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MULTIVARIATE CONVEX APPROXIMATION AND LEAST-NORM CONVEX DATA-SMOOTHING

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Multivariate convex approximation and least-norm convex data-smoothing

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Abstract

The main contents of this paper is two-fold. First, we present a method to approximate multivariate convex functions by piecewise linear upper and lower bounds. We consider a method that is based on function evaluations only. However, to use this method, the data have to be convex. Unfortunately, even if the underlying function is convex, this is not always the case due to (numerical) errors. Therefore, secondly, we present a multivariate data-smoothing method that smooths nonconvex data. We consider both the case that we have only function evaluations and the case that we also have derivative information. Furthermore, we show that our methods are polynomial time methods. We illustrate this methodology by applying it to some examples.

Keywords: approximation, convexity, data-smoothing.

JEL Classification: C60.

1 Introduction

In the field of discrete approximation, we are interested in approximating a function $y : \mathbb{R}^q \mapsto \mathbb{R}$, given a discrete dataset $\{(x^i, y^i) : 1 \leq i \leq n\}$, where $x^i \in \mathbb{R}^q$ and $y^i = y(x^i)$, and n is the number of data points. It may happen that we know beforehand that the function $y(x)$ is convex. However, many approximation methods do not make use of the information that $y(x)$ is convex and construct approximations that do not preserve the convexity. For the univariate case there is some literature on convexity preserving functions; see e.g. Kuijt (1998) and Siem et al. (2005). In Kuijt (1998), Splines are used, and in Siem et al. (2005), polynomial approximation is

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considered. For the multivariate case, Den Hertog et al. (2002), use convex quadratic polynomials to approximate convex functions. Furthermore, there is a lot of literature on so-called Sandwich algorithms; see e.g. Burkard et al. (1991), Fruhwirth et al. (1989), Rote (1992), Siem et al. (2005), and Yang and Goh (1997). In these papers, upper and lower bounds for the function $y(x)$ are constructed, based on the discrete dataset, and based on the knowledge that $y(x)$ is convex.

A problem that may occur in practice is that one may have a dataset that is subject to noise, i.e., instead of the data y^i we have $\tilde{y}^i = y(x^i) + \varepsilon_y^i$, where ε_y^i is (numerical) noise. There may also be noise in the input data, i.e., $\tilde{x}^i = x^i + \varepsilon_x^i$, and if derivative information is available, it could also be subject to noise, i.e., $\tilde{\nabla}y^i = \nabla y^i + \varepsilon_g^i$, where $\nabla y^i = \nabla y(x^i)$. Note that we assume $y(x)$ to be convex. However, due to the noise, the perturbed data might lose the convexity of $y(x)$, i.e., the noise could be such that it is not possible to fit a convex function through the perturbed data. Therefore, we are interested in data-smoothing, i.e., in shifting the data points, such that they obtain convexity, and such that the amount of movement of the data is minimized. This problem has already been tackled in literature for the univariate case; see e.g. Cullinan (1990), Demetriou and Powell (1991a), and Demetriou and Powell (1991b). Also in isotonic regression, this problem is dealt with for the univariate case; see Barlow et al. (1972).

In this paper, we will consider two problems. First, we consider how to construct piecewise linear upper and lower bounds to approximate the output for the multivariate case. This extends the method in Siem et al. (2005) for the univariate case. If derivative information is available it is easy to construct upper and lower bounds. However, derivative information is not always available, e.g., in the case of black-box functions. In this paper, it turns out that these upper and lower bounds can be found by solving linear programs (LPs).

Second, we will consider the multivariate data-smoothing problem. We consider both the case that we have only function evaluations and the case that we also have derivative information. We will show that, if we only consider errors in the output data, the first problem can be solved by using techniques, which are from linear robust optimization; see Ben-Tal and Nemirovski (2002). It turns out that this problem can be tackled by solving an LP. If we also have derivative information, we can also consider errors in the gradients and in the input variables. We then obtain a nonlinear optimization problem. However, if we assume that there are only errors in the gradients and in the output data, we obtain an LP. Also, if we assume that there are only errors in the input data and in the output data, we also obtain an LP.

The remainder of this paper is organized as follows. In Section 2, we consider the problem of constructing upper and lower bounds. In Section 3, we consider multivariate data-smoothing, and in Section 4, we give some examples of the application of the data-smoothing techniques, considered in Section 3. Finally, in Section 5, we present possible directions for further research.

2 Bounds preserving convexity

In this section we assume that $y(x)$ is convex and that the data $(x^i, y(x^i))$ for $i = 1, \dots, n$ are convex as well, i.e., there are no (numerical) errors, and there exists a convex function that

fits through the data points.

