# Randomized interval methods for global optimization

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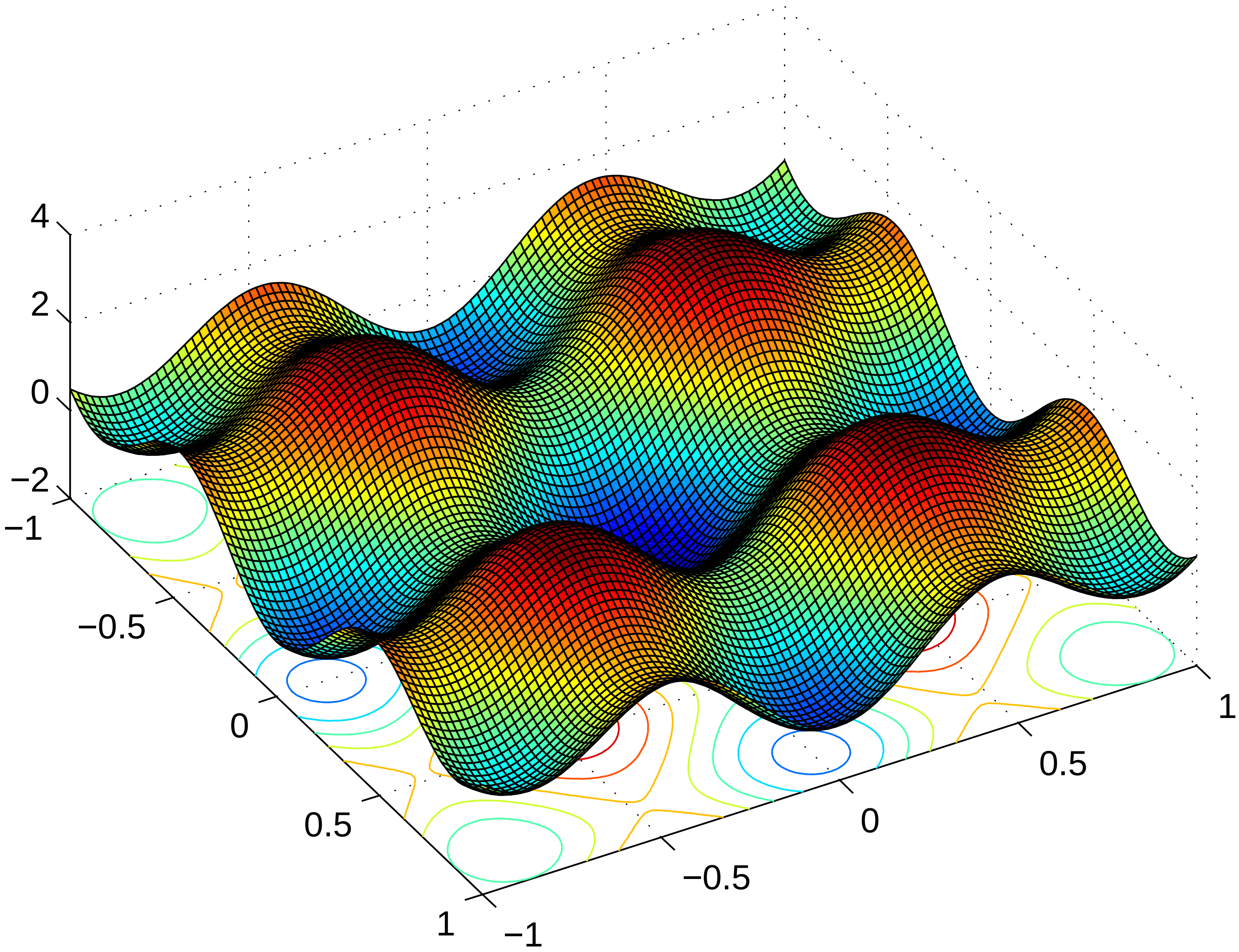
# Global optimization problem

Find the global minimum of a real-valued function $F : \mathbb{R}^n \supset \boldsymbol{X} \to \mathbb{R}$ over a rectangular axis-aligned box $\boldsymbol{X}$:

$$\text{find} \quad \min_{x \in \boldsymbol{X}} F(x)$$



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1

# Global optimization problem is NP-hard

= intractable,

i.e., its solution requires
no less than exponential
labor expenditures

A.A. Gaganov
On complexity of computing interval range
of a multivariate polynomial
// *Kibernetika*. – 1985. – №4. – P. 6–8.

