An Approach to Minimize the Number of Function Evaluations in Global Optimization

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Thesis

- Working title: Approximating the Pareto Front with Meta Models
- Supervisors: Kaisa Miettinen and Jussi Hakanen
- Monograph, 2012
- Contribution: To approximate the Pareto Front so that the decision maker can “move” on it.
- Relation to this presentation: The approach will be modified to approximate holes on the front.

Content

- Global Optimization
- Lipschitzian
- Radial Basis Functions
- The Approach
- Numerical Examples
- References

Global Optimization (1/3)

- A considered Global Optimization Problem (GOP) is

$$\min_{x \in S} f(x),$$

where

  - $S \subset \mathbb{R}^n$ is compact,
  - f is a computationally expensive continuous function from S into $\mathbb{R}$.

- In other words, the problem is to find out $x^* \in S$ so that

$$f(x^*) \leq f(x) \text{ for all } x \in S$$

with a small number of function evaluations.

Global Optimization (2/3)

Solving techniques for computationally expensive objective functions, based on a given data

$$\mathcal{D} = \{(x^1, y^1), \ldots, (x^i, y^i = f(x^i)), \ldots, (x^k, y^k)\} \subset S \times \mathbb{R},$$

- Support vector regression [Vapnik, 1998]
- A radial basis function method [Gutmann, 2001]
- The EGO algorithm [Jones et al., 1998]

However, each of the above methods requires a global optimization sub problem to be solved.

Global Optimization (3/3)

The goal and motivation of this study:

- Let us assume that we have an algorithm, which produce a solution candidate x^c to the GOP.
- If x^c is close to a vector x^j for which the corresponding y^j is far from the so-far best known minimum of f, that is,

$$y^* = \min_{i=1,\ldots,k} y^i,$$

  then $f(x^c)$ is close to y^j, because f has been assumed to be continuous.
- We can save computation time by rejecting the evaluation of $f(x^c)$.
- We want a computationally efficient approach to decide whether to evaluate $f(x^c)$ or not.

Lipschitzian (1/3)

Function f is said to be *Lipschitzian*, if there exists a *Lipschitz* constant $l > 0$ so that

$$|f(x) - f(y)| \leq l\|x - y\| \text{ for all } x, y \in S,$$

where $\|\cdot\|$ is a norm on $\mathbb{R}^n$ (for example *Euclidean* norm).

- Function f from $\mathbb{R}$ into $\mathbb{R}$, $f(x) = 2x$, is Lipschitzian.

$$|f(x) - f(y)| = |2x - 2y| \leq 2|x - y|.$$

- A differentiable function f from $\mathbb{R}^n$ into $\mathbb{R}$ is Lipschitzian, if there exists $l > 0$ so that $\|\nabla f(z)\| \leq l$ for all $z \in \mathbb{R}^n$.

$$|f(x) - f(y)| \leq \sup_{z \in \mathbb{R}^n} \|\nabla f(z)\| \|x - y\| \leq l\|x - y\|.$$

Lipschitzian (2/3)

