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THE EFFECT OF TRANSFORMATIONS ON THE APPROXIMATION OF UNIVARIATE (CONVEX) FUNCTIONS WITH APPLICATIONS TO PARETO CURVES

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# The effect of transformations on the approximation of univariate (convex) functions with applications to Pareto curves 

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#### Abstract

In the literature, methods for the construction of piecewise linear upper and lower bounds for the approximation of univariate convex functions have been proposed. We study the effect of the use of increasing convex or increasing concave transformations on the approximation of univariate (convex) functions. In this paper, we show that these transformations can be used to construct upper and lower bounds for nonconvex functions. Moreover, we show that by using such transformations of the input variable or the output variable, we obtain tighter upper and lower bounds for the approximation of convex functions than without these approximations. We show that these transformations can be applied to the approximation of a (convex) Pareto curve that is associated with a (convex) bi-objective optimization problem.


Keywords: approximation, convexity, convex/concave transformation, Pareto curve.

JEL Classification: C60.

## 1 Introduction

We consider the approximation of a univariate convex function $y: \mathbb{R} \mapsto \mathbb{R}$, which is only known in a finite set of points $x^{1}, \ldots, x^{n} \in \mathbb{R}$ with values $y\left(x^{1}\right), \ldots, y\left(x^{n}\right) \in \mathbb{R}$. In Burkard et al. (1991), Fruhwirth et al. (1989), Rote (1992), Yang and Goh (1997) and Siem et al. (2005), this is done by iteratively constructing piecewise linear upper and lower bounds. For the construction of the bounds discussed in Siem et al. (2005) and Yang and Goh (1997), only function value information, and no derivative information is needed. However, for the construction of the bounds in Burkard et al. (1991), Fruhwirth et al. (1989), and Rote (1992), also derivative information is necessary.

[^0]For the approximation of a nonconvex function, these piecewise linear upper and lower bounds cannot be used. However, in this paper, we show that if we can find an increasing transformation of either the input variable or the output variable such that the nonconvex function becomes convex, we can also obtain upper and lower bounds for this nonconvex function.

Moreover, if the function that is to be approximated is already convex, we show in this paper that by using increasing and concave transformations of the output variable $y$, we can obtain tighter upper and lower bounds. Furthermore, we show that by using increasing concave or convex transformations of the input variable $x$, we can also obtain tighter upper and lower bounds. These transformations can be applied in combination with the lower bounds based on only function value information as well as in combination with the lower bounds based on derivative information.

Furthermore, we show the relevance of our methodology for the approximation of a univariate (convex) Pareto curve that is associated with (convex) bi-objective optimization problems. The construction of a Pareto curve may be time-consuming, since the underlying optimization problems may be very large in size; see e.g. Küfer et al. (2003) and Ehrgott and Johnston (2003). The methodology in this paper accelerates the construction of an accurate Pareto curve.

The remainder of this paper is organized as follows. In Section 2, we repeat the expressions for the upper and lower bounds as presented in Siem et al. (2005). In Section 3 we study the effect of transformations of the output variables. In Section 4, we discuss the effect of transformations of the input variables. In Section 5, we show the relevance of the transformations for the approximation of a (convex) Pareto curve for (convex) bi-objective optimization problems, and consider some examples. Finally, in Section 6 we give our conclusions.

## 2 Approximating convex functions

In this section we summarize some results on piecewise linear upper and lower bounds for approximating convex functions from Siem et al. (2005). We suppose that $n$ input data points $x^{1}<\cdots<x^{n} \in \mathbb{R}$ are given together with the associated output data points $y\left(x^{1}\right), \ldots, y\left(x^{n}\right) \in$ $\mathbb{R}$. Then, it can be shown (see Siem et al. (2005)) that the straight line through the points $\left(x^{i}, y\left(x^{i}\right)\right)$ and $\left(x^{i+1}, y\left(x^{i+1}\right)\right.$ ), for $1 \leq i \leq n-1$, is an upper bound of the convex function $y(x)$, for $x \in\left[x^{i}, x^{i+1}\right]$. Furthermore, it can be shown that the straight lines through $\left(x^{i-1}, y\left(x^{i-1}\right)\right.$ ) and $\left(x^{i}, y\left(x^{i}\right)\right.$, for $2 \leq i \leq n-1$ and through $\left(x^{i+1}, y\left(x^{i+1}\right)\right)$ and $\left(x^{i+2}, y\left(x^{i+2}\right)\right)$, for $1 \leq i \leq n-2$, are lower bounds of the convex function $y(x)$, for $x \in\left[x^{i}, x^{i+1}\right]$. In the rest of the paper we define

$$
\lambda^{i}(x)=\frac{x^{i+1}-x}{x^{i+1}-x^{i}} .
$$

Theorem 1. Let $n$ input/output data points $\left(x^{1}, y\left(x^{1}\right)\right), \ldots,\left(x^{n}, y\left(x^{n}\right)\right)$, with $x^{1}<x^{2}<\cdots<$ $x^{n}$ be given, and let $y(x)$ be convex. Suppose furthermore that $x^{i} \leq x \leq x^{i+1}$, then

$$
\begin{equation*}
y(x) \leq \lambda^{i}(x) y\left(x^{i}\right)+\left(1-\lambda^{i}(x)\right) y\left(x^{i+1}\right) \quad \forall x \in\left[x^{i}, x^{i+1}\right], \forall 1 \leq i \leq n-1, \tag{1}
\end{equation*}
$$


(a)

(b)

Figure 1: Upper and lower bounds for a convex function on the interval $\left[x^{i}, x^{i+1}\right]$, using only function value information (a) and using also derivative information (b).

$$
\begin{equation*}
y(x) \geq\left(1-\lambda^{i-1}(x)\right) y\left(x^{i}\right)+\lambda^{i-1}(x) y\left(x^{i-1}\right) \quad \forall x \in\left[x^{i}, x^{i+1}\right], 2 \leq i \leq n-1, \tag{2}
\end{equation*}
$$

and

$$
y(x) \geq\left(1-\lambda^{i+1}(x)\right) y\left(x^{i+2}\right)+\lambda^{i+1}(x) y\left(x^{i+1}\right) \quad \forall x \in\left[x^{i}, x^{i+1}\right], 1 \leq i \leq n-2 .
$$

Furthermore, in case we also have derivative information, i.e., we also know $\left(x^{1}, y^{\prime}\left(x^{1}\right)\right), \ldots$, $\left(x^{n}, y^{\prime}\left(x^{n}\right)\right)$, then the tangent lines through the data points are also lower bounds. More mathematically we have:

$$
\begin{equation*}
y(x) \geq y\left(x^{i}\right)+y^{\prime}\left(x^{i}\right)\left(x-x^{i}\right), \quad \forall x \in\left[x^{1}, x^{n}\right], \forall i=1, \ldots, n . \tag{4}
\end{equation*}
$$

If $y$ is not differentiable, $y^{\prime}$ can also be a subgradient. It is shown in Siem et al. (2005), that these lower bounds are tighter than the lower bounds that are only based on function value information as given in Theorem 1. The bounds mentioned in this section are illustrated in Figure 1.

## 3 The effect of transformations of the output variable

In this section we study the effect of transformations of the output variable on the upper and lower bounds based on only function evaluations, but also on the lower bounds based on derivative information.

Suppose that we want to construct upper and lower bounds for a function $y(x)$, that is not necessarily convex, and that we know an increasing function $h: \mathbb{R} \mapsto \mathbb{R}$ such that the function
$h(y(x))$ is convex. Then, instead of constructing upper and lower bounds for the function $y(x)$, we can construct upper and lower bounds for $h(y(x))$ as mentioned in Section 2. In this section, we show that by applying the inverse transformation $h^{-1}$ to these upper and lower bounds of $h(y(x))$, we obtain bounds for $y(x)$. In this way, we are able to construct upper and lower bounds for nonconvex functions.

Moreover, suppose that $y(x)$ is convex, and that we know an increasing concave function $h: \mathbb{R} \mapsto \mathbb{R}$ such that the function $h(y(x))$ is still convex. In this section, we also show that the bounds that we obtain, after applying the inverse transformation $h^{-1}$ to the upper and lower bounds of $h(y(x))$, are even tighter than the bounds in (1), (2), (3), and (4). Without proof we first give the following well-known result.

