NUMERICA needs 86 275 s and 507820 splits. This problem has a nonconvex objective function and two nonconvex constraints. Because of the many products of variables occurring in the objective and the two constraints, we have used the well-known transformation $x_i := \exp(z_i)$ for $i = 1, \ldots, 6$. Then the transformed problem consists of a convex objective, a convex inequality and a concave inequality. In our relaxation, we have bounded the concave inequality (from below) by a linear inequality.

Table 5
Numerical results for Example 9.4

$\left[\underline{f}^*, \overline{f}^*\right]$	Splits	Time/s
[119.270 435 928, 135.076 365 935]	50	36
[127.418 523 471, 135.076 365 935]	500	624
[132.438 744 849, 135.076 365 935]	5000	5021

Table 6
Numerical results for Example 9.5

$\left[\underline{f}^*, \overline{f}^*\right]$	Splits	Time/s
[545 35:1 411; 568 25:8 870]	5	29
[566 32:4 674; 568 25:8 870]	50	496
[566 32:4 674; 568 25:8 870]	500	4557

Our numerical results for this example are displayed in Table 5. We have stopped our algorithm after 50, 500, and 5000 splits. It can be seen that after a few splits the global minimum value is enclosed rather well (for 500 splits the precision is about 5%). However, to get better enclosures much computational costs are necessary.

Example 9.5. This example (see [13, pp. 62–66]) describes a heat exchanger network of two hot streams and one cold stream. The goal is to obtain an optimal heat exchanger configuration. The modelling yields a nonconvex constrained optimization problem with 16 variables and 13 equality constraints. In [13] a best known solution is reported with the objective value 56825.

We have run NUMERICA for about two weeks without getting reasonable bounds. The computational results of our method are displayed in Table 6.

With few splits rather close bounds are computed. Increasing the number of splits increases the computational time, but not the quality of the bounds. This is because clustering occurs.

More numerical results for the special case of convex relaxations which are based on interval arithmetic can be found in [22]. Our numerical experiments show a good behaviour for problems which can be modelled well by quasiconvex lower or quasiconcave upper bound functions. However, there are several problems where our method delivers unsatisfactory results. This comprises the class of NP-hard problems (where each method has difficulties), and problems where polynomial functions of higher order occur. For such polynomials the bounds calculated by interval arithmetic drastically overestimate the corresponding ranges. One possibility to overcome these difficulties could be to use Bernstein polynomials as described by Garloff [14].

Last we want to stress that the input of a problem in NUMERICA is much easier. In NUMERICA only the original problem is given to the computer. In our code the quasiconvex relaxation must be added. This is a disadvantage of our approach. However, giving additional information like relaxations and underestimating functions to the computer seems to be an appropriate way in order to solve more complex problems.

10. Conclusions

In this paper, we have investigated the construction of quasiconvex relaxations for constrained global optimization problems and nonlinear systems. The basic idea proposed here is to take appropriate linear or quadratical estimators of the constraints and the objective. These estimators are guaranteed and use the tools of interval arithmetic. Moreover, a branch and bound algorithm for constrained global optimization problems is described which mainly uses these relaxations for computing lower bounds of subproblems. Our approach of constructing relaxations and using them in a branch and bound framework tries to overcome one of the shortcomings of classical interval branch and bound methods, namely the problem of dependence and overestimation which is mainly introduced by the constraints.

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