Quasi Convex-Concave Extensions

Christian Jansson

1 Introduction

Convexity and its generalizations have been considered in many publications during the last decades. In this paper we discuss the problem of bounding functions from below by quasiconvex functions and from above by quasiconcave functions. Moreover, applications for nonlinear systems and constrained global optimization problems are considered briefly.

For a given real-valued function $f(x)$, which is defined on some subset of $\mathbf{R^n}$ (the set of real vectors with n components), the gradient and the Hessian is denoted by $f'(x)$ and $f''(x)$, respectively. Sometimes, a function depends on parameters. In such situations the argument is seperated from the parameters by a semicolon. For example, the function $f(x; X)$ has the argument x and depends on the parameter X.

A function $f : S \to \mathbf{R}$ which is defined on a convex set $S \subseteq \mathbf{R^n}$ is called *quasiconvex*, if for all $x, y \in S, 0 \le \lambda \le 1$ the inequality

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

holds true.

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. A differentiable function $f : S \to \mathbf{R}$ is said to be *pseudoconvex*, if for all $x, y \in S$ with $f'(x)^T(x-y) \ge 0$ it is $f(y) \ge f(x)$. It can be shown that pseudoconvex functions are quasiconvex, and differentiable convex functions are pseudoconvex (see Avriel et al. (1988)).

Many quasiconvex functions are known which are not convex; for example $f(x) = -x_1 x_2$ is quasiconvex on the positive orthant, and the ratio of a nonnegative convex and a positive concave function is quasiconvex. 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 sufficient for global optimality, provided that the objective and the constraints are defined by certain quasiconvex and quasiconcave functions. Quasiconvexity (see Avriel (1976), Avriel et al. (1988), and Schaible (1972), (1981)) is of great importance in optimization theory, engineering and management science. Many applications can be found in Cambini et al.(1989).

Following, we introduce a new notion which can be viewed as a generalization of interval extensions. We assume that the reader is familiar with the basic concepts of interval arithmetic (see Alefeld and Herzberger (1983), Moore (1979), Neumaier (1990), and Ratschek and Rokne (1984)). A *quasi convex-concave extension* of a function $f : S \to \mathbf{R}$ is a mapping $[\underline{f}, \overline{f}]$ which delivers for each interval vector $X := [\underline{x}, \overline{x}] := \{x \in \mathbf{R^n} \ : \ \underline{x} \le x \le \overline{x}\}$ with $X \subseteq S$ a quasiconvex function $\underline{f}(x;X)$ and a quasiconvave function $\overline{f}(x;X)$, which are both defined on X such that

$$\underline{f}(x;X) \leq f(x) \leq \overline{f}(x;X) \text{ for all } x \in X. \tag{2}$$

In other words, the pair $\underline{f}(x;X)$ and $\overline{f}(x;X)$ contain the range of f over X. The functions $\underline{f}(x;X), \overline{f}(x;X)$ are called *lower bound function* and *upper bound function* on X, respectively.

By definition, interval extensions of f deliver real lower and upper bounds $\underline{f}(X), \overline{f}(X)$ for the range of f over X. These bounds can be interpreted as constant functions, and constant functions are both quasiconvex and quasiconcave. Hence, it follows that an interval extension is a special case of a quasi convex-concave extension.

The major goal of this paper is to give a short survey about the construction of quasi convex-concave extensions with nonconstant bound functions by using the tools of interval arithmetic. These extensions can be applied in a flexible manner such that the overestimation due to interval arithmetic can be reduced in many cases.

2 Relaxations

We will motivate quasi convex-concave extensions in this section by some applications. Consider the constrained global optimization problem

$$\min_{x \in F} f(x) \text{ where } F := \{x \in X : g_i(x) \leq 0 \text{ for } i = 1, \ldots, m\}, \tag{3}$$

and assume that f, g_i are differentiable real-valued functions defined on $X \subseteq \mathbf{R^n}$.