Lemma 1. Suppose that $h: \mathbb{R} \mapsto \mathbb{R}$ is strictly increasing and concave, then $h^{-1}: \mathbb{R} \mapsto \mathbb{R}$ exists, and is strictly increasing and convex.

Now we can show our main results. First, we consider the upper bounds, second, we consider the lower bounds based on only function value information, and third, we consider the lower bounds based on derivative information.

Theorem 2. Let $h: \mathbb{R} \mapsto \mathbb{R}$ be strictly increasing and let $y: \mathbb{R} \mapsto \mathbb{R}$ be such that $h(y(x))$ is convex. Then

$$
\begin{equation*}
y(x) \leq h^{-1}\left[\lambda^{i}(x) h\left(y\left(x^{i}\right)\right)+\left(1-\lambda^{i}(x)\right) h\left(y\left(x^{i+1}\right)\right)\right] \quad \forall x \in\left[x^{i}, x^{i+1}\right], \forall i=1, \ldots, n-1 \tag{5}
\end{equation*}
$$

i.e., the transformed upper bound is also an upper bound for the (not necessarily convex) function $y(x)$.

In addition, let $h$ be concave and $y$ be convex. Then

$$
\begin{align*}
y(x) & \leq h^{-1}\left[\lambda^{i}(x) h\left(y\left(x^{i}\right)\right)+\left(1-\lambda^{i}(x)\right) h\left(y\left(x^{i+1}\right)\right)\right]  \tag{6}\\
& \leq \lambda^{i}(x) y\left(x^{i}\right)+\left(1-\lambda^{i}(x)\right) y\left(x^{i+1}\right) \quad \forall x \in\left[x^{i}, x^{i+1}\right], \forall i=1, \ldots, n-1,
\end{align*}
$$

i.e., the transformed upper bound is tighter than the original upper bound (1).

Proof. From Theorem 1 and the convexity of $h(y(x))$ it follows that

$$
\begin{equation*}
h(y(x)) \leq \lambda^{i}(x) h\left(y\left(x^{i}\right)\right)+\left(1-\lambda^{i}(x)\right) h\left(y\left(x^{i+1}\right)\right) \quad \forall x \in\left[x^{i}, x^{i+1}\right], \forall i=1, \ldots, n-1 . \tag{7}
\end{equation*}
$$

Note that from Lemma 1, we know that $h^{-1}$ is increasing. Applying $h^{-1}$ on both sides of (7) gives (5). Next, we show (6):

$$
\begin{aligned}
y(x)=h^{-1}(h(y(x))) & \leq h^{-1}\left[\lambda^{i}(x) h\left(y\left(x^{i}\right)\right)+\left(1-\lambda^{i}(x)\right) h\left(y\left(x^{i+1}\right)\right)\right] \\
& \leq \lambda^{i}(x) y\left(x^{i}\right)+\left(1-\lambda^{i}(x)\right) y\left(x^{i+1}\right)
\end{aligned}
$$

where in the first inequality we used (7) and the fact that $h^{-1}$ is increasing, and in the second inequality that $h^{-1}$ is convex.

Theorem 3. Let $h: \mathbb{R} \mapsto \mathbb{R}$ be strictly increasing and let $y: \mathbb{R} \mapsto \mathbb{R}$ be such that $h(y(x))$ is convex, then

$$
\begin{align*}
& y(x) \geq h^{-1}\left[\lambda^{i-1}(x) h\left(y\left(x^{i-1}\right)\right)+\left(1-\lambda^{i-1}(x)\right) h\left(y\left(x^{i}\right)\right)\right]  \tag{8}\\
& \forall x \in\left[x^{i}, x^{i+1}\right], \forall i=2, \ldots, n-1 \\
& y(x) \geq h^{-1}\left[\lambda^{i+1}(x) h\left(y\left(x^{i+1}\right)\right)+\left(1-\lambda^{i+1}(x)\right) h\left(y\left(x^{i+2}\right)\right)\right]  \tag{9}\\
& \forall x \in\left[x^{i}, x^{i+1}\right], \forall i=1, \ldots, n-2
\end{align*}
$$

i.e., the transformed lower bound is also a lower bound for the (not necessarily convex) function $y(x)$.

In addition, let $h$ be differentiable and concave, and let $y$ be convex. Then

$$
\begin{align*}
y(x) & \geq h^{-1}\left[\lambda^{i-1}(x) h\left(y\left(x^{i-1}\right)\right)+\left(1-\lambda^{i-1}(x)\right) h\left(y\left(x^{i}\right)\right)\right]  \tag{10}\\
& \geq \lambda^{i-1}(x) y\left(x^{i-1}\right)+\left(1-\lambda^{i-1}(x)\right) y\left(x^{i}\right) \quad \forall x \in\left[x^{i}, x^{i+1}\right], \forall i=2, \ldots, n-1, \\
y(x) & \geq h^{-1}\left[\lambda^{i+1}(x) h\left(y\left(x^{i+1}\right)\right)+\left(1-\lambda^{i+1}(x)\right) h\left(y\left(x^{i+2}\right)\right)\right]  \tag{11}\\
& \geq \lambda^{i+1}(x) y\left(x^{i+1}\right)+\left(1-\lambda^{i+1}(x)\right) y\left(x^{i+2}\right) \quad \forall x \in\left[x^{i}, x^{i+1}\right], \forall i=1, \ldots, n-2,
\end{align*}
$$

i.e., the transformed lower bounds are tighter than the original lower bounds (2) and (3).

Proof. From Theorem 1 and the convexity of $h(y(x))$ it follows that

$$
h(y(x)) \geq \lambda^{i-1}(x) h\left(y\left(x^{i-1}\right)\right)+\left(1-\lambda^{i-1}(x)\right) h\left(y\left(x^{i}\right)\right) \quad \forall x \geq x^{i}, \forall i=2, \ldots, n-1
$$

Since $h^{-1}$ is increasing (see Lemma 1), we have that

$$
\begin{aligned}
& y(x)=h^{-1}(h(y(x))) \geq h^{-1}\left[\lambda^{i-1}(x) h\left(y\left(x^{i-1}\right)\right)+\left(1-\lambda^{i-1}(x)\right) h\left(y\left(x^{i}\right)\right)\right] \\
& \forall x \geq x^{i}, \forall i=2, \ldots, n-1,
\end{aligned}
$$

which shows (8) and the first inequality of (10).
To show the second inequality of (10) we define

$$
g_{1}^{i}(x)=h^{-1}\left[\lambda^{i-1}(x) h\left(y\left(x^{i-1}\right)\right)+\left(1-\lambda^{i-1}(x)\right) h\left(y\left(x^{i}\right)\right)\right] \quad \forall i=2, \ldots, n-1
$$

and

$$
g_{2}^{i}(x)=\lambda^{i-1}(x) y\left(x^{i-1}\right)+\left(1-\lambda^{i-1}(x)\right) y\left(x^{i}\right) \quad \forall i=2, \ldots, n-1
$$

Note that $g_{1}^{i}$ is convex since $h^{-1}$ is a convex function with a linear function as argument. Now define $g^{i}(x):=g_{1}^{i}(x)-g_{2}^{i}(x)$. Then $g^{i}(x)$ is a convex function with zeros for $x=x^{i-1}$ and $x=x^{i}$. From Theorem 2 we may conclude that

$$
h^{-1}\left[\lambda^{i-1}(x) h\left(y\left(x^{i-1}\right)\right)+\left(1-\lambda^{i-1}(x)\right) h\left(y\left(x^{i}\right)\right)\right] \leq \lambda^{i-1}(x) y\left(x^{i-1}\right)+\left(1-\lambda^{i-1}(x)\right) y\left(x^{i}\right)
$$

for $x \in\left[x^{i-1}, x^{i}\right]$, which means that $g^{i}(x) \leq 0$ for $x \in\left[x^{i-1}, x^{i}\right]$. From the mean value theorem it follows that there exists a $\xi \in\left[x^{i-1}, x^{i}\right]$, for which $\left(g^{i}\right)^{\prime}(\xi)=0$. Since $g$ is convex, we may conclude that $\left(g^{i}\right)^{\prime}(x) \geq 0$, for all $x \geq x^{i}$, so also $g^{i}(x) \geq 0$ for all $x \geq x^{i}$, which shows the second inequality. The inequalities in (9) and (11) follow in a similar way.