2.1 Upper bounds

We are interested in finding the smallest upper bound for $y(x)$, given convexity, and the data $(x^i, y(x^i))$, for $i = 1, \dots, n$. Let $x = \sum_{i=1}^n \alpha_i x^i$, where $\sum_{i=1}^n \alpha_i = 1$, and $0 \leq \alpha_i \leq 1$, i.e., x is a convex combination of the input data x^i . Then, it is well-known that convexity gives us the following inequality:

$$y(x) = y\left(\sum_{i=1}^n \alpha_i x^i\right) \leq \sum_{i=1}^n \alpha_i y(x^i). \quad (1)$$

This means that $\sum_{i=1}^n \alpha_i y(x^i)$ is an upper bound for $y(x)$. To find the smallest upper bound we should therefore solve

$$\begin{aligned} u(x) := \min_{\alpha_1, \dots, \alpha_n} & \sum_{i=1}^n \alpha_i y(x^i) \\ \text{s.t.} & x = \sum_{i=1}^n \alpha_i x^i \\ & 0 \leq \alpha_i \leq 1 \\ & \sum_{i=1}^n \alpha_i = 1. \end{aligned} \quad (2)$$

We will now show that the upper bound $u(x)$ is a continuous, convex, and piecewise linear function. Note that $u(x)$ is an optimal value function. Then it follows immediately from Theorem IV.51 in Roos et al. (1998) that $u(x)$ is continuous, convex and piecewise linear. Note that this upper bound is in fact the lower part of the convex hull of the data points (x^i, y^i) , for $i = 1, \dots, n$.

2.2 Lower bounds

If we have derivative information, it is easy to construct a lower bound. It is well-known that if $y(x)$ is convex, we have that

$$y(x) \geq y(x^i) + \nabla y(x^i)^T (x - x^i), \quad \forall x \in \mathbb{R}^q, \forall i = 1, \dots, n.$$

Therefore, $\ell(x) = \max_{i=1, \dots, n} (y(x^i) + \nabla y(x^i)^T (x - x^i))$ is a lower bound.

If we do not have derivative information, we have to do something else. We are interested in finding the largest lower bound for $y(x)$, given convexity and the data $(x^i, y(x^i))$, for $i = 1, \dots, n$. Let $x^k = \sum_{i \neq k} \alpha_i^k x^i + \alpha^k x$, where $\sum_{i \neq k} \alpha_i^k + \alpha^k = 1$, with $0 \leq \alpha_i^k \leq 1$, and $0 < \alpha^k \leq 1$, for all $k = 1, \dots, n$, i.e., x^k is a convex combination of x^i , $i \neq k$, and x . Then the following holds for all $k \in \{1, \dots, n\}$:

$$y(x^k) = y\left(\sum_{i \neq k} \alpha_i^k x^i + \alpha^k x\right) \leq \sum_{i \neq k} \alpha_i^k y(x^i) + \alpha^k y(x). \quad (3)$$

Without loss of generality we may assume that $\alpha^k > 0$. Then we can rewrite (3) as

$$y(x) \geq \frac{y(x^k) - \sum_{i \neq k} \alpha_i^k y(x^i)}{\alpha^k}, \text{ for } k = 1, \dots, n.$$

This inequality gives us a lower bound for $y(x)$. To obtain the largest lower bound we should solve the following problem:

$$\max_{k=1, \dots, n} \left\{ \begin{array}{l} \max_{\alpha^k, \alpha_i^k} \frac{y(x^k) - \sum_{i \neq k} \alpha_i^k y(x^i)}{\alpha^k} \\ \text{s.t. } x^k = \sum_{i \neq k} \alpha_i^k x^i + \alpha^k x \\ \sum_{i \neq k} \alpha_i^k + \alpha^k = 1 \\ 0 \leq \alpha_i^k \leq 1 \\ 0 < \alpha^k \leq 1 \end{array} \right\}. \quad (4)$$

This comes down to solving n nonlinear optimization problems, and taking the value of the largest solution. Note that the nonlinear optimization problems have linear constraints and a fractional objective with linear numerator and denominator. These kinds of optimization problems can be rewritten into an LP; see Charnes and Cooper (1962).

This can be done as follows. Define $t^k := 1/\alpha^k$. We can now rewrite the inner optimization problem in (4) as

$$\begin{array}{l} \max_{\alpha^k, \alpha_i^k, t^k} \quad t^k y(x^k) - \sum_{i \neq k} \alpha_i^k t^k y(x^i) \\ \text{s.t.} \quad x^k t^k = \sum_{i \neq k} \alpha_i^k t^k x^i + \alpha^k t^k x \\ \sum_{i \neq k} \alpha_i^k t^k + \alpha^k t^k = t^k \\ \alpha_i^k t^k \geq 0 \\ \alpha^k t^k = 1, \end{array}$$

where we multiplied all constraints by t^k . Now we define $z_i^k := \alpha_i^k t^k$ and $z^k := \alpha^k t^k$. We then get

$$\begin{array}{l} \max_{z^k, z_i^k, t^k} \quad t^k y(x^k) - \sum_{i \neq k} z_i^k y(x^i) \\ \text{s.t.} \quad x^k t^k = \sum_{i \neq k} z_i^k x^i + z^k x \\ \sum_{i \neq k} z_i^k + z^k = t^k \\ z_i^k \geq 0 \\ z^k = 1. \end{array} \quad (5)$$