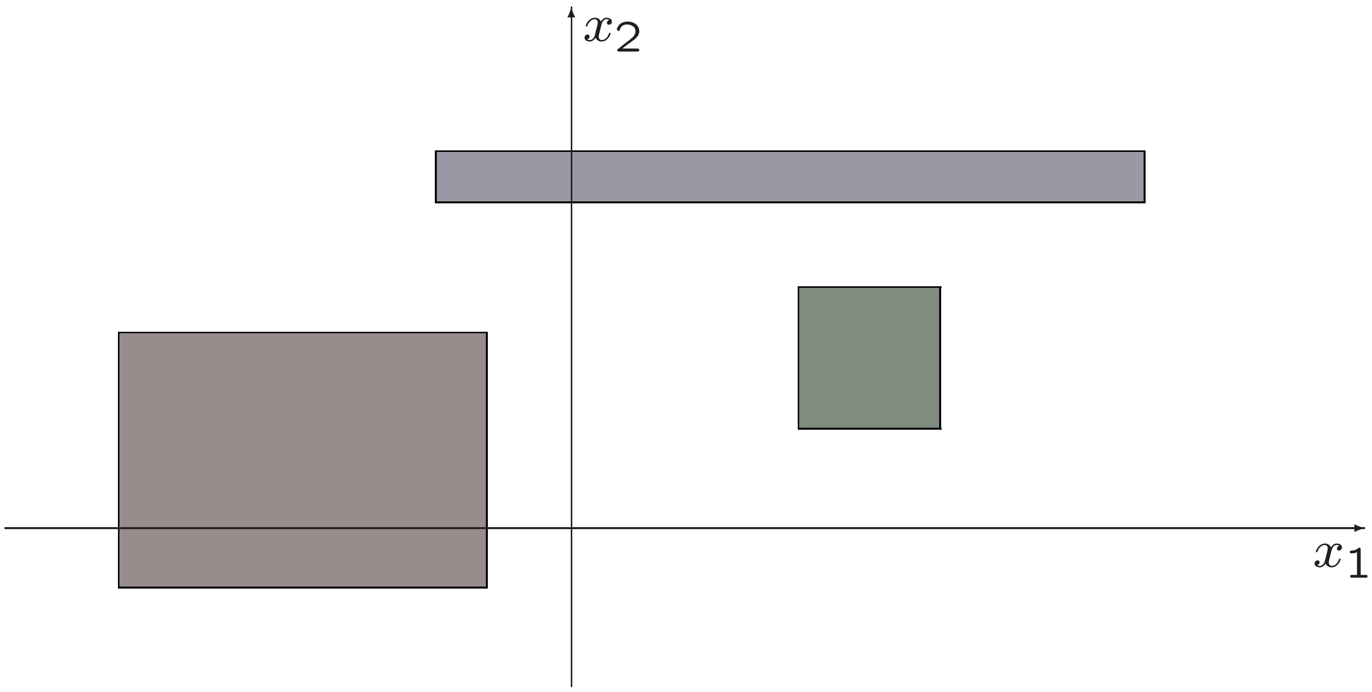
# Global optimization problem is NP-hard

Kreinovich-Kearfott theorem

Beyond the class of convex objective functions, the global optimization problem is NP-hard.

V. Kreinovich and R.B. Kearfott
Beyond convex? Global optimization is feasible only for convex objective functions: a theorem // *Journal of Global Optimization.* – 2005. – Vol. 33. – P. 617–624.