Constrained global optimization problems are NP-hard, even for quadratic functions. One approach for solving NP-hard optimization problems is to use branch and bound methods. During the last decade several methods and programs for constrained global optimization problems became available which use branch and bound techniques and are mainly based on interval arithmetic (see e.g. Hansen (1992), Kearfott (1996), Neumaier (1997), Dallwig, Neumaier and Schichl (1997), Ratschek and Rokne (1988), Schnepper and Stadtherr (1993), and Van Hentenryck, Michel and Deville (1997)).

Our approach (see Jansson (1999a),(1999b), and (2000)) for solving constrained global optimization problems uses quasiconvex relaxations, which permit to compute lower bounds for subproblems generated during a branch and bound process.

A *quasiconvex relaxation* of problem (3) is an optimization problem

$$\min_{x \in R} \underline{f}(x) \text{ where } R := \{x \in X : \underline{g}_i(x) \leq 0 \text{ for } i = 1, \ldots, m\}, \tag{4}$$

with the properties that $\underline{f}$ is a pseudoconvex lower bound function of f on X, and $\underline{g}_i$ are quasiconvex lower bound functions of g_i for $i = 1, \ldots, m$ on X. These lower bound functions can be obtained by using the results about quasi convex-concave extensions which are presented in the following sections. By definition

(4) it follows immediately that the quasiconvex relaxation has the properties (i) $F \subseteq R$, and (ii) the global minimum value of the relaxation (4) provides a lower bound for the global minimum value of the original problem (3).

The Kuhn-Tucker points x^* of the relaxation (4) are characterized as the solutions of the nonlinear system

$$\underline{f}'(x^*) + \sum_{i=1}^{m} \lambda_i \underline{g}_i'(x^*) = 0,\ \lambda_i \underline{g}_i(x^*) = 0,\ \text{for } i = 1, \dots, m \tag{5}$$

with $\lambda_i \geq 0$ and $\underline{g}_i(x^*) \leq 0$ for $i = 1, \dots, m$. It follows (cf. Avriel (1976)) that each Kuhn-Tucker point of a quasiconvex optimization problem (4) is a global minimum point. There are very efficient methods (for example interior-point methods or SQP-methods) for calculating Kuhn-Tucker points. Hence, an approximate lower bound of the global minimum value for problem (3) can be computed efficiently. Using such an approximation, rigorous bounds for the global minimum value of (4) can be obtained by applying some verified nonlinear system solver to the equations (5).

Roughly speaking, our method for solving problem (3) consists of a branch and bound framework using quasiconvex relaxations. The lower bounds of the subproblems, which are required by this branch and bound scheme, are calculated by computing the Kuhn-Tucker points of the corresponding quasiconvex relaxations. For a detailed treatment of this approach the reader is referred to Jansson (1999b) and (2000).

Methods using convex relaxations for special structured continuous global optimization problems were first introduced by Falk and Soland (1969). Their approach concerns separable nonconvex programming problems. Later, in the case of concave minimization, convex relaxations have been used by Bulatov (1977), Bulatov and Kasinkaya (1982), Emelichev and Kovalev (1970), Falk and Hoffmann (1976), and Horst (1976). For recent developements and improvements see also Zamora and Grossmann (1998) and the references cited over there.

If additionally nonlinear equations $h_i(x) = 0$ are added to (3), then these can be represented as two nonlinear inequalities $h_i(x) \leq 0, h_i(x) \geq 0$. The latter two inequalities are replaced by $\underline{h}_i(x) \leq 0$ and $\overline{h}_i(x) \geq 0$ where $\underline{h}_i(x), \overline{h}_i(x)$ are a quasiconvex lower and a quasiconcave upper bound function, respectively. Then, it can be shown that for the resulting relaxation the necessary Kuhn-Tucker conditions are sufficient for global optimality. Hence, the aforementioned method can be applied for solving problems involving also nonlinear equations.

The zeros of nonlinear systems can be viewed as the set of feasible solutions of a constrained global optimization, where the constraints consist only of nonlinear equations and the objective is the zero function. Therefore, our branch and bound method can be applied for solving nonlinear systems.

3 Bound functions of first and second order

This section treats the construction of affine and quadratical convex lower bound functions. For arithmetical expressions, these bound functions can be automatically generated on a computer by using interval arithmetic.