Note that (5) is an LP. Therefore, for the lower bound $\ell(x)$ we obtain the following:

$$\ell(x) := \max_{k=1, \dots, n} \left\{ \begin{array}{l} \max_{z^k, z_i^k, t^k} \quad t^k y(x^k) - \sum_{i \neq k} z_i^k y(x^i) \\ \text{s.t.} \quad x^k t^k = \sum_{i \neq k} z_i^k x^i + z^k x \\ \sum_{i \neq k} z_i^k + z^k = t^k \\ z_i^k \geq 0 \\ z^k = 1. \end{array} \right\}. \quad (6)$$

Note that the number of constraints in (6) is $q + 1$. The number of variables in (6) is also $q + 1$. Therefore it takes polynomial time to find the lower bound. A direct approach, i.e., an approach by enumeration of all possible binding inequalities in (3) would give $n \times \binom{n-1}{q} = O(n^{q+1})$ calculations. Note that such a direct approach is not polynomial in q , the dimension of the problem.

We can now show that the lower bound $\ell(x)$ is continuous and piecewise linear. Denote the optimal value of the k -th inner optimization problem in (6) as a function of x by $f_k(x)$. Then we can write $\ell(x) = \max_{k=1, \dots, n} f_k(x)$. Note that $f_k(x)$ is an optimal value function. From Roos et al. (1998), Theorem IV.50, it follows that $f_k(x)$ is continuous, concave, and piecewise linear. If we take the maximum of continuous, and piecewise linear functions, we obtain a continuous, piecewise linear function. Therefore, $\ell(x)$ is continuous and piecewise linear.

3 Convex data-smoothing

If the dataset is not convex, we first have to smooth the data such that it becomes convex. We distinguish between the case that we only have function evaluations and the case that we also have derivative information.

3.1 Function value information

We only consider movement of the output data \tilde{y}^i . So, we want to minimally shift the perturbed output data \tilde{y}^i such that they become convex. In the following optimization problem, we minimize the upward shifts $(\delta_y^+)^i$ and the downward shifts $(\delta_y^-)^i$ such that the new shifted output data points y_s^i become convex:

$$\begin{array}{ll} \min_{\delta_y^+, \delta_y^-, y_s} & \sum_{i=1}^n ((\delta_y^+)^i + (\delta_y^-)^i) \\ \text{s.t.} & y_s^i = \tilde{y}^i + (\delta_y^+)^i - (\delta_y^-)^i \quad \forall i = 1, \dots, n \\ & y_s^i \leq \sum_{k \neq i} \lambda_k^i y_s^k \quad (\forall \lambda_k^i \in [0, 1] | x^i = \sum_{k \neq i} \lambda_k^i x^k, \sum_{k \neq i} \lambda_k^i = 1), \forall i = 1, \dots, n \\ & \delta_y^+ \in \mathbb{R}_+^n, \delta_y^- \in \mathbb{R}_+^n. \end{array} \quad (7)$$

We minimize the ℓ_1 -norm. It is easy to see that in the optimum either $(\delta_y^+)^i = 0$ or $(\delta_y^-)^i = 0$. The second constraint forces the shifted output data points y_s^i to become convex. Note that (7) is an LP with infinitely many constraints, i.e., it is a semi-infinite LP, which can also be seen as a robust linear programming problem. We can solve this problem with methods from Ben-Tal and Nemirovski (2002). Since the "uncertainty region": $\{\forall \lambda_k^i \in [0, 1] | x^i = \sum_{k \neq i} \lambda_k^i x^k, \sum_{k \neq i} \lambda_k^i = 1\}$ of the second constraint in (7) is a polytope, we can rewrite this semi-infinite programming constraint as a collection of linear constraints without an uncertainty region. We follow the reasoning of the proof of Theorem 1 in Ben-Tal and Nemirovski (2002) to show this. Let us consider the second constraint for a certain value of i . We can write this constraint as

$$\sum_{k \neq i} \lambda_k^i y_s^k - y_s^i \geq 0 \quad \forall (\lambda_k^i \in [0, 1] | x^i = \sum_{k \neq i} \lambda_k^i x^k, \sum_{k \neq i} \lambda_k^i = 1). \quad (8)$$