# Interval technique

# Classical interval arithmetic $\mathbb{IR}$

is formed by intervals $\boldsymbol{x} = [\underline{\boldsymbol{x}}, \overline{\boldsymbol{x}}] \subset \mathbb{R}$, so that

$$\boldsymbol{x} \star \boldsymbol{y} = \left\{ x \star y \mid x \in \boldsymbol{x}, y \in \boldsymbol{y} \right\} \qquad \text{for} \quad \star \in \{+, -, \cdot, /\}$$

$$\boldsymbol{x} + \boldsymbol{y} = \left[\underline{\boldsymbol{x}} + \underline{\boldsymbol{y}},\ \overline{\boldsymbol{x}} + \overline{\boldsymbol{y}}\right]$$

$$\boldsymbol{x} - \boldsymbol{y} = \left[\underline{\boldsymbol{x}} - \overline{\boldsymbol{y}},\ \overline{\boldsymbol{x}} - \underline{\boldsymbol{y}}\right]$$

$$\boldsymbol{x} \cdot \boldsymbol{y} = \left[\min\{\underline{\boldsymbol{x}}\,\underline{\boldsymbol{y}}, \underline{\boldsymbol{x}}\,\overline{\boldsymbol{y}}, \overline{\boldsymbol{x}}\,\underline{\boldsymbol{y}}, \overline{\boldsymbol{x}}\,\overline{\boldsymbol{y}}\},\ \max\{\underline{\boldsymbol{x}}\,\underline{\boldsymbol{y}}, \underline{\boldsymbol{x}}\,\overline{\boldsymbol{y}}, \overline{\boldsymbol{x}}\,\underline{\boldsymbol{y}}, \overline{\boldsymbol{x}}\,\overline{\boldsymbol{y}}\}\right]$$

$$\boldsymbol{x} / \boldsymbol{y} = \boldsymbol{x} \cdot \left[1/\overline{\boldsymbol{y}},\ 1/\underline{\boldsymbol{y}}\right] \qquad \text{for} \quad \boldsymbol{y} \not\ni 0$$

# Interval extension of functions

**Definition**

Interval function $\boldsymbol{f} : \mathbb{IR}^n \to \mathbb{IR}^m$ is called *interval extension* of the real-valued function $f : \mathbb{R}^n \to \mathbb{R}^m$, if

1) $\boldsymbol{f}(x) = f(x)$ for $x \in \mathbb{R}^n$,

2) $\boldsymbol{f}(\boldsymbol{x})$ is inclusion monotonic.

$\Longrightarrow$ outer estimate of the range of values

$$\boldsymbol{f}(\boldsymbol{x}) \;\supseteq\; \{\, f(x) \mid x \in \boldsymbol{x} \,\}$$

# Natural interval extension

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a rational function of the arguments $(x_1, x_2, \ldots, x_n) = x$.

If, for a box $\boldsymbol{x} = (\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n)$, defined is the result $\boldsymbol{f}_\natural(\boldsymbol{x})$ of substituting the intervals $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n$ instead of the arguments of the function $f(x)$ and executing all the operations with them according to the interval arithmetic instructions, then

$$\{ f(x) \mid x \in \boldsymbol{x} \} \;\subseteq\; \boldsymbol{f}_\natural(\boldsymbol{x}),$$

i.e. $\boldsymbol{f}_\natural(\boldsymbol{x})$ contains the range of values of $f(x)$ over $\boldsymbol{x}$.

# Centered form of interval extension

$$\boldsymbol{f}_c(\boldsymbol{x}, \tilde{x}) \;=\; f(\tilde{x}) + \sum_{i=1}^{n} \boldsymbol{g}_i(\boldsymbol{x}, \tilde{x})(\,\boldsymbol{x}_i - \tilde{x}_i),$$

where $\tilde{x} = (\,\tilde{x}_1, \tilde{x}_2, \ldots, \tilde{x}_n)$ is a fixed “center”,

$\boldsymbol{g}_i(\boldsymbol{x}, \tilde{x})$ are intervals depending on $\tilde{x}$ и $\boldsymbol{x}$.

