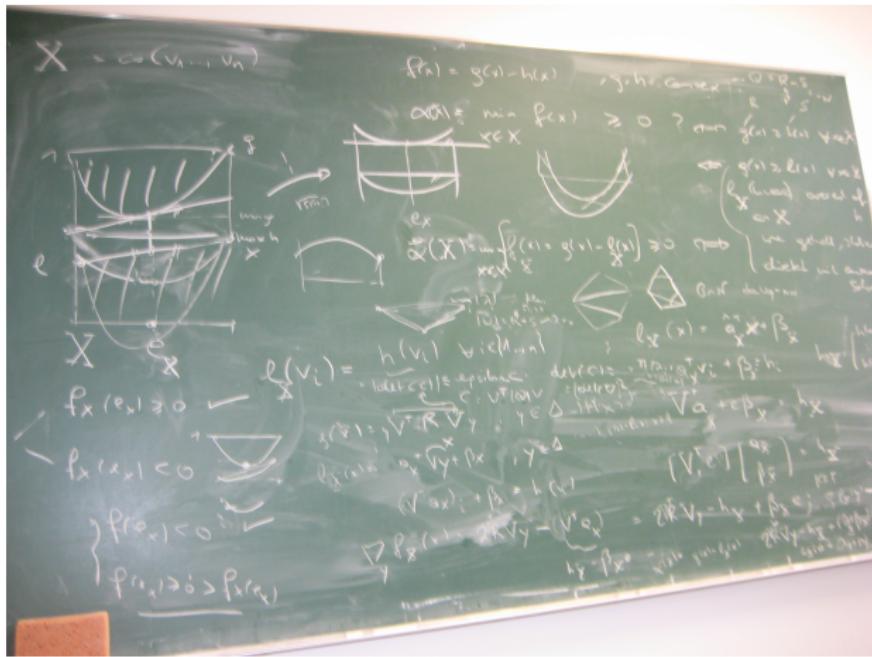


Application of Convex Underestimators to Global Multiobjective Optimization

Gabriele Eichfelder

joint work with Tobias Gerlach, Julia Niebling, and Susanne Sumi (Ilmenau)

How it started ...



(but also other great memories of Vienna!)



Copositivity test...

Matrix $A \in \mathcal{S}^n$ copositive $\Leftrightarrow \min_{x \geq 0} x^\top Ax = 0$

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- Copositivity detection via difference-of-convex approach:

Decompose $Q = Q_+ - Q_-$ with Q_+, Q_- positive semidefinite, and replace by

$$\inf\{x^\top Q_+ x \mid x^\top Q_- x = 1, x \geq 0\} \geq 1.$$

$$\text{and } \dots x^\top Q x = x^\top Q_+ x - x^\top Q_- x \geq x^\top Q_+ x - 1 \geq 0$$

Copositivity test...

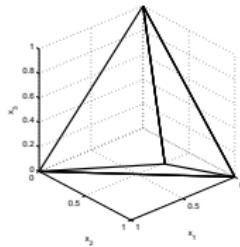
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- Branch-and-Bound by partitioning of the standard simplex:



Content

1. α BB method for global (scalar) optimization
 $f: \mathbb{R}^n \rightarrow \mathbb{R}$
2. Basics of multiobjective optimization
 $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$
3. α BB method for global multiobjective optimization
 $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$

Nonlinear Optimization

We consider the following nonlinear optimization problem

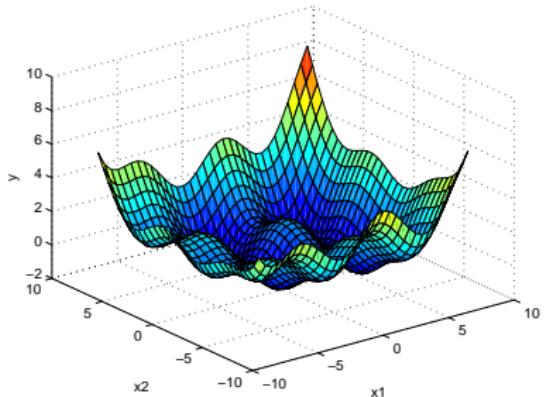
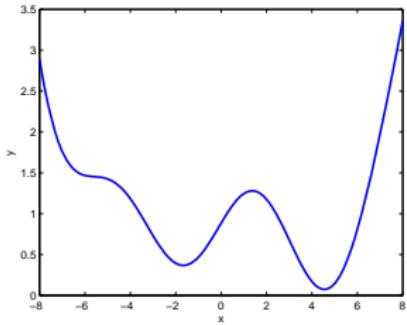
$$\min_{x \in X} f(x) \quad (P)$$

with twice continuously differentiable objective function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ and feasible set

$$X = \{x \in \mathbb{R}^n \mid \underline{x} \leq x \leq \bar{x}\} = [\underline{x}, \bar{x}]$$

with $\underline{x}, \bar{x} \in \mathbb{R}^n$, $\underline{x} \leq \bar{x}$.

Local and Global Solutions of $\min_{x \in X} f(x)$ (P)

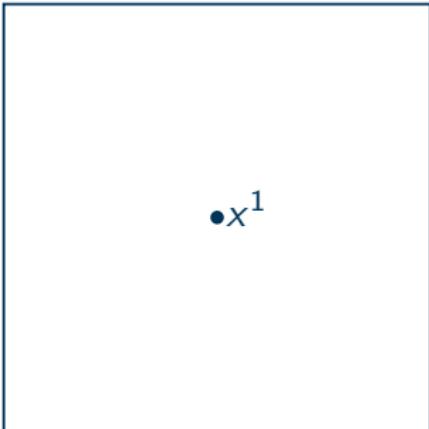


- ▶ A point $\bar{x} \in X$ is a (global) minimal solution of (P), if
$$f(\bar{x}) \leq f(x) \text{ for all } x \in X.$$