Note that this constraint is satisfied if and only if the solution of the minimization problem

$$\begin{aligned} \min_{\lambda_k^i} \quad & \sum_{k \neq i} \lambda_k^i y_s^k - y_s^i \\ \text{s.t.} \quad & x^i = \sum_{k \neq i} \lambda_k^i x^k \\ & \sum_{k \neq i} \lambda_k^i = 1 \\ & \lambda_k^i \in [0, 1] \end{aligned} \quad (9)$$

is nonnegative. The dual of this LP is given by:

$$\begin{aligned} \max_{r^i, v^i, w^i} \quad & (x^i)^T r^i + v^i + e_{n-1}^T w^i - y_s^i \\ \text{s.t.} \quad & (x^k)^T r^i + v^i + w_k^i \leq y_s^k \quad \forall k \neq i \\ & w^i \leq 0 \\ & r^i \in \mathbb{R}^q, v^i \in \mathbb{R}, w^i \in \mathbb{R}^{n-1}, \end{aligned} \quad (10)$$

where e_{n-1} is the $(n-1)$ -dimensional all-one vector. Since (10) is the dual of (9), both LP's have the same optimal solution. Note that (10) is nonnegative if and only if there **exists** a feasible solution for (10) such that the objective function of (10) is nonnegative. We can now conclude that (8) is satisfied if and only if there exist r^i , v^i , and w^i , which are feasible for (10) and have a nonnegative objective, i.e. if the following inequalities are satisfied:

$$\begin{cases} (x^i)^T r^i + v^i + e_{n-1}^T w^i \geq y_s^i \\ (x^k)^T r^i + v^i + w_k^i \leq y_s^k \quad \forall k \neq i \\ w^i \leq 0 \\ r^i \in \mathbb{R}^q, v^i \in \mathbb{R}, w^i \in \mathbb{R}^{n-1}. \end{cases} \quad (11)$$

We can now finally rewrite the second constraint in (7) as (11) for every $i = 1, \dots, n$. This means that we can rewrite (7) as

$$\begin{aligned}
& \min_{\delta_y^+, \delta_y^-, y_s, r^i, v^i, w^i} \sum_{i=1}^n ((\delta_y^+)^i + (\delta_y^-)^i) \\
& \text{s.t. } y_s^i = \tilde{y}^i + (\delta_y^+)^i - (\delta_y^-)^i \quad \forall i = 1, \dots, n \\
& (x^i)^T r^i + v^i + e_{n-1}^T w^i \geq y_s^i \quad \forall i = 1, \dots, n \\
& (x^k)^T r^i + v^i + w_k^i \leq y_s^k \quad \forall k \neq i, \forall i = 1, \dots, n \\
& w^i \leq 0 \quad \forall i = 1, \dots, n \\
& \delta_y^+ \in \mathbb{R}_+^n, \delta_y^- \in \mathbb{R}_+^n, \\
& w^i \in \mathbb{R}^{n-1}, r^i \in \mathbb{R}^q, v^i \in \mathbb{R} \quad \forall i = 1, \dots, n,
\end{aligned} \tag{12}$$

which is an LP. Note that, after substituting the equality constraints for y_s^i , the number of constraints in (12) is $n(n-1) + n = n^2$. The number of variables in (12) is $n^2 + (q+2)n$. A direct approach, i.e., an approach by enumeration of possible binding constraints for the uncertainty region in (7), would give $n \times \binom{n-1}{q+1} = O(n^{q+2})$ constraints, which is certainly a lot more. However, a direct approach would give $2n$ variables. Note also that such a direct approach is not polynomial in q , the dimension of the problem. However, since (12) is an LP, and the number of constraints and variables are polynomial in n and q , the proposed method is polynomial.

Above, we minimized the sum of the absolute values of the shifts, i.e. the ℓ_1 -norm. However, we can also choose to minimize other norms, such as e.g., the ℓ_∞ -norm or the ℓ_2 -norm. Using the ℓ_∞ -norm, we also obtain an LP, which is similar to (12). Using the ℓ_2 -norm, we obtain a convex quadratic program. This quadratic program has a quadratic objective with the same constraints as in (12).

3.2 Derivative information

Next, we consider the case in which we also have gradient information. Suppose that the underlying function is convex, but the data are not convex, due to (numerical) errors. Again, we are interested in shifting the data such that they become convex. We consider perturbed output values \tilde{y}^i , perturbed gradients $\tilde{\nabla}y(x^i)$, and perturbed input values \tilde{x}^i . Therefore in this case we want to minimize the shifts in the output values, in the gradients, and in the inputs. So, in the following optimization problem, we minimize the sum of upward and downward shifts $(\delta_y^+)^i$ and $(\delta_y^-)^i$ of the output values, the upward and downward shifts $(\delta_g^+)^i$ and $(\delta_g^-)^i$ of the gradient, and the upward and downward shifts $(\delta_x^+)^i$ and $(\delta_x^-)^i$ of the input values such that the

data become convex:

$$\begin{aligned}
& \min_{\substack{(\delta_y^+)^i, (\delta_y^-)^i, (\delta_g^+)^i, \\ (\delta_g^-)^i, (\delta_x^+)^i, (\delta_x^-)^i, \\ x_s^i, y_s^i, (\nabla y^i)_s}} \sum_{i=1}^n \left((\delta_y^+)^i + (\delta_y^-)^i + e_q^T (\delta_g^+)^i + e_q^T (\delta_g^-)^i + e_q^T (\delta_x^+)^i + e_q^T (\delta_x^-)^i \right) \\
& \text{s.t.} \quad (\nabla y^i)_s = \tilde{\nabla} y^i + (\delta_g^+)^i - (\delta_g^-)^i \quad \forall i = 1, \dots, n \\
& \quad \quad x_s^i = \tilde{x}^i + (\delta_x^+)^i - (\delta_x^-)^i \quad \forall i = 1, \dots, n \\
& \quad \quad y_s^i = \tilde{y}^i + (\delta_y^+)^i - (\delta_y^-)^i \quad \forall i = 1, \dots, n \\
& \quad \quad (\nabla y^i)_s^T (x_s^j - x_s^i) + y_s^i \leq y_s^j \quad \forall i, j = 1, \dots, n, i \neq j \\
& \quad \quad (\delta_y^+)^i \in \mathbb{R}_+, (\delta_y^-)^i \in \mathbb{R}_+, (\delta_g^+)^i \in \mathbb{R}_+^q \quad \forall i = 1, \dots, n \\
& \quad \quad (\delta_g^-)^i \in \mathbb{R}_+^q, (\delta_x^+)^i \in \mathbb{R}_+^q, (\delta_x^-)^i \in \mathbb{R}_+^q \quad \forall i = 1, \dots, n,
\end{aligned} \tag{13}$$

where $\nabla y^i = \nabla y(x^i)$, and e_q is the q -dimensional all-one vector. The 4-th constraint in (13) is a necessary and sufficient condition for convexity of the data; see page 338 in Boyd and Vandenberghe (2004). However optimization problem (13) is a nonconvex optimization problem, and therefore not tractable.

If there is no uncertainty in the input values x^1, \dots, x^n , we obtain

$$\begin{aligned}
& \min_{\substack{(\delta_y^+)^i, (\delta_y^-)^i, (\delta_g^+)^i, \\ (\delta_g^-)^i, (\nabla y^i)_s, y_s^i}} \sum_{i=1}^n \left((\delta_y^+)^i + (\delta_y^-)^i + e_q^T (\delta_g^+)^i + e_q^T (\delta_g^-)^i \right) \\
& \text{s.t.} \quad (\nabla y^i)_s = \tilde{\nabla} y^i + (\delta_g^+)^i - (\delta_g^-)^i \quad \forall i = 1, \dots, n \\
& \quad \quad y_s^i = y^i + (\delta_y^+)^i - (\delta_y^-)^i \quad \forall i = 1, \dots, n \\
& \quad \quad (\nabla y^i)_s^T (x^j - x^i) + y_s^i \leq y_s^j \quad \forall i, j = 1, \dots, n, i \neq j \\
& \quad \quad (\delta_y^+)^i \in \mathbb{R}_+, (\delta_y^-)^i \in \mathbb{R}_+, (\delta_g^+)^i \in \mathbb{R}_+^q, (\delta_g^-)^i \in \mathbb{R}_+^q \quad \forall i = 1, \dots, n,
\end{aligned} \tag{14}$$

which is an LP.

If we may assume there is no uncertainty in the values of the gradients, but only in the input data and the output data we obtain

$$\begin{aligned}
& \min_{\substack{(\delta_y^+)^i, (\delta_y^-)^i, (\delta_x^+)^i, \\ (\delta_x^-)^i, y_s^i, x_s^i}} \sum_{i=1}^n \left((\delta_y^+)^i + (\delta_y^-)^i + e_q^T (\delta_x^+)^i + e_q^T (\delta_x^-)^i \right) \\
& \text{s.t.} \quad y_s^i = \tilde{y}^i + (\delta_y^+)^i - (\delta_y^-)^i \quad \forall i = 1, \dots, n \\
& \quad \quad x_s^i = \tilde{x}^i + (\delta_x^+)^i - (\delta_x^-)^i \quad \forall i = 1, \dots, n \\
& \quad \quad (\nabla y^i)_s^T (x_s^j - x_s^i) + y_s^i \leq y_s^j \quad \forall i, j = 1, \dots, n, i \neq j \\
& \quad \quad (\delta_y^+)^i \in \mathbb{R}_+, (\delta_y^-)^i \in \mathbb{R}_+, (\delta_x^+)^i \in \mathbb{R}_+^q, (\delta_x^-)^i \in \mathbb{R}_+^q \quad \forall i = 1, \dots, n,
\end{aligned} \tag{15}$$

which is an LP. An example of a problem, where the gradient information is exact, and we only have errors in the input variables and output variables is in the field of multiobjective optimization. In the so-called weighted sum method, to determine a point on the Pareto curve/surface the weights determine the exact value of the gradient, whereas due to numerical errors of the

Table 1: Data and results of smoothing in Example 4.1.

number	x_1	x_2	y	\tilde{y}	y_s
1	-0.0199	-1.9768	3.9081	6.1588	6.1588
2	0.0925	1.3411	1.8071	0.4628	0.4628
3	1.4427	0.3253	2.1872	2.7214	2.7214
4	-1.8056	-1.1961	4.6908	4.6208	4.6208
5	-0.4435	-0.3444	0.3153	2.2718	<i>2.0578</i>
6	-1.2952	0.8811	2.4539	3.7644	3.7644
7	1.7826	1.6795	5.9984	5.7807	5.7807
8	0.8074	-1.3585	2.4974	0.0899	<i>0.4842</i>
9	-0.8714	0.5089	1.0183	2.6254	2.6254
10	0.5779	-0.7205	0.8531	0.5766	0.5766

solver, the input value and the output value might be subject to noise.