For an interval vector $X = [\underline{x}, \overline{x}] \in \mathbf{IR^n}$ the 2^n vertices $x(\sigma)$ can be described by

$$x(\sigma) = \underline{x} + \sum_{i=1}^{n} \sigma_i(\overline{x}_i - \underline{x}_i)e_i, \tag{6}$$

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 i-th unit vector. 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 $x(0) = \underline{x},\ x(1) = \overline{x}$.

Theorem 1 *Given a continuously differentiable function $f : S \to \mathbf{R}$ with $S \subseteq \mathbf{R^n}$, and given an interval vector $X \subseteq S$. Suppose further that there exist two vectors $\underline{d}, \overline{d} \in \mathbf{R^n}$ such that the inequalities*

$$\underline{d} \leq f'(x) \leq \overline{d} \tag{7}$$

are valid 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 affine function

$$\underline{f}(x; X, \sigma) := d(\sigma)^T \cdot x + \{f(x(\sigma)) - d(\sigma)^T \cdot x(\sigma)\} \tag{8}$$

satisfies for all $x \in X$ the inequality

$$\underline{f}(x; X, \sigma) \leq f(x), \tag{9}$$

and moreover

$$\underline{f}(x(\sigma); X, \sigma) = f(x(\sigma)). \tag{10}$$

This theorem is a special case of Theorem 1 in Jansson (2000), and it allows 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, the calculation of these bounds can be fully automatized using automatic differentiation (see for example Griewank and Corliss (1991). Then, a fixed vector $\sigma \in \{0,1\}^n$ is chosen. Formula (8) yields an affine function $\underline{f}(x; X, \sigma)$. The inequality (9) implies that $\underline{f}(x; X, \sigma)$ is a lower bound function of f over X. Equation (10) shows that this lower bound function coincides with the original function f in the vertex $x(\sigma)$.

A similar formula can be derived for affine upper bound functions. One way is to construct a corresponding lower bound function of $-f$, and then to take the negative bound function. Therefore, in this paper we will present only formulae for lower bound functions.

Summarizing, we obtain a convex-concave extension of $f : S \to \mathbf{R}$ in the following way: fix a vector $\sigma \in \{0,1\}^n$, and for each interval vector $X \subseteq S$ calculate, by using some interval extension, an interval vector $D := [\underline{d}, \overline{d}]$ such that (7) is satisfied. Then the lower bound function (cf. (8)) and the upper bound function provide a corresponding quasi convex-concave extension where the bounds are affine functions.

In a large variety of engineering applications nonlinear systems and constrained global optimization problems occur where many of the constraints are defined by bilinear functions. In Jansson (2000) it is proved that for the bilinear functions $f(x_1, x_2) := x_1 \cdot x_2$ Theorem 1 generates automatically the convex envelope, that is the uniformly best possible underestimating function: The function

$$\underline{f}(x) := \max\{\underline{f}(x; X, 0), \underline{f}(x, X, 1)\}, \tag{11}$$

where

$$\begin{aligned} \underline{f}(x; X, 0) &= \underline{x}_2 x_1 + \underline{x}_1 x_2 - \underline{x}_1 \underline{x}_2 \\ \underline{f}(x; X, 1) &= \overline{x}_2 x_1 + \overline{x}_1 x_2 - \overline{x}_1 \overline{x}_2 \end{aligned} \tag{12}$$

is the convex envelope of f on $X = [\underline{x}_1, \overline{x}_1] \times [\underline{x}_2, \overline{x}_2]$. A similar formula is valid for the concave envelope. Originally, the convex envelope of a bilinear function is given in Al-Kayal and Falk (1983). However, it is interesting that this convex envelope is generated by applying Theorem 1.

Last, we mention that Theorem 1 remains also valid if in (7) the bounds $[\underline{d}, \overline{d}]$ are replaced by corresponding bounds for slopes (cf. for example Hansen (1992), Krawczyk and Neumaier (1985), and Rump (1996)). Therefore, also nondifferentiable functions may be bounded by affine functions.

The following theorem, which is proved in Jansson (1999b), is concerned with quadratic lower bound functions.