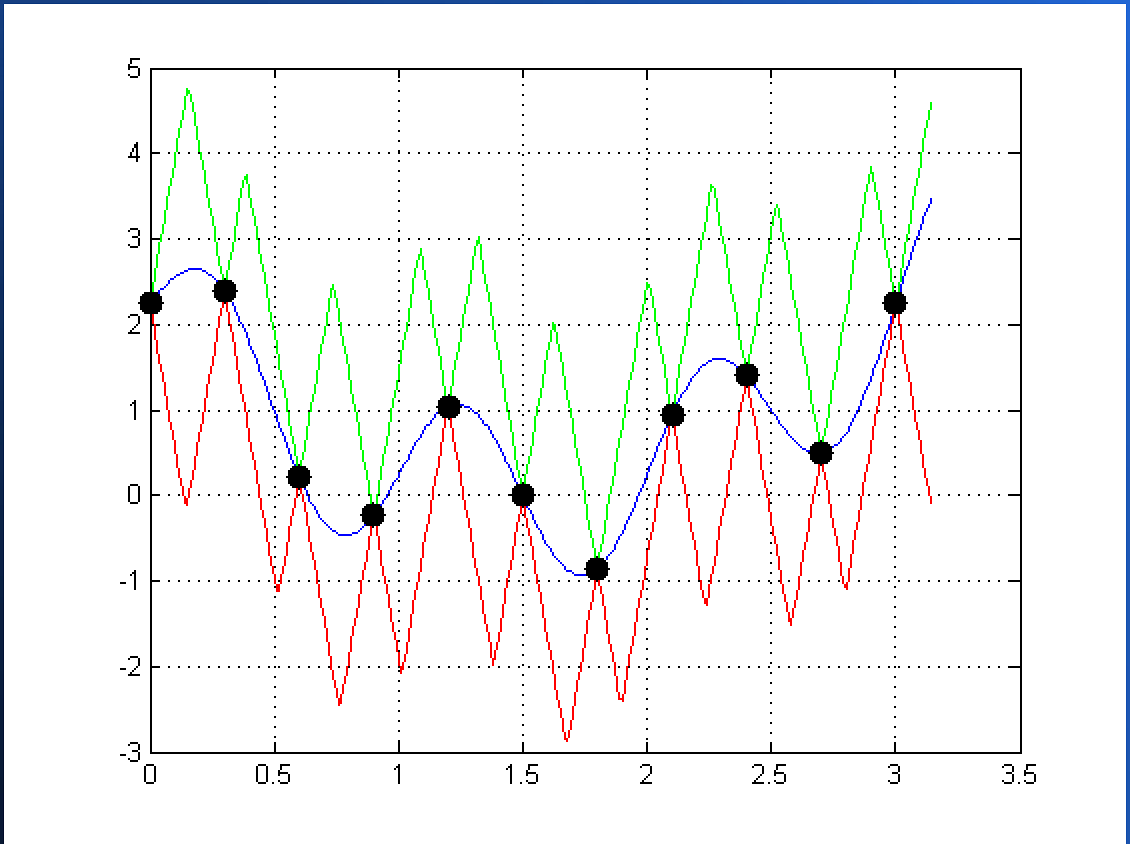
Global optimization solving algorithms based on the Lipschitzian property

- The DIRECT algorithm [Jones et al., 1993]
- Partition methods [Pintér, 1996]
  - Lower and upper approximations based on l and $\mathcal{D}$

$$f_l(x) = \max_{i=1,\ldots,k} \left(y^i - l\|x - x^i\| \right),$$
$$f_u(x) = \min_{i=1,\ldots,k} \left(y^i + l\|x - x^i\| \right).$$

  - However, the Lipschitz constant l must be known or approximated.

Lipschitzian (3/3)



Radial Basis Functions (1/3)

A basic Radial Basis Function [Buhmann, 2003] (RBF) g from S into $\mathbb{R}$, based on $\mathcal{D}$, is

$$g(x) = \sum_{i=1}^{k} \lambda_i \phi(\|x - x^i\|),$$

where

- coefficients λ_i are solution of a system of linear equations

$$\begin{bmatrix} \phi(\|x^1 - x^1\|) & \cdots & \phi(\|x^1 - x^k\|) \\ \vdots & \ddots & \vdots \\ \phi(\|x^k - x^1\|) & \cdots & \phi(\|x^k - x^k\|) \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \vdots \\ \lambda_k \end{bmatrix} = \begin{bmatrix} y^1 \\ \vdots \\ y^k \end{bmatrix},$$

- function ϕ from $\mathbb{R}$ into $\mathbb{R}$ is a given *basis function*.

Radial Basis Functions (2/3)