Next, we show a similar result for the lower bounds based on derivative information.

Theorem 4. Let $h: \mathbb{R} \mapsto \mathbb{R}$ be continuously differentiable, and strictly increasing. Furthermore, suppose that $y: \mathbb{R} \mapsto \mathbb{R}$, such that $h(y(x))$ is convex. Then

$$
\begin{equation*}
y(x) \geq h^{-1}\left[h\left(y\left(x^{i}\right)\right)+h^{\prime}\left(y\left(x^{i}\right)\right) y^{\prime}\left(x^{i}\right)\left(x-x^{i}\right)\right] \quad \forall x \in\left[x^{1}, x^{n}\right], \forall i=1, \ldots, n, \tag{12}
\end{equation*}
$$

i.e., the transformed lower bound is also a lower bound for the (not necessarily convex) function $y(x)$.

In addition, let $h$ be concave and let $y$ be convex. Then

$$
\begin{align*}
y(x) & \geq h^{-1}\left[h\left(y\left(x^{i}\right)\right)+h^{\prime}\left(y\left(x^{i}\right)\right) y^{\prime}\left(x^{i}\right)\left(x-x^{i}\right)\right]  \tag{13}\\
& \geq y\left(x^{i}\right)+y^{\prime}\left(x^{i}\right)\left(x-x^{i}\right) \quad \forall x \in\left[x^{1}, x^{n}\right], \forall i=1, \ldots, n
\end{align*}
$$

i.e., the transformed lower bound is tighter than the original lower bound (4).

Proof. From (4) and the convexity of $h(y(x))$ it follows that

$$
h(y(x)) \geq h\left(y\left(x^{i}\right)\right)+h^{\prime}\left(y\left(x^{i}\right)\right) y^{\prime}\left(x^{i}\right)\left(x-x^{i}\right) \quad \forall x \in\left[x^{1}, x^{n}\right], \forall i=1, \ldots, n .
$$

Since we know from Lemma 1 that $h^{-1}$ is increasing, we have that

$$
y(x)=h^{-1}(h(y(x))) \geq h^{-1}\left[h\left(y\left(x^{i}\right)\right)+h^{\prime}\left(y\left(x^{i}\right)\right) y^{\prime}\left(x^{i}\right)\left(x-x^{i}\right)\right] \quad \forall x \in\left[x^{1}, x^{n}\right], \forall i=1, \ldots, n,
$$

which shows (12) and the first inequality of (13). To show the second inequality of (13) we define

$$
g_{1}^{i}(x)=h^{-1}\left[h\left(y\left(x^{i}\right)\right)+h^{\prime}\left(y\left(x^{i}\right)\right) y^{\prime}\left(x^{i}\right)\left(x-x^{i}\right)\right] \quad \forall i=1, \ldots, n
$$

and

$$
g_{2}^{i}(x)=y\left(x^{i}\right)+y^{\prime}\left(x^{i}\right)\left(x-x^{i}\right) \quad \forall i=1, \ldots, n
$$

Note that $g_{1}^{i}$ is convex since $h^{-1}$ is a convex function (see Lemma 1) with a linear function as argument. Now define $g^{i}(x):=g_{1}^{i}(x)-g_{2}^{i}(x)$. Then $g^{i}(x)$ is a convex function, which is zero for $x=x^{i}$. Differentiating $g_{1}^{i}(x)$ gives:

$$
\begin{aligned}
\left(g_{1}^{i}\right)^{\prime}(x) & =\left(h^{-1}\right)^{\prime}\left[h\left(y\left(x^{i}\right)\right)+h^{\prime}\left(y\left(x^{i}\right)\right) y^{\prime}\left(x^{i}\right)\left(x-x^{i}\right)\right] h^{\prime}\left(y\left(x^{i}\right)\right) y^{\prime}\left(x^{i}\right) \\
& =\frac{1}{h^{\prime}\left[h^{-1}\left[h\left(y\left(x^{i}\right)\right)+h^{\prime}\left(y\left(x^{i}\right)\right) y^{\prime}\left(x^{i}\right)\left(x-x^{i}\right)\right]\right]} h^{\prime}\left(y\left(x^{i}\right)\right) y^{\prime}\left(x^{i}\right),
\end{aligned}
$$

where we used the inverse function theorem. This means that

$$
\left(g_{1}^{i}\right)^{\prime}\left(x^{i}\right)=\left(g_{1}^{i}\right)^{\prime}\left(x^{i}\right)-\left(g_{2}^{i}\right)^{\prime}\left(x^{i}\right)=y^{\prime}\left(x^{i}\right)-y^{\prime}\left(x^{i}\right)=0
$$

Since $g^{i}(x)$ is convex, we have that $\left(g^{i}\right)^{\prime}(x) \geq 0$, for all $x \geq x^{i}$, and $\left(g^{i}\right)^{\prime}(x) \leq 0$, for all $x \leq x^{i}$. This implies that $g^{i}(x) \geq 0$ for all $x \in\left[x^{1}, x^{n}\right]$, which shows the second inequality of (13).

In a similar way it can be shown that if $h: \mathbb{R} \mapsto \mathbb{R}$ is strictly increasing and convex, and $h(y(x))$ is convex, the upper and lower bounds that we obtain by applying the inverse transformation $h^{-1}$ to the upper and lower bounds of $h(y(x))$ are looser than the original upper and lower bounds of $y(x)$.

## 4 The effect of transformations of the input variable

In this section we study the effect of transformations of the input variable on the upper and lower bounds based on only function evaluations, but also on the lower bounds based on derivative information.

Suppose we want to construct upper and lower bounds for a function $y(x)$ that is not necessarily convex. If we know a function $h: \mathbb{R} \mapsto \mathbb{R}$ such that the function $y(h(x))$ is convex, we can construct upper and lower bounds for $y(h(x))$ as mentioned in Section 2. In this section, we show that by applying the inverse transformation $h^{-1}$ to these upper and lower bounds of $y(h(x))$, we obtain bounds for $y(x)$. In this way, we are able to construct upper and lower bounds for nonconvex functions.

If $y(x)$ is convex, and we know an increasing function $h: \mathbb{R} \mapsto \mathbb{R}$ such that the function $y(h(x))$ is still convex, we can also show that under certain conditions, the bounds that we obtain after applying the inverse transformation $h^{-1}$ to the upper and lower bounds of $y(h(x))$, are tighter than the bounds in (1), (2), (3), and (4).

We have to distinguish between the case that $y(x)$ is decreasing and the case that $y(x)$ is increasing. If $y(x)$ is decreasing, then $h$ has to be convex to obtain tighter bounds. If $y(x)$ is increasing, then $h$ has to be concave to obtain tighter bounds.

### 4.1 Decreasing output

Without proof we first give a well-known lemma, which is a similar result as Lemma 1.
Lemma 2. Suppose that $h: \mathbb{R} \mapsto \mathbb{R}$ is strictly increasing and convex, then $h^{-1}: \mathbb{R} \mapsto \mathbb{R}$ exists, and is strictly increasing and concave.

In the rest of this paper we define

$$
\mu^{i}(x)=\frac{h^{-1}\left(x^{i+1}\right)-h^{-1}(x)}{h^{-1}\left(x^{i+1}\right)-h^{-1}\left(x^{i}\right)}
$$

Theorem 5. Let $h: \mathbb{R} \mapsto \mathbb{R}$ and $y: \mathbb{R} \mapsto \mathbb{R}$ be such that $y(h(x))$ is convex. Then

$$
\begin{equation*}
y(x) \leq \mu^{i}(x) y\left(x^{i}\right)+\left(1-\mu^{i}(x)\right) y\left(x^{i+1}\right) \quad \forall x \in\left[x^{i}, x^{i+1}\right], \forall i=1, \ldots, n-1 \tag{14}
\end{equation*}
$$

i.e., the transformed upper bound is also an upper bound for the (not necessarily convex) function $y(x)$.