- ▶ A point $\bar{x} \in X$ is a local minimal solution of (P), if a neighbourhood $U_{\bar{x}}$ of \bar{x} exists with

$$f(\bar{x}) \leq f(x) \text{ for all } x \in X \cap U_{\bar{x}}.$$

Basic Branch and Bound Algorithm

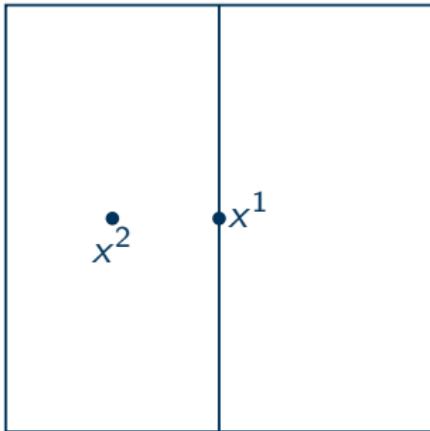


Feasible set $X \subset \mathbb{R}^2$

- ▶ Branch: Partitioning rule, partition in subboxes X^i
- ▶ Selection rule
(e.g. $f(x^i)$ with midpoints x^i of subboxes X^i)
- ▶ Bound: Discarding tests
- ▶ Termination rule

Basic idea: $\min_{x \in X} f(x) = \min \left\{ \min_{x \in X^i} f(x) \right\}$ if $X = \bigcup_i X^i$

Basic Branch and Bound Algorithm

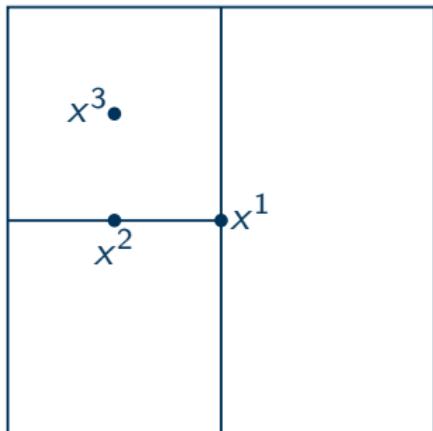


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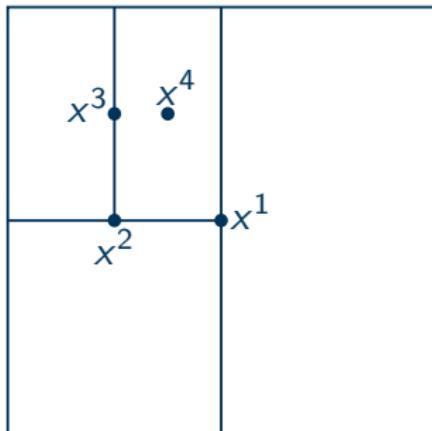


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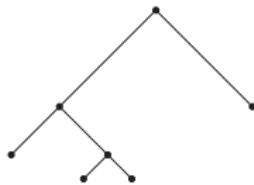
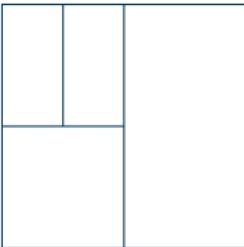


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Discarding tests scalar-valued case $f: X \rightarrow \mathbb{R}$



- ▶ upper bound for the (global) minimum by $\min_i f(x^i)$ (with midpoints x^i)
- ▶ lower bounds by interval arithmetic or convex underestimators for the values $f(x)$ with $x \in X^j$ for each subbox X^j ,
i.e. u^j with $u^j \leq \min_{x \in X^j} f(x)$
- ▶ Discard subbox X^j if

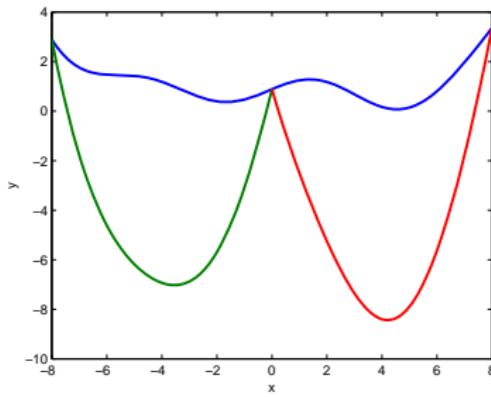
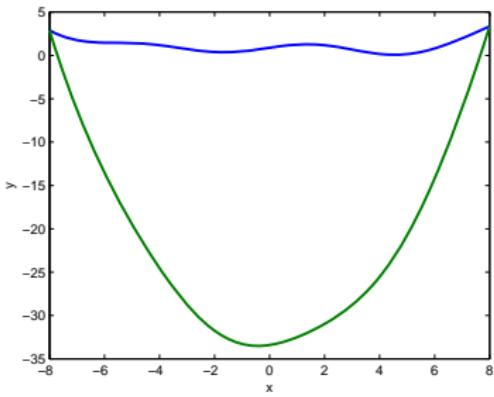
$$\min_i f(x^i) < u^j.$$

α BB: Bounds by Convex Underestimator

Definition

As before let $X \subset \mathbb{R}^n$ and $f: \mathbb{R}^n \rightarrow \mathbb{R}$. A function $\tilde{f}: X \rightarrow \mathbb{R}$ is called a **convex underestimator** of f on X , if

- ▶ \tilde{f} is convex on X and
- ▶ $\tilde{f}(x) \leq f(x)$ for all $x \in X$.



Convex Underestimator by α BB

Lemma (Maranas, Floudas '94)

As before let $X = [\underline{x}, \bar{x}]$. Then $f_{\alpha,X} : X \rightarrow \mathbb{R}$,

$$f_{\alpha,X}(x) := f(x) + \alpha \sum_{i=1}^n \underbrace{(\underline{x}_i - x_i)(\bar{x}_i - x_i)}_{\leq 0},$$

is a convex underestimator of f w.r.t. X if and only if

$$\alpha \geq \max \left\{ 0, -\frac{1}{2} \min \{ \lambda_{\min}(H_f(x)) \mid x \in X \} \right\}.$$

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$$u_j := \min_{x \in X^j} f_{\alpha,X^j}(x) \leq \min_{x \in X^j} f(x)$$

and

$$\max_{x \in X} (f(x) - f_{\alpha,X}(x)) = \frac{\alpha}{8} \|\bar{x} - \underline{x}\|_2^2.$$

Algorithm for (ε, δ) -minimal set

Aim: Cover/representation of the set $\operatorname{argmin}\{f(x) \mid x \in X\}$.

Definition

Let $\varepsilon > 0$, $\delta > 0$ and $\operatorname{argmin}_{x \in X} f(x) \neq \emptyset$.