Note that in the formulation of (13), (14), and (15), we have minimized the shifts $(\delta_y^+)^i$, $(\delta_y^-)^i$, $(\delta_g^+)^i$, $(\delta_g^-)^i$, $(\delta_x^+)^i$, $(\delta_x^-)^i$, and have given them all equal importance. However, we might want to give the error in the gradient more weight.

4 Numerical Examples

In this section we will consider some examples of the theory discussed in Section 3.

Example 4.1 (artificial, no derivative information)

In this example we apply the theory that we developed in Section 3.1. We consider the function $y : \mathbb{R}^2 \mapsto \mathbb{R}$, given by $y(x_1, x_2) = x_1^2 + x_2^2$. We take a sample of 10 input data points x^1, \dots, x^{10} from $[-2, 2] \times [-2, 2]$, and calculate the output values $y(x^1), \dots, y(x^{10})$. Furthermore, we add some noise to it, i.e., we add a noise ε_y^i , where the ε_y^i 's are independent and uniformly distributed on $[-2.5, 2.5]$, such that the data become nonconvex. We obtain values $\tilde{y}^i = y^i + \varepsilon_y^i$. The values are given in Table 4.1. We solved (12) for this problem, and the shifted data y_s^i are also given in Table 4.1. The values that are really shifted, are shown in italics. \square

Example 4.2 (radio therapy, no derivative information)

In radiotherapy the main goal is to give the tumour enough radiation dose, such that the surrounding organs do not receive too much radiation dose. This problem can be formulated mathematically by a multiobjective optimization problem. With the tumour and each healthy surrounding organ, an objective function is associated. One of the problems is that the calculation of a point on the Pareto surface can be very time-consuming. Therefore, we are interested in approximating the Pareto surface; see e.g. Hoffmann et al. (2005). Under certain conditions, we may assume that this Pareto surface is convex. However, due to numerical errors, the Pareto points may not be convex. Therefore we should first smooth them to make them convex.

We have data from a patient of the Radboud University Nijmegen Medical Centre, in Nijmegen, the Netherlands. This data is from a multiobjective optimization problem with 3

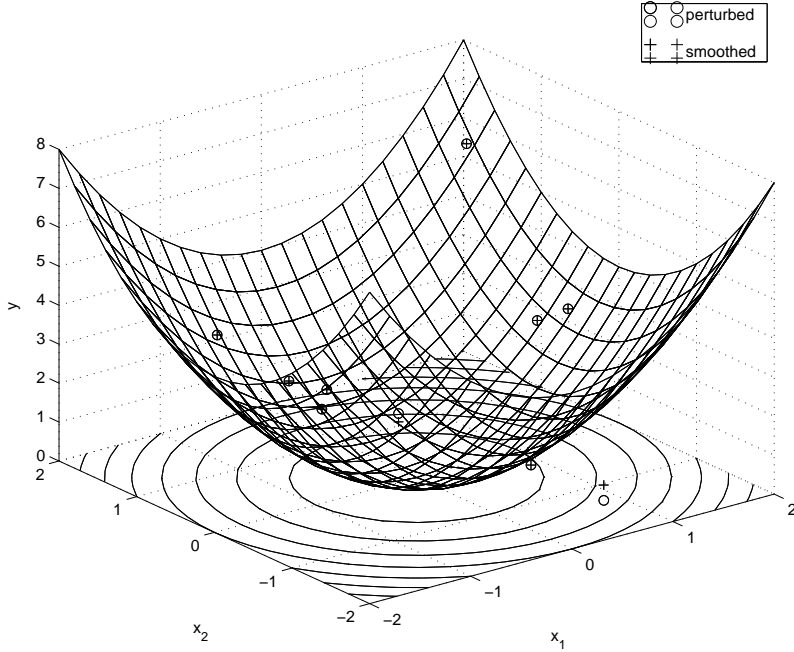


Figure 1: The exact function, the perturbed data, and the smoothed data of Example 4.1.

objectives, and has 69 data points. The data are shown in Figure 2. The Pareto surface is a convex and decreasing function. However, it turned out that the data is not convex. By solving (12), the data is smoothed such that the data becomes convex. The smoothed data points are also shown in Figure 2.