In addition, let $h$ be strictly increasing and convex. Let $y$ be convex and let $y\left(x^{i}\right) \geq y\left(x^{i+1}\right)$, $\forall i=1, \ldots, n-1$. Then

$$
\begin{align*}
y(x) & \leq \mu^{i}(x) y\left(x^{i}\right)+\left(1-\mu^{i}(x)\right) y\left(x^{i+1}\right)  \tag{15}\\
& \leq \lambda^{i}(x) y\left(x^{i}\right)+\left(1-\lambda^{i}(x)\right) y\left(x^{i+1}\right) \quad \forall x \in\left[x^{i}, x^{i+1}\right], \forall i=1, \ldots, n-1
\end{align*}
$$

i.e., the transformed upper bounds are tighter than the original upper bounds.

Proof. Since the original dataset is given by $\left(x^{i}, y\left(x^{i}\right)\right)$, for all $i=1, \ldots, n$, the transformed dataset is given by $\left(h^{-1}\left(x^{i}\right), y\left(h\left(h^{-1}\left(x^{i}\right)\right)\right)\right.$ ). Note that it is not given by $\left(x^{i}, y\left(h\left(x^{i}\right)\right)\right)$, since the value of $y(x)$ is not known in $x=h\left(x^{i}\right)$, but in $x=x^{i}=h\left(h^{-1}\left(x^{i}\right)\right)$. From Theorem 1 and the convexity of $y(h(x))$ it follows that

$$
\begin{array}{r}
y(h(x)) \leq \frac{h^{-1}\left(x^{i+1}\right)-x}{h^{-1}\left(x^{i+1}\right)-h^{-1}\left(x^{i}\right)} y\left(h\left(h^{-1}\left(x^{i}\right)\right)\right)+\frac{x-h^{-1}\left(x^{i}\right)}{h^{-1}\left(x^{i+1}\right)-h^{-1}\left(x^{i}\right)} y\left(h\left(h^{-1}\left(x^{i+1}\right)\right)\right) \\
\forall x \in\left[h^{-1}\left(x^{i}\right), h^{-1}\left(x^{i+1}\right)\right]
\end{array}
$$

Applying the transformation $h^{-1}$ to the variable $x$ yields

$$
y(x) \leq \mu^{i}(x) y\left(x^{i}\right)+\left(1-\mu^{i}(x)\right) y\left(x^{i+1}\right) \quad \forall x \in\left[x^{i}, x^{i+1}\right]
$$

which shows (14) and the first inequality of (15). The second inequality in (15) is equivalent with

$$
\mu^{i}(x)\left(y\left(x^{i}\right)-y\left(x^{i+1}\right)\right) \leq \lambda^{i}(x)\left(y\left(x^{i}\right)-y\left(x^{i+1}\right)\right)
$$

Since we assumed that $y\left(x^{i}\right) \geq y\left(x^{i+1}\right)$ we only have to show that $\mu^{i}(x) \leq \lambda^{i}(x)$, i.e.,

$$
\begin{equation*}
\frac{h^{-1}\left(x^{i+1}\right)-h^{-1}(x)}{h^{-1}\left(x^{i+1}\right)-h^{-1}\left(x^{i}\right)} \leq \frac{x^{i+1}-x}{x^{i+1}-x^{i}} \tag{16}
\end{equation*}
$$

From Lemma 2, it follows that $h^{-1}$ is strictly increasing and concave. Let $\ell_{i}(x)$ be the straight line through the points $\left(x^{i}, h^{-1}\left(x^{i}\right)\right)$ and $\left(x^{i+1}, h^{-1}\left(x^{i+1}\right)\right)$, i.e.,

$$
\ell_{i}(x)=h^{-1}\left(x^{i}\right)+\frac{h^{-1}\left(x^{i+1}\right)-h^{-1}\left(x^{i}\right)}{x^{i+1}-x^{i}}\left(x-x^{i}\right)
$$

We can now write for $x \in\left[x^{i}, x^{i+1}\right]$

$$
\frac{x^{i+1}-x}{x^{i+1}-x^{i}}=\frac{\ell_{i}\left(x^{i+1}\right)-\ell_{i}(x)}{\ell_{i}\left(x^{i+1}\right)-\ell_{i}\left(x^{i}\right)} \geq \frac{h^{-1}\left(x^{i+1}\right)-h^{-1}(x)}{h^{-1}\left(x^{i+1}\right)-h^{-1}\left(x^{i}\right)},
$$

where in the inequality we used the concavity of $h^{-1}$, the fact that $\ell_{i}(x)$ is linear and that $\ell_{i}\left(x^{i}\right)=h^{-1}\left(x^{i}\right)$ and $\ell_{i}\left(x^{i+1}\right)=h^{-1}\left(x^{i+1}\right)$, which implies $\ell_{i}(x) \leq h^{-1}(x), \forall x \in\left[x^{i}, x^{i+1}\right]$.

Theorem 6. Let $h: \mathbb{R} \mapsto \mathbb{R}$ and $y: \mathbb{R} \mapsto \mathbb{R}$ be such that $y(h(x))$ is convex. Then

$$
\begin{align*}
& y(x) \geq \mu^{i-1}(x) y\left(x^{i-1}\right)+\left(1-\mu^{i-1}(x)\right) y\left(x^{i}\right)  \tag{17}\\
& y(x) \geq \mu^{i+1}(x) y\left(x^{i+1}\right)+\left(1-\mu^{i+1}(x)\right) y\left(x^{i+2}\right), \tag{18}
\end{align*}
$$

i.e., the transformed lower bound is also a lower bound for the (not necessarily convex) function $y(x)$.

In addition, let $h$ be differentiable, strictly increasing, and convex. Let $y$ be convex and let $y\left(x^{i}\right) \geq y\left(x^{i+1}\right), \forall i=1, \ldots, n-1$. Then

$$
\begin{align*}
y(x) & \geq \mu^{i-1}(x) y\left(x^{i-1}\right)+\left(1-\mu^{i-1}(x)\right) y\left(x^{i}\right)  \tag{19}\\
& \geq \lambda^{i-1}(x) y\left(x^{i-1}\right)+\left(1-\lambda^{i-1}(x)\right) y\left(x^{i}\right) \quad \forall x \in\left[x^{i}, x^{i+1}\right], \forall i=2, \ldots, n-1, \\
y(x) & \geq \mu^{i+1}(x) y\left(x^{i+1}\right)+\left(1-\mu^{i+1}(x)\right) y\left(x^{i+2}\right)  \tag{20}\\
& \geq \lambda^{i+1}(x) y\left(x^{i+1}\right)+\left(1-\lambda^{i+1}(x)\right) y\left(x^{i+2}\right) \quad
\end{align*}
$$

i.e., the transformed lower bounds are tighter than the original lower bounds.

Proof. From Theorem 1 and the convexity of $y(h(x))$ it follows that

$$
\begin{array}{r}
y(h(x)) \geq \frac{h^{-1}\left(x^{i}\right)-x}{h^{-1}\left(x^{i}\right)-h^{-1}\left(x^{i-1}\right)} y\left(h\left(h^{-1}\left(x^{i-1}\right)\right)\right)+\frac{x-h^{-1}\left(x^{i-1}\right)}{h^{-1}\left(x^{i}\right)-h^{-1}\left(x^{i-1}\right)} y\left(h\left(h^{-1}\left(x^{i}\right)\right)\right) \\
\forall x \geq h^{-1}\left(x^{i}\right) .
\end{array}
$$

Applying the transformation $h^{-1}(x)$ yields

$$
y(x) \geq \mu^{i-1}(x) y\left(x^{i-1}\right)+\left(1-\mu^{i-1}(x)\right) y\left(x^{i}\right) \quad \forall x \geq h^{-1}\left(x^{i}\right),
$$

which shows (17) and the first inequality in (19). To show the second inequality in (19), we first define

$$
g_{1}^{i}(x)=\mu^{i-1}(x) y\left(x^{i-1}\right)+\left(1-\mu^{i-1}(x)\right) y\left(x^{i}\right) \quad \forall i=2, \ldots, n-1,
$$

and

$$
g_{2}^{i}(x)=\lambda^{i-1}(x) y\left(x^{i-1}\right)+\left(1-\lambda^{i-1}(x)\right) y\left(x^{i}\right) \quad \forall i=2, \ldots, n-1 .
$$

Note that $g_{1}^{i}(x)$ is a convex function, since $h^{-1}$ is concave (see Lemma 2) and $y\left(x^{i-1}\right) \geq y\left(x^{i}\right)$.