(a) $\tilde{x} \in X$ is an ε -minimal point of f w.r.t. X , if

$$f(\tilde{x}) \leq \min_{x \in X} f(x) + \varepsilon.$$

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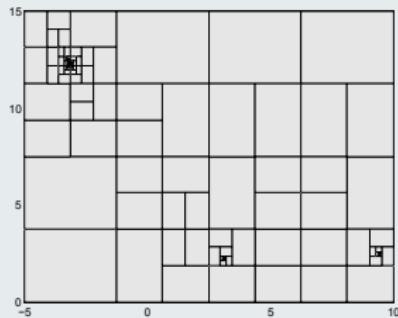
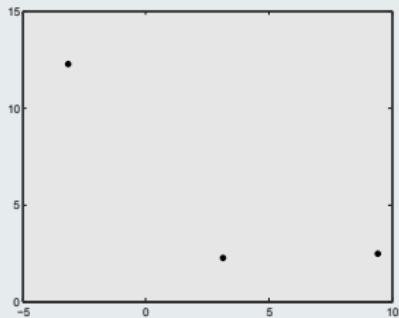
$$f(\tilde{x}) \leq \min_{x \in X} f(x) + \varepsilon.$$

(b) A finite subset A of ε -minimal points of f w.r.t. X is an (ε, δ) -minimal set of f w.r.t. X if for all $\bar{x} \in \operatorname{argmin}_{x \in X} f(x)$ there exists $\hat{x} \in A$ such that $\|\hat{x} - \bar{x}\|_2 \leq \delta$.

Modified α BB Algorithm

Beispiel (Branin, Hoo '72)

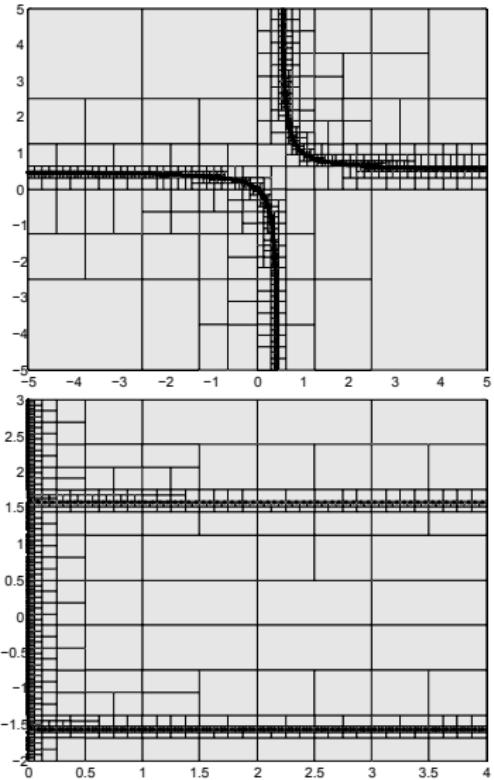
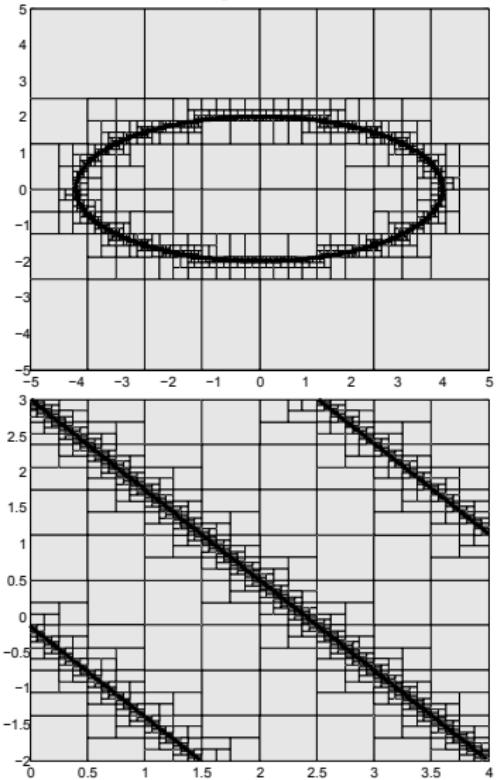
$$f(x) := \left(x_2 - \frac{5.1}{4\pi^2} x_1^2 + \frac{5}{\pi} x_1 - 6 \right)^2 + 10 \left(1 - \frac{1}{8\pi} \right) \cos(x_1) + 10$$
$$X = [-5, 10] \times [0, 15].$$



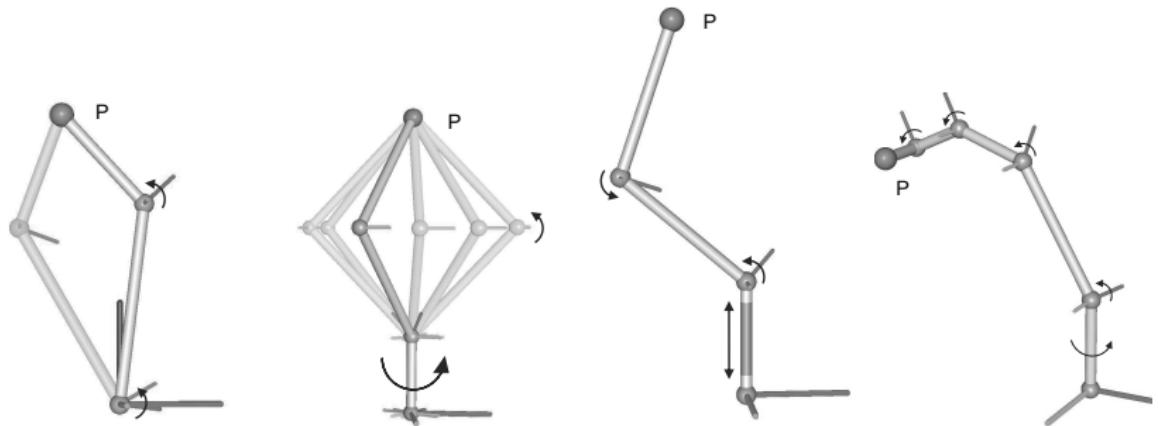
Theorem (E./Gerlach/Sumi '16)

The modified α BB algorithm terminates after finitely many iterations with an (ε, δ) -minimal set of f w.r.t. X .

Some examples



Robot arm (Tetra GmbH, Ilmenau)



2

Basics of multiobjective optimization

Multiobjective Optimization

$$\min \begin{pmatrix} f_1(x) \\ \vdots \\ f_m(x) \end{pmatrix} \text{ s.t. } x \in X \quad (\text{MOP})$$

with twice continuously differentiable functions

$f_i: \mathbb{R}^n \rightarrow \mathbb{R}$, $i = 1, \dots, m$,

and feasible set

$$X = \{x \in \mathbb{R}^n \mid \underline{x} \leq x \leq \bar{x}\} = [\underline{x}, \bar{x}]$$

where $\underline{x}, \bar{x} \in \mathbb{R}^n$ with $\underline{x} \leq \bar{x}$.