The given basis function can be, for example,

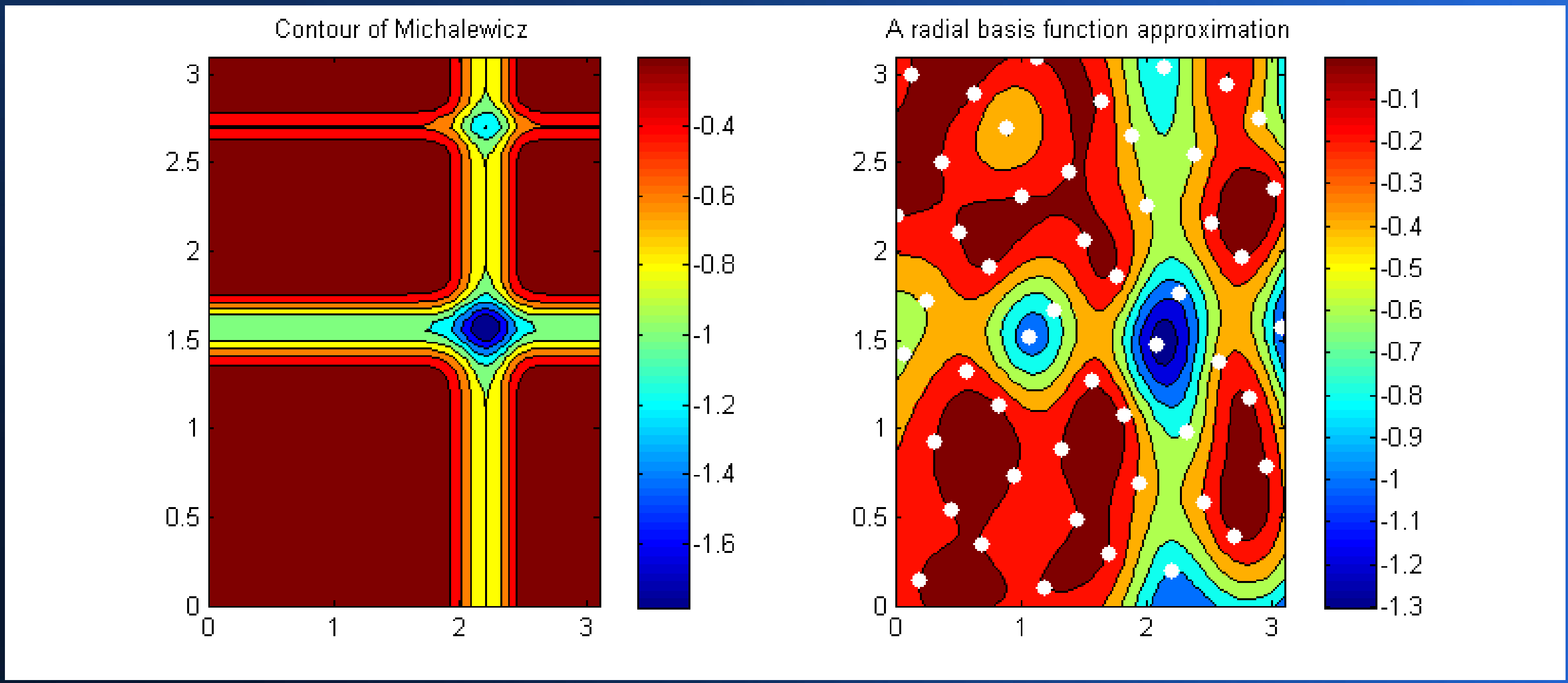
- a polyharmonic spline: $\phi(r) = r^d$, $d = 1, 3, 5, \ldots$
- thin plate spline: $\phi(r) = r^d \ln r$, $d = 2, 4, 6, \ldots$
- multiquadric: $\phi(r) = \sqrt{r^2 + \varepsilon^2}$, $\varepsilon > 0$
- Gaussian: $\phi(r) = e^{-\varepsilon r^2}$, $\varepsilon > 0$

We consider an RBF with a polyharmonic spline of third degree ($d = 3$), because it is smooth and Lipschitzian on S. Let such an RBF be denoted by f_{RBF} and let the Lipschitz constant be l_{RBF}.

- We have an approximation l_{RBF} for l.
- We have lower and upper approximations for f.

Radial Basis Functions (3/3)

- Michalewicz function: $f(x) = -\sum_{i=1}^{2} \sin(x_i) \left(\sin \left(\frac{i x_i^2}{\pi} \right) \right)^{20}$
- f_{RBF} with 50 *Hammersley* points [Kalagnanam and Diwekar, 1997]



The Approach (1/3)