Theorem 2 *Let $f : S \to \mathbf{R}$ be a twice continuously differentiable function where $S \subseteq \mathbf{R^n}$. Let X 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*

$$\underline{H} \le f''(x) \le \overline{H} \quad \text{for all } x \in X; \tag{13}$$

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

$$\underline{H}_{ij}(\sigma) := \begin{cases} \underline{H}_{ij} & \text{if } \sigma_i = \sigma_j \\ \overline{H}_{ij} & \text{otherwise} \end{cases} \tag{14}$$

for $0 \le i, j \le n$;

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

$$Y := \frac{1}{2}\underline{H}(\sigma) \cdot (X - x(\sigma)), \tag{15}$$

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

Then the following results are valid:

(a) *The quadratic function*

$$\begin{array}{rcl} \underline{f}(x; X, \sigma) & := & f(x(\sigma)) + f'(x(\sigma))^T (x - x(\sigma)) \\ & + & \frac{1}{2}(x - x(\sigma))^T \underline{H}(\sigma)(x - x(\sigma)) \end{array} \tag{16}$$

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*

$$\underline{g}(x; X, \sigma) := f(x(\sigma)) + f'(x(\sigma))^T (x - x(\sigma)) + \sum_{i=1}^{m} \max\{q_i^1(x), q_i^2(x)\} \tag{17}$$

where

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

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

As in the case of the previous affine bound functions, this theorem gives the possibility to generate convex quadratical bound functions. The only difference is that now bounds $\underline{H}, \overline{H}$ for the Hessian of f with respect to X have to be calculated by using interval arithmetic. As before, also these bound functions define a quasi convex-concave extension.

4 Splittings

Interval arithmetic is capable to compute lower and upper bounds for the range of arithmetical expressions over a box. These bounds can be obtained by replacing each real operation and real variable in an arithmetical expression by a corresponding interval operation and interval variable, respectively. This process yields bounds which can be computed very fast, but which may overestimate the range because of the dependence of variables (see e.g. Neumaier (1990)).

In order to reduce the overestimation due to the problem of dependence, the question arises whether it is possible to bound and to work appropriately with arithmetical expressions itself rather than with interval variables and interval operations. In other words: Is it possible to bound an arithmetical expression by quasiconvex lower and quasiconcave upper bound functions, provided the arithmetical expression is splitted into two parts with respect to one of the real operations $+, -, *, /$.

In general this seems to be not possible for nonconstant bound functions: Indeed, the sum of two convex arithmetical expressions is convex, but this property is not valid for the product and the ratio.

However, the following theorem shows that at least in several cases quasiconvexity of lower bound functions for the product and the ratio of arithmetical expressions can be proved, provided these expressions satisfy certain sign and convexity properties.

Theorem 3 *Let $X \subseteq \mathbf{R^n}$ be convex, $g, h : X \to \mathbf{R}$, and assume that $\underline{g}, \underline{h}, \overline{g}, \overline{h}$ are convex lower and concave upper bound functions of g and h on X, respectively. Then:*

1. *$\underline{g} + \underline{h}$ is a convex lower bound function of the sum $g + h$ on X.*
2. *$\underline{g} - \overline{h}$ is a convex lower bound function of the difference $g - h$ on X.*
3. *If g is nonpositive and h is nonnegative on X, then $\underline{g} \cdot \overline{h}$ is a quasiconvex lower bound function of the product $g \cdot h$ on X.*
4. *If $\underline{g}$ and $\underline{h}$ are positive, and $1/\underline{g}$ or $1/\underline{h}$ is concave on X, then $\underline{g} \cdot \underline{h}$ is a quasiconvex lower bound function of the product $g \cdot h$ on X.*
5. *If $\overline{g}$ and $\overline{h}$ are negative, and $1/\overline{g}$ or $1/\overline{h}$ is convex on X, then $\overline{g} \cdot \overline{h}$ is a quasiconvex lower bound function of the product $g \cdot h$ on X.*
6. *If h is positive on X, then $1/\overline{h}$ is a convex lower bound function of the reciprocal $1/h$ on X.*
7. *If $\underline{g}$ is nonnegative and h is positive on X, then $\underline{g}/\overline{h}$ is a quasiconvex lower bound function of the ratio g/h on X.*

PROOF. 1. and 2. follow by observing that the sum of two convex functions is convex.