Now, define $g^{i}(x):=g_{1}^{i}(x)-g_{2}^{i}(x)$. Then $g^{i}(x)$ is a convex function with zeros in $x=x^{i-1}$ and $x=x^{i}$. From Theorem 5 we may conclude that

$$
\mu^{i-1}(x) y\left(x^{i-1}\right)+\left(1-\mu^{i-1}(x)\right) y\left(x^{i}\right) \leq \lambda^{i-1}(x) y\left(x^{i-1}\right)+\left(1-\lambda^{i-1}(x)\right) y\left(x^{i}\right)
$$

for $x \in\left[x^{i-1}, x^{i}\right]$, with $y\left(x^{i-1}\right) \geq y\left(x^{i}\right)$, which means that $g^{i}(x) \leq 0, \forall x \in\left[x^{i-1}, x^{i}\right]$. From the mean value theorem it follows that there exists a $\xi \in\left[x^{i-1}, x^{i}\right]$, for which $\left(g^{i}\right)^{\prime}(\xi)=0$. Since $g$ is convex, we may conclude that $\left(g^{i}\right)^{\prime}(x) \geq 0$, for all $x \geq x^{i}$, so also $g^{i}(x) \geq 0$ for all $x \geq x^{i}$, which shows the second inequality. The inequalities in (18) and (20) follow in a similar way.

Next, we show a similar result for the lower bound based on derivative information.
Theorem 7. Let $h: \mathbb{R} \mapsto \mathbb{R}$ and $y: \mathbb{R} \mapsto \mathbb{R}$ be such that $y(h(x))$ is convex. Then

$$
\begin{equation*}
y(x) \geq y\left(x^{i}\right)+y^{\prime}\left(x^{i}\right) h^{\prime}\left(h^{-1}\left(x^{i}\right)\right)\left(h^{-1}(x)-h^{-1}\left(x^{i}\right)\right) \quad \forall x \in\left[x^{1}, x^{n}\right], \forall i=1, \ldots, n \tag{21}
\end{equation*}
$$

i.e., the transformed lower bound is also a lower bound for the (not necessarily convex) function $y(x)$.

Let $h$ be continuously differentiable, strictly increasing, and convex. Let $y: \mathbb{R} \mapsto \mathbb{R}$ be convex, and let $y^{\prime}(x) \leq 0 \forall x \in\left[x^{1}, x^{n}\right]$. Then

$$
\begin{align*}
y(x) & \geq y\left(x^{i}\right)+y^{\prime}\left(x^{i}\right) h^{\prime}\left(h^{-1}\left(x^{i}\right)\right)\left(h^{-1}(x)-h^{-1}\left(x^{i}\right)\right)  \tag{22}\\
& \geq y\left(x^{i}\right)+y^{\prime}\left(x^{i}\right)\left(x-x^{i}\right) \quad \forall x \in\left[x^{1}, x^{n}\right], \forall i=1, \ldots, n
\end{align*}
$$

i.e., the transformed lower bound is tighter than the original lower bound.

Proof. We first consider (21) and the first inequality of (22). From Theorem 1 and the convexity of $y(h(x))$ it follows that

$$
\begin{aligned}
& y(h(x)) \geq y\left(h\left(h^{-1}\left(x^{i}\right)\right)\right)+y^{\prime}\left(h\left(h^{-1}\left(x^{i}\right)\right)\right) h^{\prime}\left(h^{-1}\left(x^{i}\right)\right)\left(x-h^{-1}\left(x^{i}\right)\right) \\
& \forall \forall\left[h^{-1}\left(x^{1}\right), h^{-1}\left(x^{n}\right)\right], \forall i=1, \ldots, n
\end{aligned}
$$

By applying the transformation $h^{-1}$, we obtain
$y(x)=y\left(h\left(h^{-1}(x)\right)\right) \geq y\left(x^{i}\right)+y^{\prime}\left(x^{i}\right) h^{\prime}\left(h^{-1}\left(x^{i}\right)\right)\left(h^{-1}(x)-h^{-1}\left(x^{i}\right)\right) \quad \forall x \in\left[x^{1}, x^{n}\right], \forall i=1, \ldots, n$.
We now prove the second inequality in (22). Since $y^{\prime}(x) \leq 0$ we only have to show that

$$
h^{\prime}\left(h^{-1}\left(x^{i}\right)\right)\left(h^{-1}(x)-h^{-1}\left(x^{i}\right)\right) \leq x-x^{i}
$$

Now define

$$
g^{i}(x)=h^{\prime}\left(h^{-1}\left(x^{i}\right)\right)\left(h^{-1}(x)-h^{-1}\left(x^{i}\right)\right)-\left(x-x^{i}\right)
$$

Note that $g^{i}(x)$ is concave, since it follows from Lemma 2 that $h^{-1}$ is concave. Also note that
$g^{i}\left(x^{i}\right)=0$. With the inverse function theorem it follows that

$$
\left(g^{i}\right)^{\prime}\left(x^{i}\right)=h^{\prime}\left(h^{-1}\left(x^{i}\right)\right) \frac{1}{h^{\prime}\left(h^{-1}\left(x^{i}\right)\right)}-1=0 .
$$

Since $g^{i}(x)$ is concave, it follows that $g^{i}(x) \leq 0$. This shows the second inequality in (22).
In a similar way it can be shown for the case that $y\left(x^{i}\right) \geq y\left(x^{i+1}\right)$, for $i=1, \ldots, n-1$, that if $h: \mathbb{R} \mapsto \mathbb{R}$ is strictly increasing and concave, the upper and lower bounds that we obtain by applying the inverse transformation $h^{-1}$ to the upper and lower bounds of $y(h(x))$ are looser than the original upper and lower bounds of $y(x)$.

### 4.2 Increasing output

We have similar theorems for the case that $y\left(x^{i}\right) \leq y\left(x^{i+1}\right)$. However, to obtain tighter bounds, we now need $h(x)$ to be strictly increasing and concave. We give the theorems without proofs, since they follow in a similar way as Theorems 5,6 , and 7 .

Theorem 8. Let $h: \mathbb{R} \mapsto \mathbb{R}$ and $y: \mathbb{R} \mapsto \mathbb{R}$ be such that $y(h(x))$ is convex. Then

$$
\begin{equation*}
y(x) \leq \mu^{i}(x) y\left(x^{i}\right)+\left(1-\mu^{i}(x)\right) y\left(x^{i+1}\right) \quad \forall x \in\left[x^{i}, x^{i+1}\right], \forall i=1, \ldots, n-1, \tag{23}
\end{equation*}
$$

i.e., the transformed upper bound is also an upper bound for the (not necessarily convex) function $y(x)$.

In addition, let $h$ be strictly increasing and concave. Let $y$ be convex and let $y\left(x^{i}\right) \leq y\left(x^{i+1}\right)$, $\forall i=1, \ldots, n-1$. Then

$$
\begin{align*}
& y(x) \leq \mu^{i}(x) y\left(x^{i}\right)+\left(1-\mu^{i}(x)\right) y\left(x^{i+1}\right)  \tag{24}\\
& \leq \\
& \leq \lambda^{i}(x) y\left(x^{i}\right)+\left(1-\lambda^{i}(x)\right) y\left(x^{i+1}\right) \\
& \forall x \in\left[x^{i}, x^{i+1}\right], \forall i=1, \ldots, n-1,
\end{align*}
$$

i.e., the transformed upper bounds are tighter than the original upper bounds.

Theorem 9. Let $h: \mathbb{R} \mapsto \mathbb{R}$ and $y: \mathbb{R} \mapsto \mathbb{R}$ be such that $y(h(x))$ is convex. Then

$$
\begin{aligned}
& y(x) \geq \mu^{i-1}(x) y\left(x^{i-1}\right)+\left(1-\mu^{i-1}(x)\right) y\left(x^{i}\right) \\
& y(x) \geq \mu^{i+1}(x) y\left(x^{i+1}\right)+\left(1-\mu^{i+1}(x)\right) y\left(x^{i+2}\right),
\end{aligned}
$$

i.e., the transformed lower bound is also a lower bound for the (not necessarily convex) function $y(x)$.