Efficient solutions in multi-objective optimization

Consider

$$\min_{x \in X} f(x) \text{ with } f: \mathbb{R}^n \rightarrow \mathbb{R}^m, f(x) = (f_1(x), \dots, f_m(x))^\top.$$

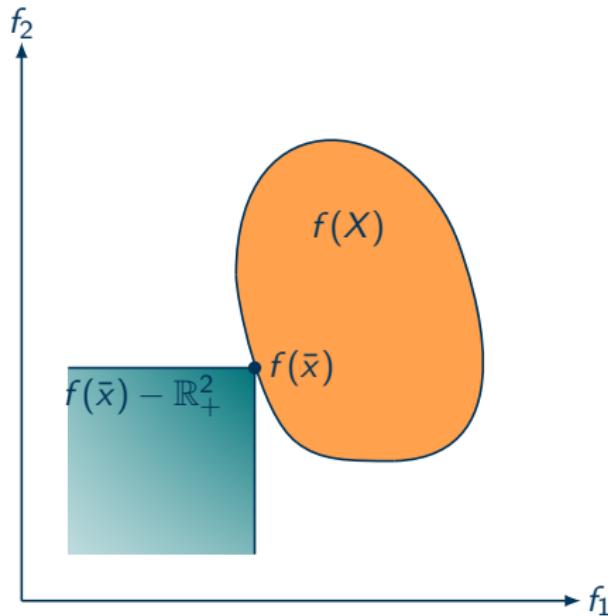
The point $\bar{x} \in X$ is an **efficient solution** of $\min_{x \in X} f(x)$ if there exists **no** $x \in X$ with

$$\begin{aligned} f_i(x) &\leq f_i(\bar{x}) \text{ for all } i = 1, \dots, m, \\ \text{and } f_j(x) &< f_j(\bar{x}) \text{ for at least one } j \in \{1, \dots, m\}. \end{aligned}$$

Hence if

$$(\{f(\bar{x})\} - \mathbb{R}_+^m) \cap f(X) = \{f(\bar{x})\} .$$

Efficient solutions with $m = 2$



\bar{x} is efficient $\iff (\{f(\bar{x})\} - \mathbb{R}_+^2) \cap f(X) = \{f(\bar{x})\}$

Scalarization

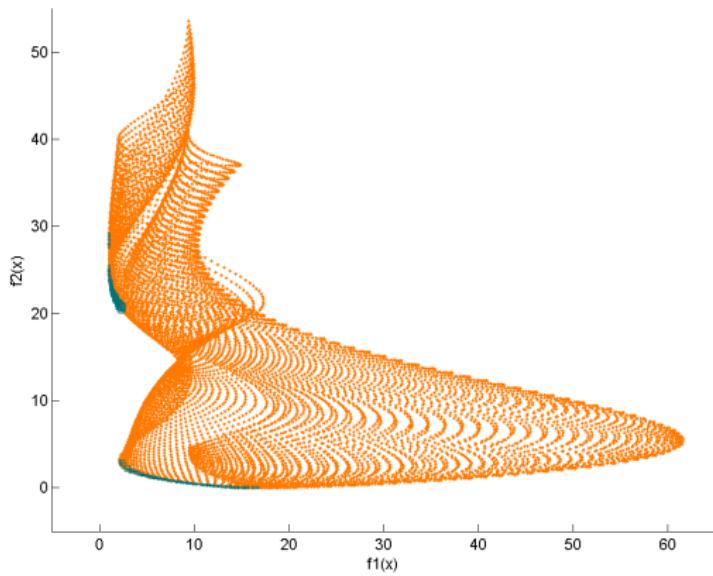
- Weighted sum

$$\min_{x \in X} \mathbf{w}^T f(x) = \sum_{i=1}^m w_i f_i(x) = w_1 f_1(x) + \dots + w_m f_m(x).$$

- ε -constraint method

$$\begin{aligned} & \min \quad f_m(x) \\ & \text{s.t.} \\ & f_1(x) \leq \varepsilon_1 \\ & \quad \vdots \\ & f_{m-1}(x) \leq \varepsilon_{m-1} \\ & x \in X \end{aligned}$$

Local efficient solutions: Poloni function



α BB method for global multiobjective optimization

Basic Branch-and-Bound for biobjective problems

$$\min \begin{pmatrix} f_1(x) \\ f_2(x) \end{pmatrix} \text{ s.t. } x \in X_0 = [\underline{x}, \bar{x}] \quad (\text{MOP})$$

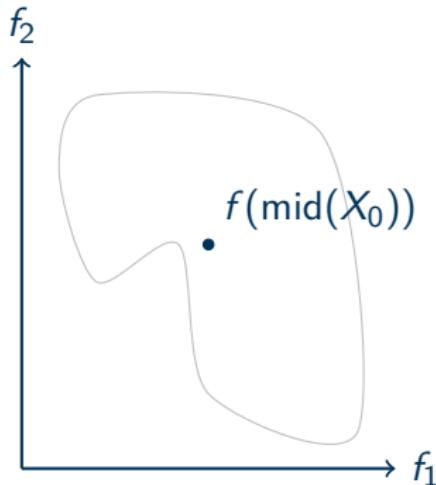
- ▶ Branch: Partitioning rule
- ▶ Selection rule
- ▶ Bound: Discarding tests
 - ▶ upper bound?
 - ▶ lower bound on subboxes?
- ▶ Termination rule

[Fernández, Tóth '09]

Multiobjective optimization: upper bounds?

„Provisional nondominated solutions“ \mathcal{L}_{PNS} :

List with known objective values, which do not dominate each other.

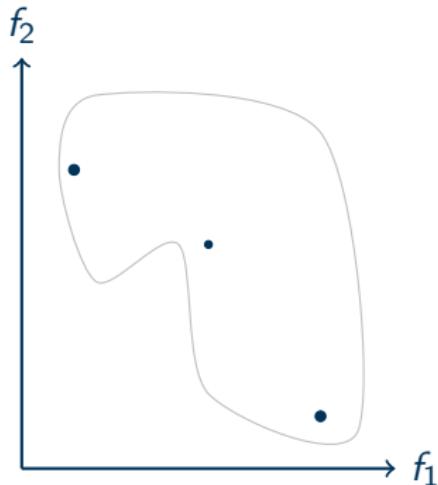


wobei $\text{mid}(X_0) := \frac{1}{2}(\bar{x} + \underline{x})$ für $X_0 = [\underline{x}, \bar{x}]$.