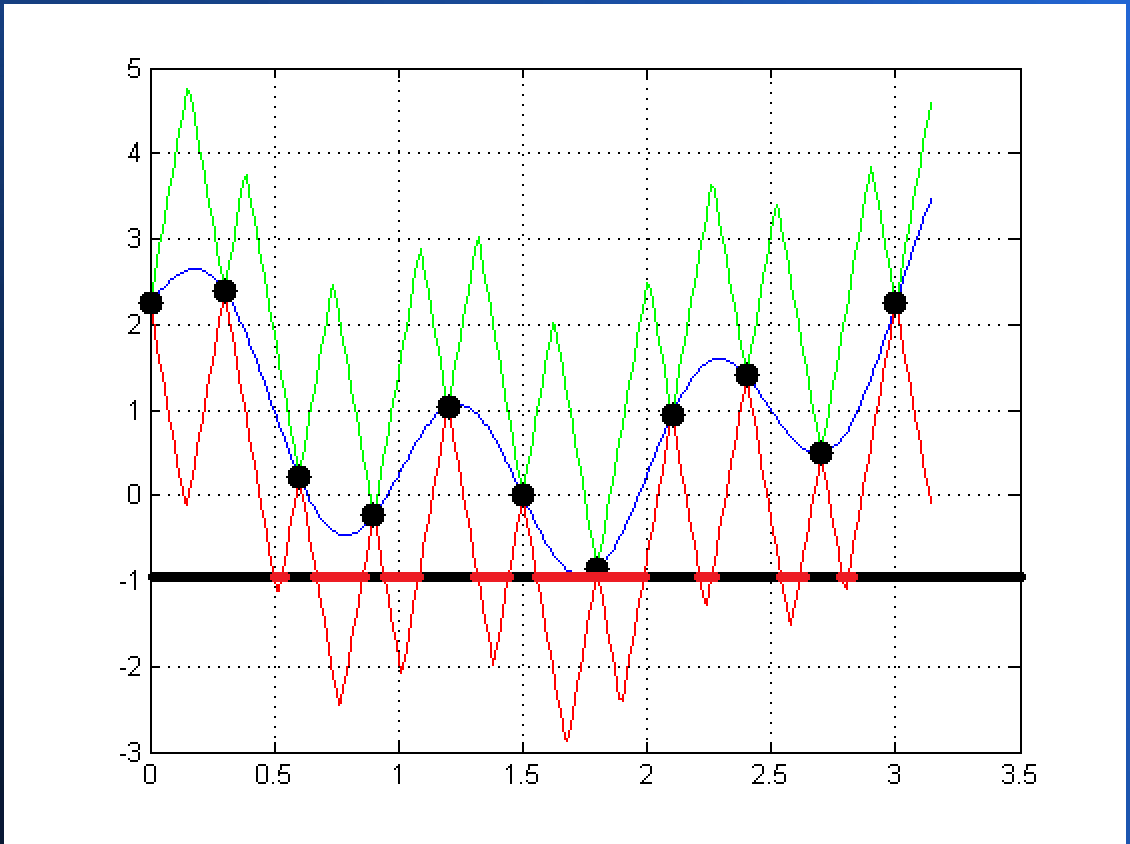
By using the Lipschitzian property (Partition methods), l_{RBF} and $\mathcal{D}$, we can separate S into two regions:

- The most promising region A_1 is a region where x^* of the GOP may exists.
  - $A_1 = \{x \in S : f_l(x) \leq y^*\}$
- The region A_{-1}, which is out of interest, is a region where x^* does not exists.
  - $A_{-1} = \{x \in S : f_l(x) > y^*\}$

In this way, we

- can reject the costly evaluation of $f(x^c)$, in the case that $x^c \in A_{-1}$,
- and try to focus on evaluations on A_1.

The Approach (2/3)



The Approach (3/3)

However,

- the approach does not produce solution candidates
- it only approximates whether to evaluate or not.

This is based on how well f_{RBF} approximates f.

- It is possible that f_{RBF} fails to approximate f, that is, $l_{RBF} < l$ caused by the lack of given information of f in $\mathcal{D}$.
- In this case, the most promising region A_1 may loose the track to the true minimum of the GOP.