3. Using the assumptions $\underline{g}(x) \leq g(x) \leq 0$, $0 \leq h(x) \leq \overline{h}(x)$ it follows that $\underline{g}(x) \cdot \overline{h}(x) \leq \underline{g}(x) \cdot h(x) \leq g(x) \cdot h(x)$ for every $x \in X$.

Hence, $\underline{g} \cdot \overline{h}$ is a lower bound function of $g \cdot h$ on X. Since $-\underline{g}$ is nonnegative and concave, and $\overline{h}$ is nonnegative and concave, Table 5.1 in Avriel et al. (1988) implies the quasiconcavity of the product $-\underline{g} \cdot \overline{h}$. Therefore, $\underline{g} \cdot \overline{h}$ is quasiconvex.

4. The positivity of $\underline{g}$ and $\underline{h}$ implies that $\underline{g} \cdot \underline{h}$ is a lower bound function of $g \cdot h$. Since $1/\underline{g}$ or $1/\underline{h}$ is concave, Table 5.1 in Avriel et al. (1988) yields the quasiconvexity of the product $\underline{g} \cdot \underline{h}$.

5. The assumption is equivalent to $-\overline{g}, -\overline{h}$ are positive and $-1/\overline{g}$ or $-1/\overline{h}$ is concave. Table 5.1 in Avriel et al. (1988) yields the quasiconvexity of the

product $-\overline{g}\cdot(-\overline{h})$. Observing that $-\overline{g}(x) \leq -g(x), -\overline{h}(x) \leq -h(x)$ implies that $-\overline{g}\cdot(-\overline{h})$ is a quasiconvex lower bound function of $-g\cdot(-h)$.

Property 6. follows from the fact that the reciprocal function of a positive concave function is convex on X.

To prove 7., we observe that $\underline{g}/\overline{h}$ is a lower bound function of g/h because of the sign restrictions. The quasiconvexity of $\underline{g}/\overline{h}$ follows from Table 5.4 in Avriel et al. (1988) by using the convexity of $\underline{g}$ and the concavity of $\overline{h}$. □

The following theorem is concerned with the composition of functions.

Theorem 4 *Let $X \subseteq \mathbf{R^n}$ be convex, and let $f_i : X \to \mathbf{R}$ with convex lower bound functions $\underline{f}_i$ for $i = 1,\ldots,m$ be given. Let g be a nondecreasing quasiconvex function on the convex hull of the range of $(f_1,\ldots,f_m)$ over X. Then $g(\underline{f}_1,\ldots,\underline{f}_m)$ is a quasiconvex lower bound function of the composition $g(f_1,\ldots,f_m)$ on X.*

Proof. Since g is nondecreasing, the inequalities $\underline{f}_i(x) \leq f_i(x)$ for $i = 1,\ldots,m$ imply $g(\underline{f}_1(x),\ldots,\underline{f}_m(x)) \leq g(f_1(x),\ldots,f_m(x))$ for all $x \in X$. Hence, $g(\underline{f}_1(x),\ldots,\underline{f}_m(x))$ is a lower bound function of the composition. The remaining quasiconvexity follows from Theorem 5.3 in Avriel et al. (1988). □

Several other special rules can be derived in a similar manner. But this is out of the scope of this paper. However, there are situations where a function can be decomposed into two parts, but only one part can be well bounded by a convex or quasiconvex function. In this case the other part should be bounded by using an interval extension yielding a constant bound function. Then, because one of the parts is a constant, the sum, difference, product or ratio of these two parts can be bounded as usual.