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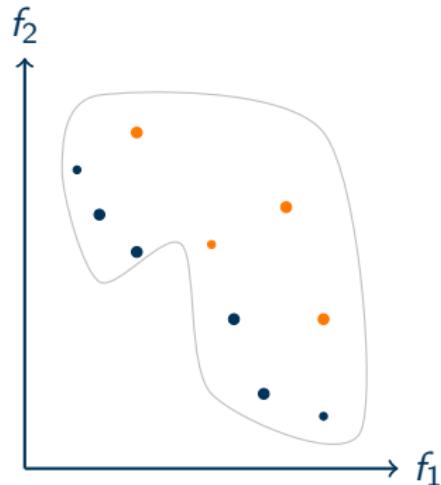


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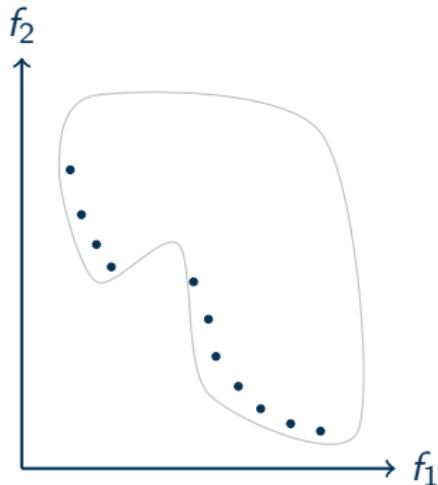


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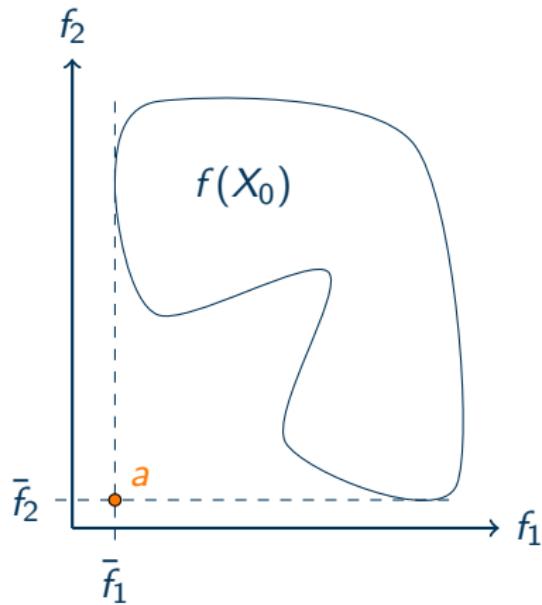
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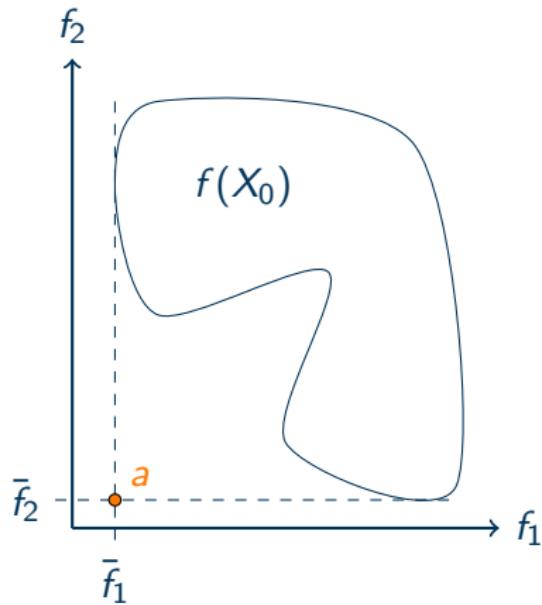
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Lower bounds? Ideal point



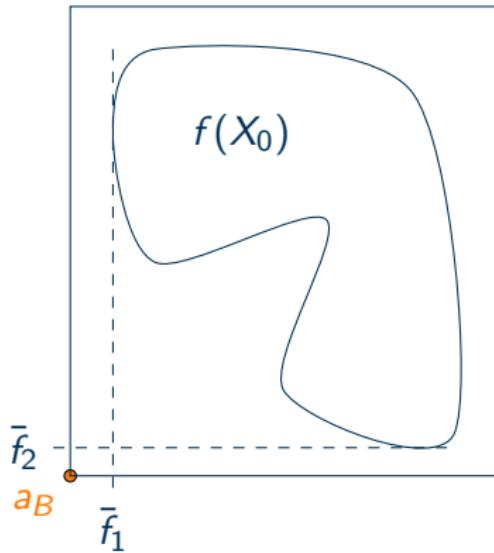
- ▶ Solve
 $\bar{f}_1 := \min_{x \in X_0} f_1(x)$ and
 $\bar{f}_2 := \min_{x \in X_0} f_2(x)$
- ▶ Set $a = (\bar{f}_1, \bar{f}_2)^\top$

Lower bounds? Ideal point



- ▶ Solve
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Ideal point and interval arithmetic

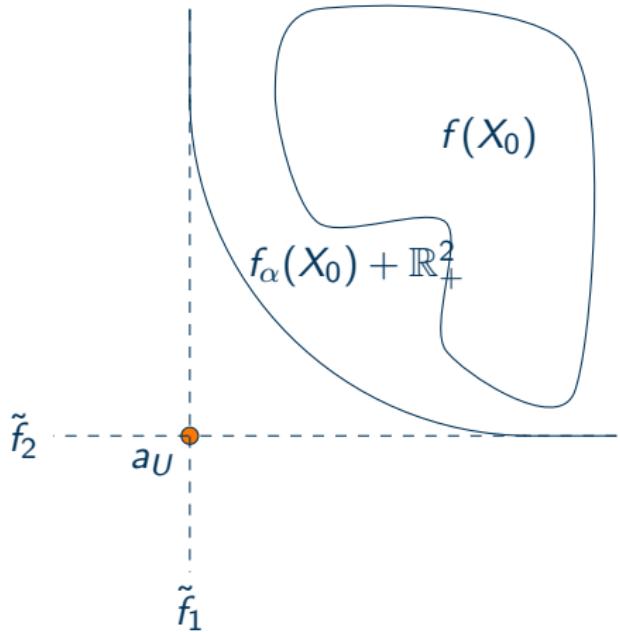


- ▶ Determine interval extensions F_1 of f_1 and F_2 of f_2 and use that for calculating a box $B \subset \mathbb{R}^2$ with