□

Example 4.3 (artificial, derivative information)

In this example we apply the theory of Section 3.2. We consider the function $y : \mathbb{R} \mapsto \mathbb{R}$, given by $y(x) = 1/x$. We assume that we have derivative information, and that there are errors in the outputs and in the gradients. We take 9 equidistant input points and calculate the function value $y(x)$ and its derivative $y'(x) = -1/x^2$ in these 9 input points, and perturb the data such that we get the data \tilde{y} , and \tilde{y}' . Then, to smooth the data we have to solve the LP (14). Note that the method can also be used for multivariate functions, however the results can be visualized clearer for the univariate case. The data is given in Table 4.3 and also shown in Figure 3. After solving (14), we obtain the shifted data y_s and y'_s , which are given in Table 4.3, and also shown in Figure 3. The values that are really shifted, are shown in italics.

□

5 Further Research

As interesting topics for further research we mention several possible applications of the methods developed in this paper.

Possible applications for the construction of the bounds in Section 2 are:

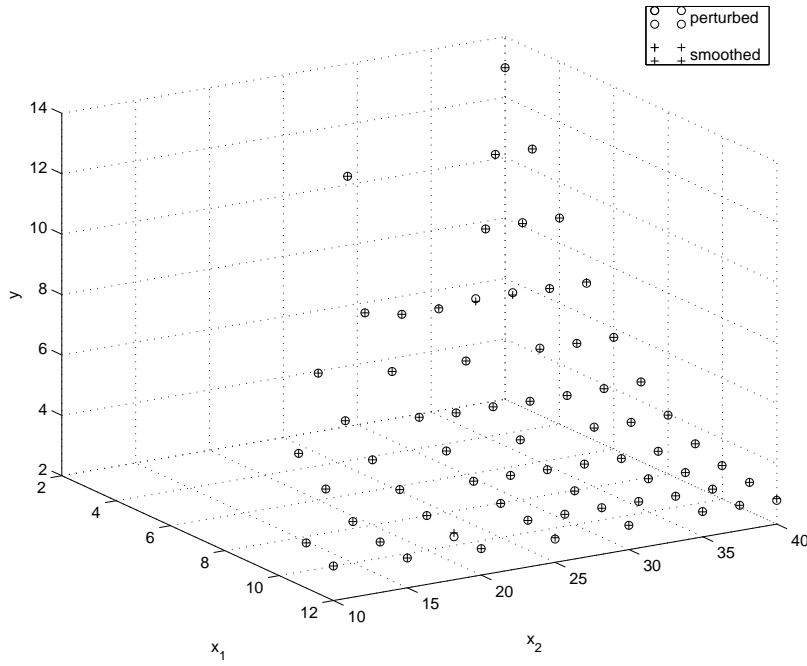


Figure 2: The the perturbed data and the smoothed data of Example 4.2.

Table 2: Data and results of smoothing in Example 4.3.

number	x	y	y'	\tilde{y}	\tilde{y}'	y_s	y'_s
1	0.2	5.0000	-25.0000	5.2701	-25.3226	5.2701	-25.3226
2	0.3	3.3333	-11.1111	3.3974	-11.1279	3.3974	-11.1279
3	0.4	2.5000	-6.2500	2.7348	-5.9355	2.7348	-5.9355
4	0.5	2.0000	-4.0000	1.9739	-4.5778	<i>2.1413</i>	-4.5778
5	0.6	1.6667	-2.7778	1.8595	-2.8441	1.8568	-2.8441
6	0.7	1.4286	-2.0408	1.4978	-1.6905	<i>1.5724</i>	-1.6905
7	0.8	1.2500	-1.5625	1.5031	-1.2767	<i>1.4418</i>	-1.3058
8	0.9	1.1111	-1.2346	0.9169	-1.3477	<i>1.3113</i>	-1.3058
9	1	1.0000	-1.0000	1.2613	-0.4997	1.2613	-0.4997

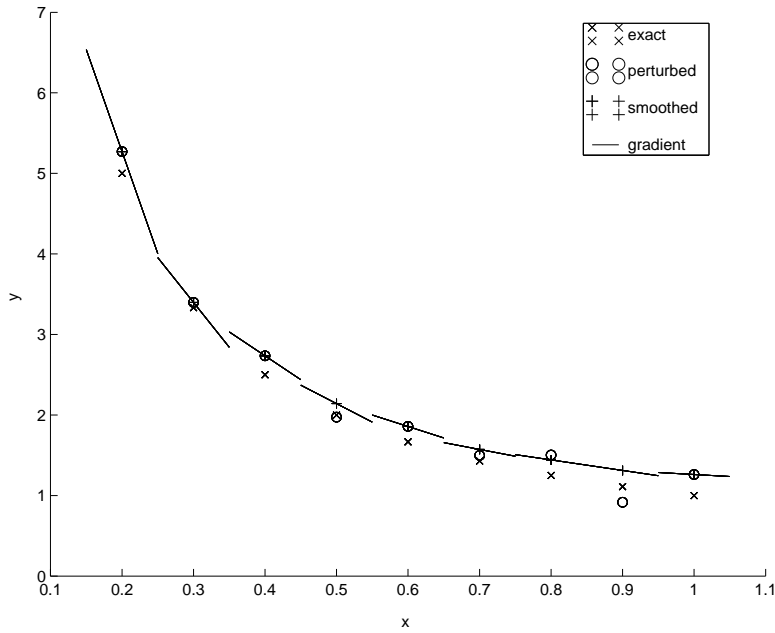


Figure 3: The exact data, the perturbed data, and the smoothed data with its smoothed gradient of Example 4.3.