Numerical Examples (1/2)

Test functions:

- Rosenbrock:

$$f(x) = 100(x_1^2 - x_2)^2 + (x_1 - 1)^2$$

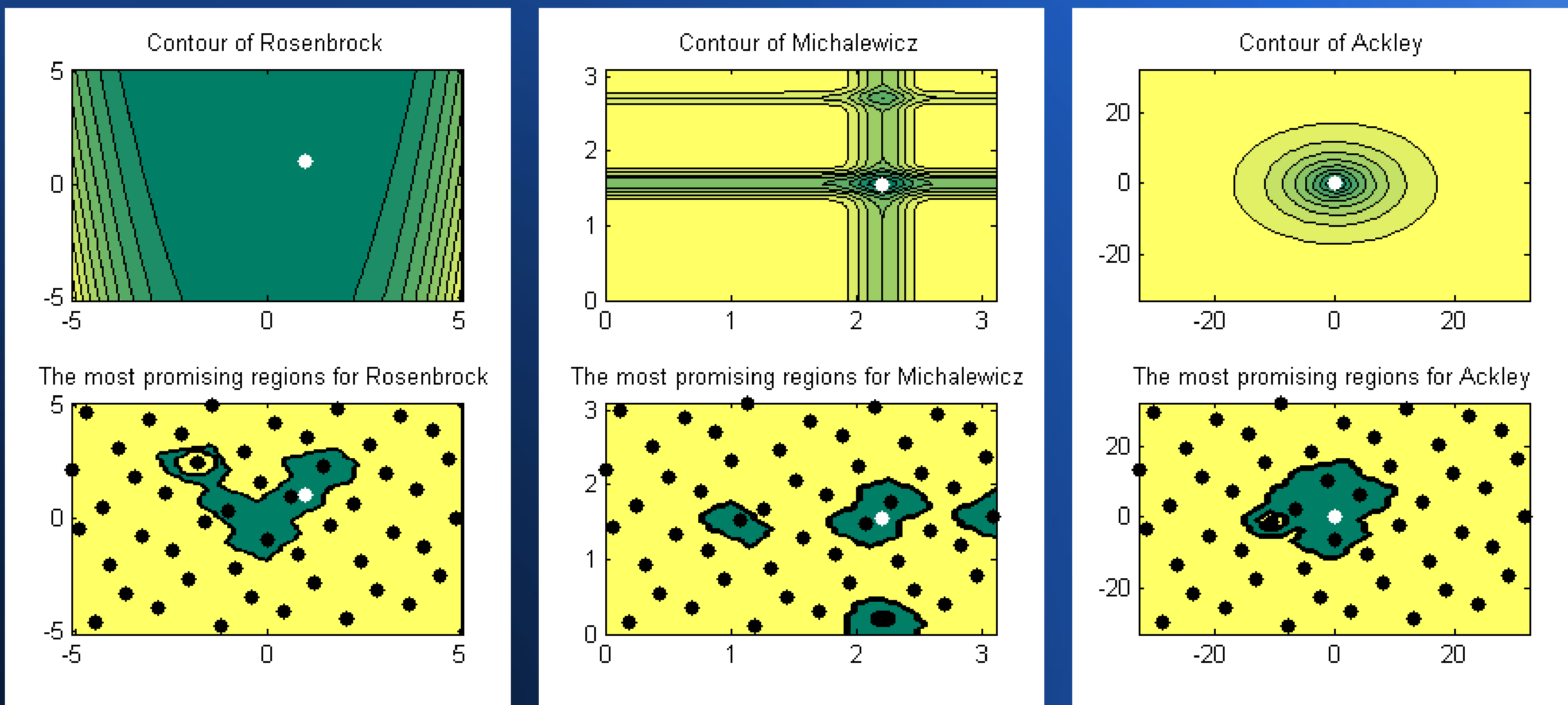
- Michalewicz:

$$f(x) = -\sum_{i=1}^{2} \sin(x_i) \left(\sin \left(\frac{i x_i^2}{\pi} \right) \right)^{20}$$

- Ackley:

$$f(x) = 20 + e - 20 e^{-\sqrt{\frac{1}{5} \sum_{i=1}^{2} x_i^2}} - e^{-\frac{1}{2} \sum_{i=1}^{2} \cos(2\pi x_i)}$$

Numerical Examples (2/2)



Conclusion

- A computationally efficient approach has been constructed to approximate the most promising region where the true minimum of the GOP may exists.
  - The approach is based on lower and upper approximations and a required approximation for the Lipschitz constant is derived from a radial basis function.
- The approach is able to decide whether to evaluate the computationally expensive objective function or not.
  - One can save computation time by rejecting the function evaluation for which an approximated value is not going to be smaller than the known minimum value of GOP.

Thank you!

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