$$f(X_0) \subset B$$

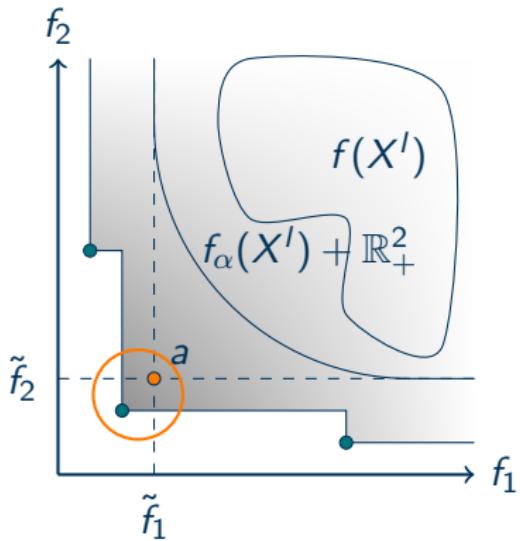
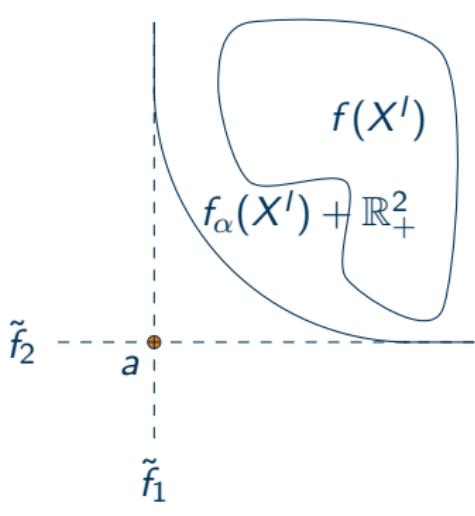
- ▶ Choose a_B als lower bound of the box B

Ideal point and convex underestimators



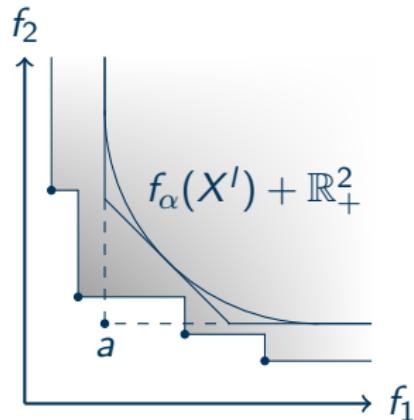
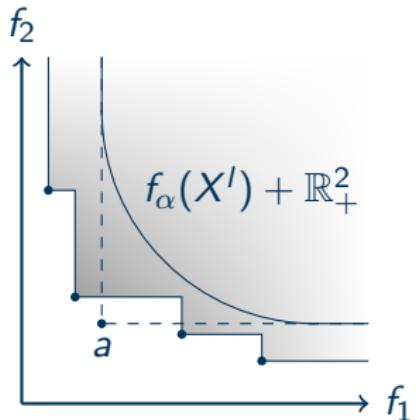
- ▶ Determine convex underestimators $f_{1,\alpha}$ of f_1 and $f_{2,\alpha}$ of f_2 on X_0
- ▶ Calculate $\tilde{f}_1 := \min_{x \in X_0} f_{1,\alpha}(x)$ and $\tilde{f}_2 := \min_{x \in X_0} f_{2,\alpha}(x)$
- ▶ Set $a_U := (\tilde{f}_1, \tilde{f}_2)^\top$

Fist discarding test for a box X'



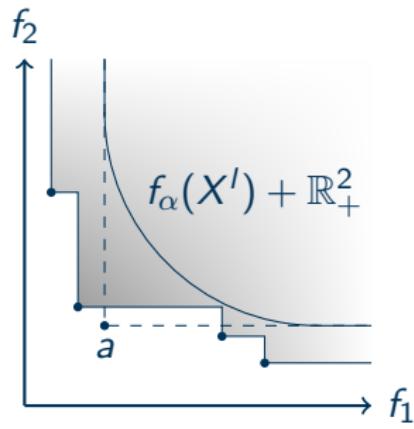
Compare a with points from the list \mathcal{L}_{PNS} (=upper bounds) and discard X' , if a is componentwise larger than any point from \mathcal{L}_{PNS} !

Improved discarding test

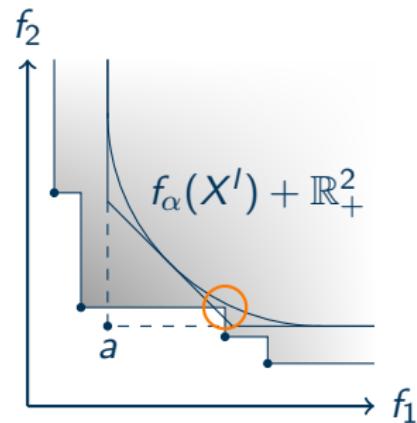


Improve lower bound by applying one step of **Benson's algorithm**
[Benson '98, Ehrgott, Shao, Schöbel '11, Löhne, Rudloff, Ulus '14]
with objective function f_α in X^I .