5 Example

In order to illustrate how the previous results may be applied, we consider the function

$$f(x) = (5 + 2x(1-x) + 0.5x\exp(1.5x) + \frac{1}{4}\cos(6\pi x))/(x+0.5)$$

on the interval $X = [0,1]$. The function f (see Figure 1, solid) is a nonconvex function. The nonconvex numerator of f can be split into two parts: $g_1(x) := 5 + 2x + 0.5x\exp(1.5x)$ and $g_2(x) := -2x^2 + \frac{1}{4}\cos(6\pi x)$. The first part is convex, and we set $\underline{g}_1(x) := g_1(x)$ for all $x \in X$. Using Theorem 1, we bound g_2 from below by the affine functions

$$\underline{g}_2(x; X, \sigma) = d(\sigma)^T x + \{g_2(x(\sigma)) - d(\sigma)^T \cdot x(\sigma)\},$$

where $\sigma \in \{0,1\}$, and the interval $D = [\underline{d},\overline{d}]$ is computed by using the slope arithmetic which is contained in INTLAB (Rump (1999)). By Theorem 3, assertion 1 it follows that the two functions

$$\underline{g}(x; X, \sigma) := \underline{g}_1(x) + \underline{g}_2(x; X, \sigma), \quad \sigma \in \{0,1\}$$

are convex lower bound functions of the numerator of f. A short calculation using interval arithmetic shows that both functions $\underline{g}(x; X, \sigma)$ are positive. The denominator $h(x) := x + 0.5$ is also positive on X. Setting $\overline{h}(x) = h(x)$ for all $x \in X$, Theorem 3 assertion 7 implies that the functions $\underline{g}(x; X, \sigma)/\overline{h}(x)$ are quasiconvex lower bound functions of the ratio g/h on X. These lower bound functions are displayed for $\sigma = 0$ (dotted) and for $\sigma = 1$ (dash-dotted) in Figure 1. In the case $\sigma = 1$ the lower bound function is not convex but quasiconvex.

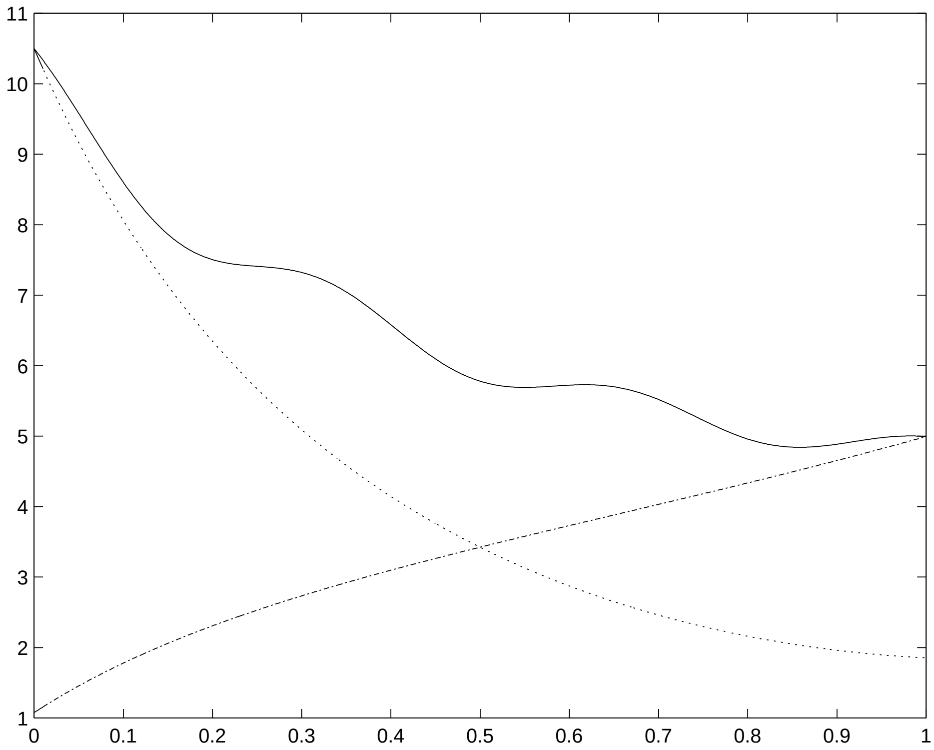

Fig. 1. Function f and two quasiconvex lower bound functions

Several other numerical examples including constrained global optimization problems of large scale are presented in Jansson (1999b), (2000).

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