In addition, let $h$ be differentiable, strictly increasing, and concave. Let $y$ be convex and let

|  |  | transformation of |  |  |
| :---: | :---: | :---: | :---: | :---: |
|  |  | $x$ |  |  |
|  |  | $y$ increasing | $y$ decreasing |  |
| convex | looser | looser | tighter |  |
| concave | tighter | tighter | looser |  |

Table 1: The effect of strictly increasing transformations $h$ on the upper and lower bounds for different scenarios of the input variable $x$ and output variable $y$
$y\left(x^{i}\right) \leq y\left(x^{i+1}\right), \forall i=1, \ldots, n-1$. Then

$$
\begin{align*}
& y(x) \geq \mu^{i-1}(x) y\left(x^{i-1}\right)+\left(1-\mu^{i-1}(x)\right) y\left(x^{i}\right) \\
& \geq \lambda^{i-1}(x) y\left(x^{i-1}\right)+\left(1-\lambda^{i-1}(x)\right) y\left(x^{i}\right)  \tag{25}\\
& \forall x \in\left[x^{i}, x^{i+1}\right], \forall i=2, \ldots, n-1 \\
& y(x) \geq \mu^{i+1}(x) y\left(x^{i+1}\right)+\left(1-\mu^{i+1}(x)\right) y\left(x^{i+2}\right) \\
& \geq \lambda^{i+1}(x) y\left(x^{i+1}\right)+\left(1-\lambda^{i+1}(x)\right) y\left(x^{i+2}\right)  \tag{26}\\
& \forall x \in\left[x^{i}, x^{i+1}\right], \forall i=1, \ldots, n-2
\end{align*}
$$

i.e., the transformed lower bounds are tighter than the original lower bounds.

Theorem 10. Let $h: \mathbb{R} \mapsto \mathbb{R}$ and $y: \mathbb{R} \mapsto \mathbb{R}$ be such that $y(h(x))$ is convex. Then

$$
\begin{equation*}
y(x) \geq y\left(x^{i}\right)+y^{\prime}\left(x^{i}\right) h^{\prime}\left(h^{-1}\left(x^{i}\right)\right)\left(h^{-1}(x)-h^{-1}\left(x^{i}\right)\right) \quad \forall x \in\left[x^{1}, x^{n}\right], \forall i=1, \ldots, n \tag{27}
\end{equation*}
$$

i.e., the transformed lower bound is also a lower bound for the (not necessarily convex) function $y(x)$.

In addition, let $h$ be continuously differentiable, strictly increasing, and concave. Let $y$ be convex, and let $y^{\prime}(x) \geq 0 \forall x \in\left[x^{1}, x^{n}\right]$. Then

$$
\begin{align*}
y(x) & \geq y\left(x^{i}\right)+y^{\prime}\left(x^{i}\right) h^{\prime}\left(h^{-1}\left(x^{i}\right)\right)\left(h^{-1}(x)-h^{-1}\left(x^{i}\right)\right)  \tag{28}\\
& \geq y\left(x^{i}\right)+y^{\prime}\left(x^{i}\right)\left(x-x^{i}\right) \quad \forall x \in\left[x^{1}, x^{n}\right], \forall i=1, \ldots, n
\end{align*}
$$

i.e., the transformed lower bound is tighter than the original lower bound.

It can be shown in a similar way for the case that $y\left(x^{i}\right) \geq y\left(x^{i+1}\right)$, for $i=1, \ldots, n-1$, that if $h: \mathbb{R} \mapsto \mathbb{R}$ is strictly increasing and convex, the upper and lower bounds that we obtain by applying the inverse transformation $h^{-1}$ to the upper and lower bounds of $y(h(x))$, are looser than the original upper and lower bounds of $y(x)$.

We have summarized a part of the results of Sections 3 and 4 in Table 1.

## 5 Application to the approximation of the Pareto efficient frontier

An application of the methodology presented in this paper is the approximation of a convex Pareto curve (or Pareto efficient frontier) associated with a bi-objective optimization problem. First, in Section 5.1 we repeat some theory on bi-objective optimization. In Section 5.2, we show how we can apply the theory discussed in Sections 3 and 4 to obtain tighter upper and lower bounds of convex Pareto curves, and also to obtain upper and lower bounds of nonconvex Pareto curves.

### 5.1 Bi-objective optimization

Bi-objective optimization problems can in general be written in the form

$$
\begin{array}{ll}
\min _{v} & f(v)=\left[\begin{array}{ll}
f_{1}(v) & f_{2}(v)
\end{array}\right]^{T}  \tag{29}\\
\text { s.t. } & v \in S,
\end{array}
$$

where $f_{1}$ and $f_{2}$ are objective functions, and $S \subseteq \mathbb{R}^{p}$ is the feasible decision space. We want to minimize both functions $f_{1}$ and $f_{2}$ simultaneously. However, if there is a conflict between the objectives, this is not possible. In general, this optimization problem does not have a unique solution, since usually there is no solution that minimizes both objectives simultaneously. Actually, we are interested in those objective vectors, of which none of the components can be improved without worsening the other component, i.e., we are interested in the so-called Pareto optimal points.

Definition 5.1 (Pareto optimality of a decision vector). A decision vector $v^{*} \in S$ is Pareto optimal if there does not exist another decision vector $v \in S$ such that $f_{i}(v) \leq f_{i}\left(v^{*}\right)$, for all $i=1,2$ and $f_{j}(v)<f_{j}\left(v^{*}\right)$ for at least one index $j$.

The set of Pareto optimal points is called the Pareto optimal set and will be denoted by $S^{*}$. Let $Z:=f(S)$ be the feasible objective space. Now we can define Pareto optimality in the objective space.

Definition 5.2 (Pareto optimality of an objective vector). An objective vector $z^{*} \in Z$ is Pareto optimal if there does not exist another objective vector $z \in Z$ such that $z_{i} \leq z_{i}^{*}$ for all $i=1,2$ and $z_{j}<z_{j}^{*}$ for at least one index $j$.

This means that the vector $z^{*}$ is Pareto optimal if the corresponding decision vector $v^{*}$ for which $z^{*}=f\left(v^{*}\right)$ is Pareto optimal. The image of the Pareto optimal set $f\left(S^{*}\right)$ is called the Pareto curve (or Pareto efficient frontier).

Two common methods to find Pareto optimal points are the weighting method and the $\varepsilon$-constraint method; see e.g. Miettinen (1999). In the latter method, we need to solve the
following convex optimization problem for $\ell=1,2$ :

$$
\begin{array}{cl}
\min _{v} & f_{\ell}(v) \\
\text { s.t. } & f_{j}(v) \leq \varepsilon_{j} \quad \forall j=1,2, j \neq \ell  \tag{30}\\
& v \in S .
\end{array}
$$

We now give the following theorem, which can be found in Miettinen (1999).
Theorem 11. A decision vector $v^{*} \in S$ is Pareto optimal if and only if it is a solution of the $\varepsilon$-constraint problem (30) for every $\ell=1,2$, where $\varepsilon_{j}=f_{j}\left(v^{*}\right)$ for $j=1,2, j \neq \ell$.

Proof. See Miettinen (1999), page 85.
Let $\mathcal{E}=\left\{\varepsilon_{2} \in \mathbb{R}: \exists v \in S: f_{2}(v) \leq \varepsilon_{2}\right\}$. Now define the function $p: \mathcal{E} \mapsto \mathbb{R}$ as $p\left(\varepsilon_{2}\right)=$ $f_{1}\left(v^{*}\left(\varepsilon_{2}\right)\right)$, where $v^{*}\left(\varepsilon_{2}\right)$ is the solution of (30) for $\ell=1,2$. The following theorem states that the Pareto curve $p\left(\varepsilon_{2}\right)$ is convex, provided that both $f_{1}$ and $f_{2}$ are convex, and $S$ is a convex set.

Theorem 12. Suppose that $f_{1}$ and $f_{2}$ are convex functions and $S$ is a convex set, then the Pareto curve $p: \mathcal{E} \mapsto \mathbb{R}$ corresponding with bi-objective optimization problem (29) is convex.