Further Improvement

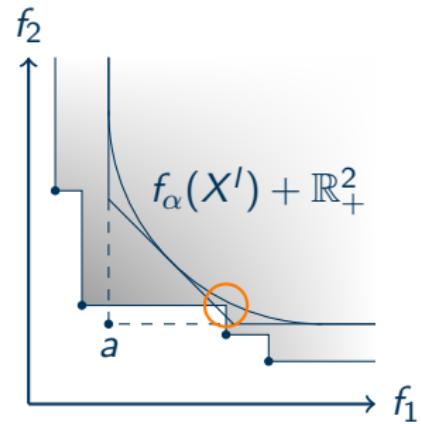


ideal point with
convex underestimator



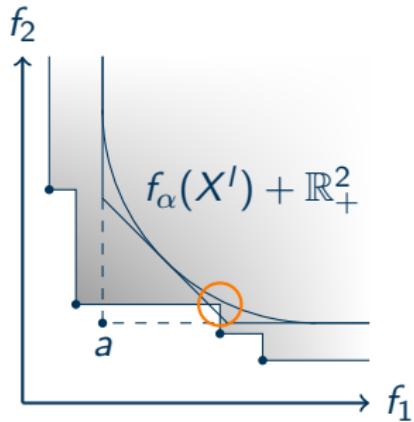
Benson step

Further Improvement



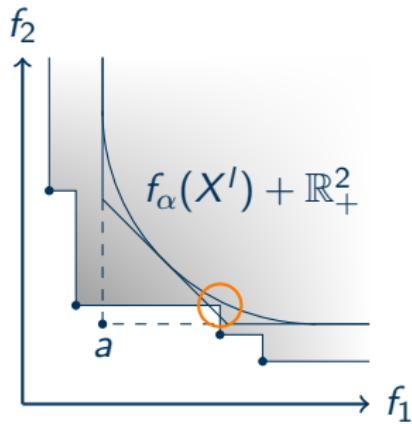
Benson step

Further Improvement

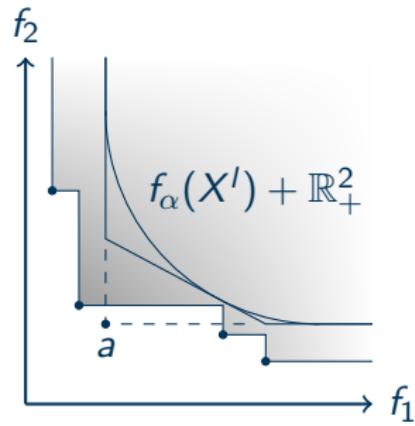


Benson step

Further Improvement

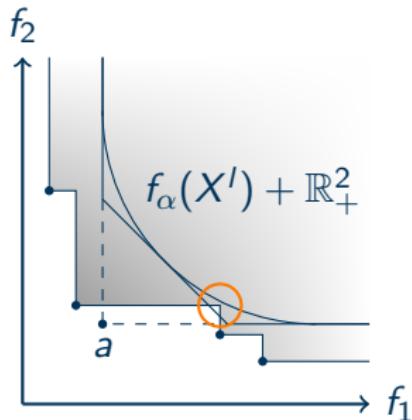


Benson step

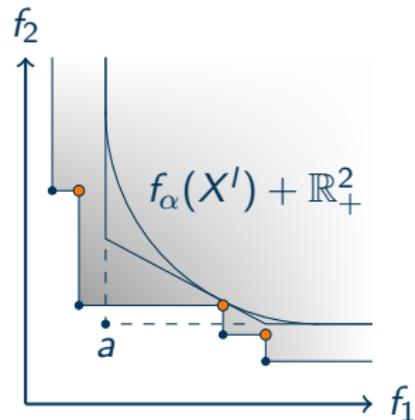


Improvement

Further Improvement



Benson step



Improvement

Apply Bensons algorithm at *local upper bounds*.

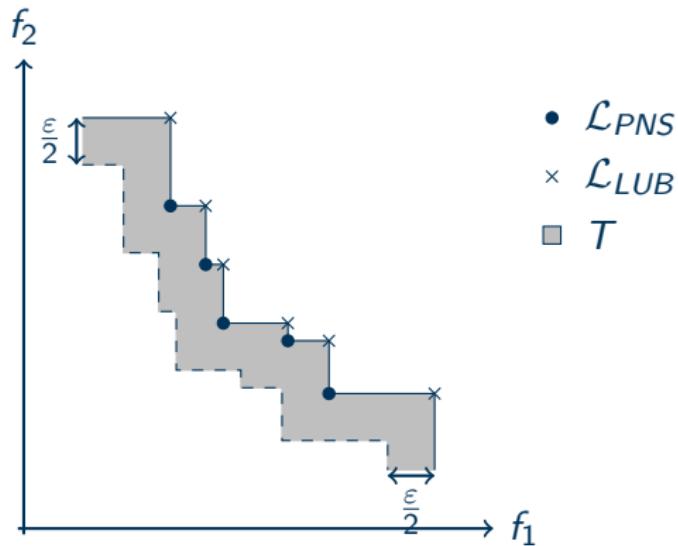
Interval arithmetic vs. Benson improved

n -dimensional Fonseca Fleming function:

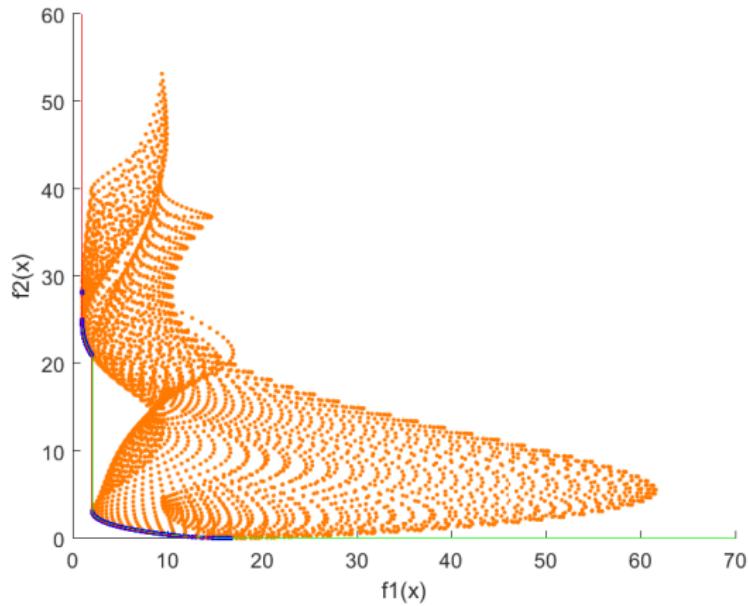
$$f(x) = \begin{pmatrix} 1 - \exp\left(-\sum_{i=1}^n \left(x_i - \frac{1}{\sqrt{n}}\right)^2\right) \\ 1 - \exp\left(-\sum_{i=1}^n \left(x_i + \frac{1}{\sqrt{n}}\right)^2\right) \end{pmatrix}, x_0 = \left[\begin{pmatrix} -2 \\ \vdots \\ -2 \end{pmatrix}, \begin{pmatrix} 2 \\ \vdots \\ 2 \end{pmatrix}\right] \subset \mathbb{R}^n$$

n	Interval arithmetic			Benson improved		
	$ \mathcal{L}_S $	iterations	time [s]	$ \mathcal{L}_S $	iterations	time [s]
2	258	373	74.12	177	273	84.65
3	2108	3563	664.98	810	1795	634.98
4	17934	33394	6.71e+3	3925	11466	4.81e+3
5	199460	325595	9.91e+4	19622	53221	2.94e+4