- Extend the Sandwich algorithms as exist for the approximation of univariate convex functions to the multivariate case by using the lower and upper bounds. More specifically, this may be useful for approximating convex Pareto curves and black-box functions (e.g. deterministic computer simulation).
- Use the lower bounds in convex optimization. For each new candidate proposed by the nonlinear programming solver, we can calculate the lower bound, and if this lower bound is larger than the best known objective value up to now, we reject the candidate before evaluating its function value. This may reduce computation time, especially when the function evaluation is time-consuming. In Den Boef and Den Hertog (2004) promising results are shown for the univariate case.

Possible applications for the data smoothing method of Section 3 are:

- Apply data smoothing before applying Sandwich type algorithms. This may be necessary because of (numerical) noise. This noise occurs e.g., when we want to estimate a Pareto surface in the field of multiobjective optimization. For the so-called weighted sum method (see Miettinen (1999)), formulation (15) can be used, since in this method the derivatives are exact. For the so-called ε -constraint method (see again Miettinen (1999)) formulation (14) can be used, since in this method the x values are exact.
- Apply data smoothing to multivariate isotonic regression problems.

References

- Barlow, R., R. Bartholomew, J. Bremner, and H. Brunk (1972). *Statistical inference under order restrictions*. Chichester: Wiley.
- Ben-Tal, A. and A. Nemirovski (2002). Robust optimization - methodology and applications. *Mathematical Programming, Series B*, **92**, 453–480.
- Boef, E. den and D. den Hertog (2004). Efficient line searching for convex functions. CentER Discussion Paper 2004-52, Tilburg University, Tilburg.
- Boyd, S. and L. Vandenberghe (2004). *Convex optimization*. Cambridge: Cambridge University Press.
- Burkard, R., H. Hamacher, and G. Rote (1991). Sandwich approximation of univariate convex functions with an application to separable convex programming. *Naval Research Logistics*, **38**, 911–924.
- Charnes, A. and W. Cooper (1962). Programming with linear fractional functional. *Naval Research Logistics Quarterly*, **9**, 181–186.
- Cullinan, M. (1990). Data smoothing using non-negative divided differences and ℓ_2 approximation. *IMA Journal of Numerical Analysis*, **10**, 583–608.
- Demetriou, I. and M. Powell (1991a). Least squares smoothing of univariate data to achieve piecewise monotonicity. *IMA Journal of Numerical Analysis*, **11**, 411–432.
- Demetriou, I. and M. Powell (1991b). The minimum sum of squares change to univariate data that gives convexity. *IMA Journal of Numerical Analysis*, **11**, 433–448.
- Fruhworth, B., R. Burkard, and G. Rote (1989). Approximation of convex curves with application to the bi-criteria minimum cost flow problem. *European Journal of Operational Research*, **42**, 326–338.
- Hertog, D. den, E. de Klerk, and K. Roos (2002). On convex quadratic approximation. *Statistica Neerlandica*, **563**, 376–385.
- Hoffmann, A., A. Siem, D. den Hertog, J. Kaanders, and H. Huizenga (2005). Dynamic generation and interpolation of Pareto optimal IMRT treatment plans for convex objective functions. Working paper, Radboud University Nijmegen Medical Centre, Nijmegen.
- Kuijt, F. (1998). *Convexity preserving interpolation – Stationary nonlinear subdivision and splines*. Ph. D. thesis, University of Twente, Enschede, The Netherlands.
- Miettinen, K. (1999). *Nonlinear Multiobjective Optimization*. Boston: Kluwer Academic Publishers.

- Roos, C., T. Terlaky, and J.-P. Vial (1998). *Theory and algorithms for linear optimization*. Chichester: John Wiley & Sons.
- Rote, G. (1992). The convergence rate of the Sandwich algorithm for approximating convex functions. *Computing*, **48**, 337–361.
- Siem, A., D. den Hertog, and A. Hoffmann (2005). A method for approximating univariate convex functions using only function evaluations with applications to Pareto curves. Working paper, Tilburg University, Tilburg.
- Siem, A., E. de Klerk, and D. den Hertog (2005). Discrete least-norm approximation by nonnegative (trigonometric) polynomials and rational functions. CentER Discussion Paper 2005-73, Tilburg University, Tilburg.
- Yang, X. and C. Goh (1997). A method for convex curve approximation. *European Journal of Operational Research*, **97**, 205–212.