Proof. Let $0 \leq \lambda \leq 1, \varepsilon^{1}, \varepsilon^{2} \in \mathcal{E}$. We then have $f_{2}\left(v^{*}\left(\varepsilon^{1}\right)\right) \leq \varepsilon^{1}$, and $f_{2}\left(v^{*}\left(\varepsilon^{2}\right)\right) \leq \varepsilon^{2}$. Let $v^{0}=\lambda v^{*}\left(\varepsilon^{1}\right)+(1-\lambda) v^{*}\left(\varepsilon^{2}\right)$, and $\varepsilon^{0}=\lambda \varepsilon^{1}+(1-\lambda) \varepsilon^{2}$. Then, $f_{2}\left(v^{0}\right)=f_{2}\left(\lambda v^{*}\left(\varepsilon^{1}\right)+(1-\lambda) v^{*}\left(\varepsilon^{2}\right)\right) \leq$ $\lambda f_{2}\left(v^{*}\left(\varepsilon^{1}\right)\right)+(1-\lambda) f_{2}\left(v^{*}\left(\varepsilon^{2}\right)\right) \leq \lambda \varepsilon^{1}+(1-\lambda) \varepsilon^{2}=\varepsilon^{0}$. Also, $v^{0} \in S$. Therefore, $v^{0}$ is a feasible point for optimization problem (30) with $\varepsilon=\varepsilon^{0}$ and $\ell=1$. Furthermore

$$
\begin{aligned}
p\left(\varepsilon^{0}\right) & =p\left(\lambda \varepsilon^{1}+(1-\lambda) \varepsilon^{2}\right) \\
& =f_{1}\left(v^{*}\left(\lambda \varepsilon^{1}+(1-\lambda) \varepsilon^{2}\right)\right) \\
& \leq f_{1}\left(v^{0}\right) \\
& =f_{1}\left(\lambda v^{*}\left(\varepsilon^{1}\right)+(1-\lambda) v^{*}\left(\varepsilon^{2}\right)\right) \\
& \leq \lambda f_{1}\left(v^{*}\left(\varepsilon^{1}\right)\right)+(1-\lambda) f_{1}\left(v^{*}\left(\varepsilon^{2}\right)\right) \\
& =\lambda p\left(\varepsilon^{1}\right)+(1-\lambda) p\left(\varepsilon^{2}\right)
\end{aligned}
$$

where we used in the first inequality that $v^{0}$ is feasible, and in the second inequality that $f_{1}$ is convex. Therefore $p$ is convex.

If the objective functions are not convex, the Pareto curve $p(\varepsilon)$ is not necessarily convex. In Figure 2 the feasible objective region is shown with both convex and nonconvex Pareto curves. There is a vast literature on methods to find Pareto optimal points; see e.g. Miettinen (1999).

Given a set of Pareto optimal points, we can now use the upper and lower bounds, given in Section 2, to approximate a convex Pareto curve $p(\varepsilon)$. However, Pareto curves are decreasing by definition. As a consequence of this, we can add the additional lower bound $p\left(\varepsilon^{n}\right) \leq p(\varepsilon)$, for $\varepsilon^{n-1} \leq \varepsilon \leq \varepsilon^{n}$. This is illustrated in Figure 3.


Figure 2: The sets $Z$ representing the feasible objective region with both nonconvex (a) and convex (b) Pareto curves.


Figure 3: Upper and lower bounds for a convex and decreasing function, based on function value information.

### 5.2 Approximation of the Pareto efficient frontier

We can use the results of Sections 3 and 4, to obtain tighter bounds of the Pareto curve, by transforming one or both of the objectives. Suppose we want to minimize $f_{1}$ and $f_{2}$ simultaneously, and that $f_{1}$ and $f_{2}$ are convex. If we know an increasing and concave function $h$, such that $h\left(f_{1}(v)\right)$ is convex, then also

$$
\begin{array}{rl}
h(p(\varepsilon))=\min _{v} & h\left(f_{1}(v)\right) \\
\text { s.t. } & f_{2}(v) \leq \varepsilon  \tag{31}\\
& v \in S
\end{array}
$$

is convex, and by applying Theorems 2,3 , and 4 , we can obtain tighter bounds for $p(\varepsilon)$.
Furthermore, if we can find an increasing and concave function $\tilde{h}: \mathbb{R} \mapsto \mathbb{R}$, such that $\tilde{h}\left(f_{2}(v)\right)$ is convex, then the function

$$
\begin{align*}
\tilde{p}(\varepsilon)=\min _{v} & f_{1}(v) \\
\text { s.t. } & \tilde{h}\left(f_{2}(v)\right) \leq \varepsilon  \tag{32}\\
& v \in S
\end{align*}
$$

is convex. We can rewrite this into

$$
\begin{aligned}
p\left(\tilde{h}^{-1}(\varepsilon)\right)=\min _{v} & f_{1}(v) \\
\text { s.t. } & f_{2}(v) \leq \tilde{h}^{-1}(\varepsilon) \\
& v \in S
\end{aligned}
$$

Since $\tilde{h}^{-1}$ is increasing and convex, $p\left(\tilde{h}^{-1}(\varepsilon)\right)$ is still convex, and $p\left(\varepsilon^{i}\right) \geq p\left(\varepsilon^{i+1}\right)$, for $i=$ $1, \ldots, n-1$, by applying Theorems 5,6 , and 7 , we can obtain tighter upper and lower bounds for $p(\varepsilon)$. This means that if we can find a concave and increasing function $\tilde{h}$ such that $\tilde{h}\left(f_{2}(v)\right)$ is convex, we can obtain tighter bounds for $p(\varepsilon)$.

Furthermore, if $f_{1}$ in (31) is not convex, $h$ is increasing and such that $h\left(f_{1}(v)\right)$ is convex, then by applying Theorems 2,3 , and 4 , we can obtain upper and lower bounds for the nonconvex Pareto curve. If in (32) $f_{2}$ is not convex and $h$ is such that $h\left(f_{2}(x)\right)$ is convex, then by applying Theorems 5, 6, and 7, we can obtain upper and lower bounds for the nonconvex Pareto curve.

Example 5.1 ( $p$-norm)
For example, let $f_{1}(v)=v^{T} A v$ and $f_{2}(v)=v^{T} B v$, with $A$ and $B$ positive semi-definite, both be convex quadratic functions, we can choose $h(u)=\tilde{h}(u)=\sqrt{u}$. Note that both $h\left(f_{1}(v)\right)$ and $\tilde{h}\left(f_{2}(v)\right)$ are convex, since $h\left(f_{1}(v)\right)=\sqrt{v^{T} A v}$ and $h\left(f_{2}(v)\right)=\sqrt{v^{T} B v}$ are norms. Then, the Pareto curve, associated with optimization problem

$$
\begin{array}{cl}
\min _{v} & \sqrt{v^{T} A v} \\
\text { s.t. } & \sqrt{v^{T} B v} \leq \varepsilon \\
& v \in S
\end{array}
$$

| Category | $i$ | $E R_{i}$ | $\operatorname{Cov}\left[R_{i}, R_{j}\right]$ |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  | 1 | $j$ | 3 |
|  | 1 | 10.8 | 2.250 | -0.120 | 0.450 |
| bonds | 2 | 7.600 | -0.120 | 0.640 | 0.336 |
| real estate | 3 | 9.500 | 0.450 | 0.336 | 1.440 |

Table 2: Expected returns and covariances.
is convex. After applying the inverse transformation to the constructed bounds, we obtain tighter bounds, than without the transformations $h(x)$ and $\tilde{h}(x)$. More generally we can apply this to convex functions of the form $f(v)=\sum_{i}\left(a_{i}^{T} v\right)^{p}$, where $a_{i}^{T}$ is the $i$-th row of a squared matrix $A$. We can apply the transformation $h(u)=\sqrt[p]{u}$. Since $h(f(v))=\sqrt[p]{\sum_{i}\left(a_{i}^{T} v\right)^{p}}$ is a norm (known as the $p$-norm), $h(f(v))$ is convex. The family of functions $f(v)=\sum_{i}\left(a_{i}^{T} v\right)^{p}$ play an important role in $l_{p}$-programming; see Terlaky (1985).