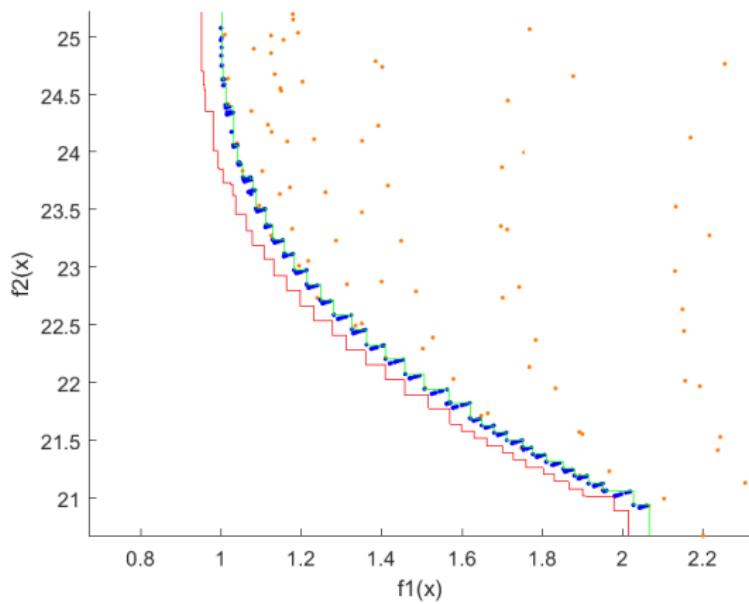
Some theoretical results



Poloni function



Poloni function



Some theoretical results

- ▶ Let for some predefined $\varepsilon > 0$

$$T := \left(\bigcup_{\bar{p} \in \mathcal{L}_{LUB}} \{\bar{p}\} - \mathbb{R}_+^m \right) \setminus \left(\bigcup_{\bar{p} \in \mathcal{L}_{LUB}} \left\{ \bar{p} - \frac{\varepsilon}{2} e \right\} - \text{int}(\mathbb{R}_+^m) \right).$$

Then $\mathcal{L}_{PNS} \subseteq T$ and for any efficient point \bar{x} it holds $f(\bar{x}) \in T$.

Some theoretical results

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- ▶ Let \mathcal{A} be the set generated by the algorithm. Then any $\tilde{x} \in \mathcal{A}$ is an ε -minimal point. And for any efficient point y there is a point $\tilde{x} \in \mathcal{A}$ with $\|\tilde{x} - y\| < \delta$.

Some theoretical results

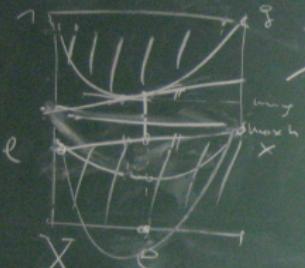
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- ▶ All while loops in the algorithm are finite.

$$X = \text{co}(v_1, \dots, v_n)$$



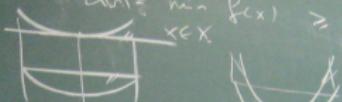
$$f_x(e_{x_i} \geq 0)$$

$$f_x(e_{x_i} < 0)$$

$$\left\{ \begin{array}{l} f_x(e_x) \leq 0 \\ P_{e_x} \geq 0 > P_x(e_x) \end{array} \right.$$

$$f(x) = g(x) - h(x)$$

$$\alpha(x) = \min_{x \in X} f(x) \geq 0$$



$$\alpha(x) = \inf_{x \in X} f(x) = g(x) - h(x) \geq 0$$



$$l(v_i)$$

$$l(x) = \alpha x + \beta$$

$$g(x) = \sqrt{R} V_y, \quad y \in \Delta \quad (\text{inner product})$$

$$h(x) = \sqrt{R} V_x + \beta$$

$$(\sqrt{R} x)_i + \beta = h(x)$$

$$(V, e) \left[\begin{smallmatrix} \alpha \\ \beta \end{smallmatrix} \right] = b$$

$$\nabla_{\frac{\partial}{\partial x}}(x) = 2RVy - (V^T x) = 2RVy - h(x) + \beta x; \quad \nabla^2 y = \frac{\partial^2}{\partial x^2} y = \frac{\partial^2}{\partial x^2} V^T x = R^2 I_n$$

$$h_x - \beta x = \frac{1}{2} x^T R^2 x - \frac{1}{2} x^T R^2 V^T V x = \frac{1}{2} x^T (R^2 - R^2 V^T V) x = \frac{1}{2} x^T Q x$$

$$Q = R^2 - R^2 V^T V = R^2 (I_n - V^T V)$$



Literature

- ▶ A. Neumaier.
Interval methods for systems of equations.
Cambridge University Press, 1990.
- ▶ S.M. Rump.
INTLAB - INTerval LABoratory.
In Tibor Csendes, *Developments in Reliable Computing*: 77-104, Kluwer, 1999.
<http://www.ti3.tuhh.de/rump/>.
- ▶ C. D. Maranas and C. A. Floudas.
Global minimum potential energy conformations of small molecules.
J. of Global Optim., 4(2):135–170, 1994.
- ▶ G. Eichfelder, T. Gerlach and S. Sumi.
A modification of the α BB method for box-constrained optimization and an application to inverse kinematics.
EURO J. on Comput. Optim., 4:93-121, 2016.
- ▶ J. Fernández and B. Tóth.
Obtaining the efficient set of nonlinear biobjective optimization problems via interval branch-and-bound methods.
Comp. Optim. and Appl., 42:393–419, 2009.
- ▶ H. P. Benson.
An outer approximation algorithm for generating all efficient extreme points in the outcome set of a multiple objective linear programming problem.
J. of Global Optim., 13:1–24, 1998.
- ▶ M. Ehrgott, L. Shao, and A. Schöbel.
An approximation algorithm for convex multi-objective programming problems.
J. of Global Optim., 50:397–416, 2011.
- ▶ A. Löhne, B. Rudloff, and F. Ulus.
Primal and dual approximation algorithms for convex vector optimization problems.
J. of Global Optim., 60(4):713–736, 2014.
- ▶ K. Klamroth, R. Lacour and D. Vanderpooten.
On the representation of the search region in multi-objective optimization.
EJOR, 245: 767–778, 2015.
- ▶ J. Niebling und G. Eichfelder.
A Branch-and-Bound based algorithm for nonconvex multiobjective optimization.
Preprint-Series, 2018.