Example 5.2 (Strategic investment model)
In this example we consider a strategic investment model. There exist many sorts of investment categories, such as deposits, saving accounts, bonds, stocks, real estate, commodities, foreign currencies, and derivatives. Each category has its own expected return, and its own risk characteristic. The strategic investment model can be used to model how top management could spread an overall budget over several investment categories. The objective is to minimize the portfolio risk (measured by the variance of the return), such that a certain minimal desired expected return is achieved. The model was introduced by Markowitz (1952), and is given by:

$$
\begin{array}{cl}
\min _{v} & v^{T} \Sigma v \\
\text { s.t. } & r^{T} v \geq M  \tag{33}\\
& e_{p}^{T} v=1 \\
& v \in \mathbb{R}_{+}^{p},
\end{array}
$$

where $\Sigma$ is a positive semi-definite covariance matrix consisting of elements $\Sigma_{i j}$ of covariances between investment categories $i$ and $j, r$ is the vector consisting of elements $r_{i}$ of expected return of investment category $i, M$ is the desired expected portfolio return, $e_{p}$ is the $p$-dimensional allone vector, $v$ is the vector with elements $v_{i}$ of fractions of the budget invested in each category, and $p$ is the number of investment categories.

In Table 2, a simple problem instance is given, which we took from Bisschop (2000), Chapter 18. It contains three investment categories: stocks, bonds, and real estate. The stochastic variable $R_{i}$ denotes the expected return of investment category $i$. Based on four equidistant data points, we calculate the upper and lower bounds (1), (2), (3), and (4). Then, we apply the concave and increasing transformation $h(u)=\sqrt{u}$ to the objective in (33). Note that since the function $f(v)=\sqrt{v^{T} \Sigma v}$ is convex (it is a norm), the conditions of Theorems 2, 3, and 4 are satisfied. Then, we calculate the transformed upper and lower bounds from (6),(10), (11),


Figure 4: Transformed and not transformed upper and lower bounds of Pareto efficient frontier associated with (33).
and (13). The transformed and nontransformed bounds are shown in Figure 4. Indeed, as we can see in Figure 4, the transformed bounds are tighter than the nontransformed bounds, as we showed in Theorems 2, 3, and 4.

Next, we exchange the objective and the first constraint in (33):

$$
\begin{array}{cl}
\min _{v} & -r^{T} v \\
\text { s.t. } & v^{T} \Sigma v \leq M  \tag{34}\\
& e_{p}^{T} v=1 \\
& v \in \mathbb{R}_{+}^{p} .
\end{array}
$$

We calculate the upper and lower bounds (1), (2), (3), and (4). Again, we apply the transformation $h(u)$ to the portfolio risk, i.e., the first constraint in (34). By calculating the transformed bounds as given in (15), (19), (20), and (22), we obtain tighter bounds of the Pareto efficient frontier. The transformed and nontransformed upper and lower bounds are shown in Figure 5.

Example 5.3 (Nonconvex Pareto efficient frontier)
In this example we consider the estimation of a nonconvex Pareto efficient frontier. The objective is to minimize

$$
f_{1}(v)=\left[1-\prod_{i=1}^{n}\left[1-\left(e^{-\exp \left(-\alpha v_{i}-\beta v_{i}^{2} / n\right)}\right)^{s}\right]^{\Delta c_{i}}\right]^{1 / s}
$$

where $\alpha, \beta, s, \Delta c_{i}=c_{i} / \sum_{i=1}^{n} c_{i}$, and $c_{i}$ are constants, and at the same time maximize

$$
f_{2}(v)=\sum_{i=1}^{n} v_{i}
$$



Figure 5: Transformed and not transformed upper and lower bounds of Pareto efficient frontier associated with (34).

The origin of $f_{1}(v)$ can be found in Brahme and Agren (1987). The associated $\varepsilon$-constraint optimization problem is given as

$$
\begin{align*}
\min _{v} & {\left[1-\prod_{i=1}^{n}\left[1-\left(e^{-\exp \left(-\alpha v_{i}-\beta v_{i}^{2} / n\right)}\right)^{s}\right]^{\Delta c_{i}}\right]^{1 / s} } \\
\text { s.t. } & \sum_{i=1}^{n} v_{i} \geq \varepsilon  \tag{35}\\
& v \in \mathbb{R}_{+}^{n}
\end{align*}
$$

It can be shown that $f_{1}(v)$ is not convex. This implies that the Pareto efficient frontier that is associated with (35) is not necessarily convex. However, by applying the convex and increasing transformation $h(u)=-\log \left(1-u^{s}\right)$ to $f_{1}$ we obtain a convex function $h\left(f_{1}(v)\right)$; see Hoffmann et al. (2006). We take $n=5, \alpha=1, \beta=5, s=2, c_{1}=5, c_{2}=6, c_{3}=4, c_{4}=3$, and $c_{5}=8$. Now, we can construct the transformed upper and lower bounds both using only function value information and using also derivative information as given in (5), (8), (9), and (12). The bounds are shown in Figure 6.

Next, we consider the $\varepsilon$-constraint problem with $f_{1}$ as a constraint and $f_{2}$ as objective:

$$
\begin{array}{ll}
\min _{v} & -\sum_{i=1}^{n} v_{i} \\
\text { s.t. } & {\left[1-\prod_{i=1}^{n}\left[1-\left(e^{-\exp \left(-\alpha v_{i}-\beta v_{i}^{2} / n\right)}\right)^{s}\right]^{\Delta c_{i}}\right]^{1 / s} \leq \varepsilon} \tag{36}
\end{array}
$$

$$
v \in \mathbb{R}_{+}^{n}
$$

Again, we apply the transformation $h(u)$ to $f_{1}$, and construct the transformed upper and lower bounds using only function value information and using also derivative information as given in (14), (17), (18), and (21). These bounds are shown in Figure 7.


Figure 6: Upper and lower bounds of Pareto efficient frontier associated with (35).


Figure 7: Upper and lower bounds of Pareto efficient frontier associated with (36).

## 6 Conclusions

In this paper, we studied the effect of transformations on the approximation of univariate (convex) functions. By using increasing transformations on the input or the output variables, we can transform nonconvex functions into convex functions, for which upper and lower bounds are given. We showed that applying the inverse transformation to these upper and lower bounds gives us bounds for the original nonconvex function.

Moreover, we showed that if the function that is to be approximated is convex, we can obtain tighter upper and lower bounds than the original piecewise linear upper and lower bounds. We can achieve this by using increasing and concave transformations of the output variable $y$ and concave or convex transformations of the input variable $x$.

Furthermore, we applied the developed theory to the approximation of a convex Pareto curve and a nonconvex Pareto curve, associated with bi-objective optimization problems. Finally, we gave some examples of these applications.

## References

Bisschop, J. (2000). AIMMS optimization modeling. Technical report, Haarlem.
Brahme, A. and A.K. Agren (1987). Optimal dose distribution for eradication of heterogeneous tumours. Acta Oncologica, 26, 377-356.

Burkard, R.E., H.W. Hamacher, and G. Rote (1991). Sandwich approximation of univariate convex functions with an application to separable convex programming. Naval Research Logistics, 38, 911-924.

Ehrgott, M. and R. Johnston (2003). Optimisation of beam directions in intensity modulated radiation therapy planning. OR Spectrum, 25, 251-264.

Fruhwirth, B., R.E. 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.

Hoffmann, A.L., D. den Hertog, and A.Y.D. Siem (2006). Convexity analysis of LQ-model based radiobiological objective functions for radiation therapy planning optimization. Working paper.

Küfer, K.-H., A. Scherrer, M. Monz, F. Alonso, H. Trinkaus, T. Bortfeld, and C. Thieke (2003). Intensity-modulated radiotherapy - a large scale multi-criteria programming problem. $O R$ Spectrum, 25, 223-249.

Markowitz, H.M. (1952). Portfolio selection. Journal of Finance, 7, 77-91.

Miettinen, K. (1999). Nonlinear Multiobjective Optimization. Boston: Kluwer Academic Publishers.

Rote, G. (1992). The convergence rate of the Sandwich algorithm for approximating convex functions. Computing, 48, 337-361.

Siem, A.Y.D., D. den Hertog, and A.L. Hoffmann (2005). A method for approximating univariate convex functions using function only evaluations. Working paper.

Terlaky, T. (1985). On $l_{p}$ programming. European Journal of Operational Research, 22, 70-100.
Yang, X.Q. and C.J. Goh (1997). A method for convex curve approximation. European Journal of Operational Research, 97, 205-212.


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