$\boldsymbol{g}_i(\boldsymbol{x}, \tilde{x})$ can be interval enclosures for $\dfrac{\partial f(x)}{\partial x_i}$ over $\boldsymbol{x}$

or interval slopes for $f$ over $\boldsymbol{x}$

G. Alefeld, J. Herzberger, *Introduction to Interval Computations.* – New York: Academic Press, 1983.

R.E. Moore, R.B. Kearfott, M. Cloud, *Introduction to Interval Analysis.* – Philadelphia: SIAM, 2009.

A. Neumaier, *Interval methods for systems of equations.* – Cambridge: Cambridge University Press, 1990.

R.B. Kearfott, *Rigorous Global Search: Continuous Problems.* – Dordrecht: Kluwer, 1996.

Hansen E., Walster G.W. *Global Optimization Using Interval Analysis.* – New York: Marcel Dekker, 2004.

# Accuracy of interval evaluation

crucially depends on the width of the box over which we evaluate

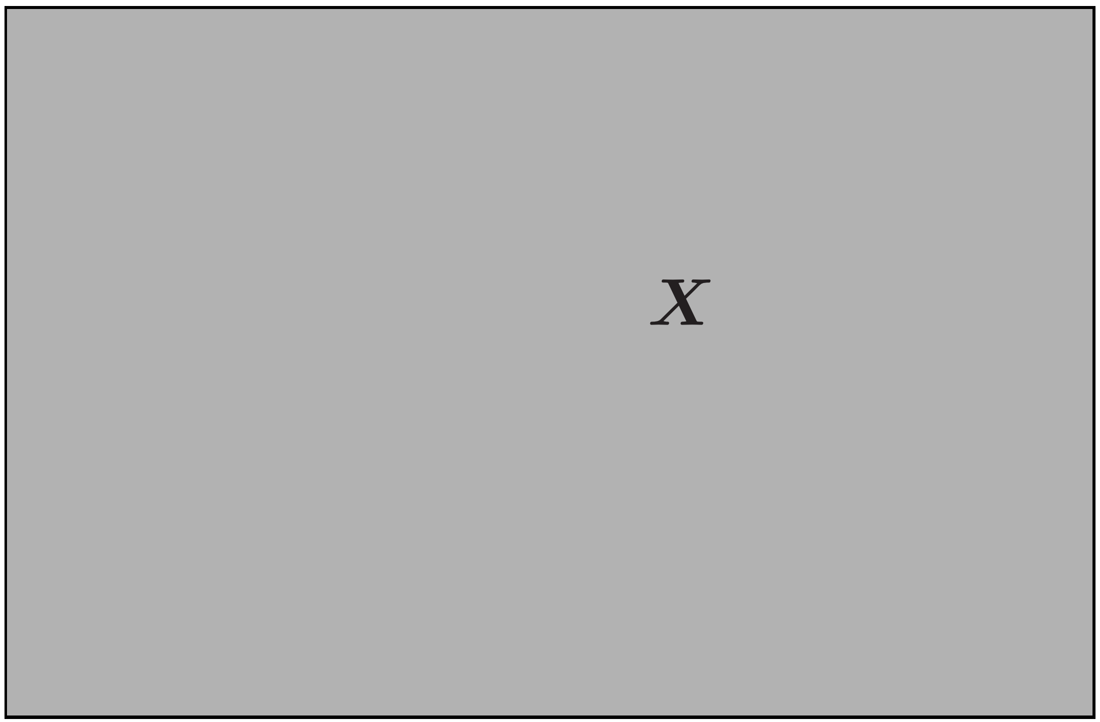
For natural interval extension,

$$\text{dist}\left(\, \boldsymbol{f}_{\natural}(\boldsymbol{x}, \tilde{x}), f(\boldsymbol{x})\,\right) \;\leq\; C\,\|\text{wid}\,\boldsymbol{x}\|$$

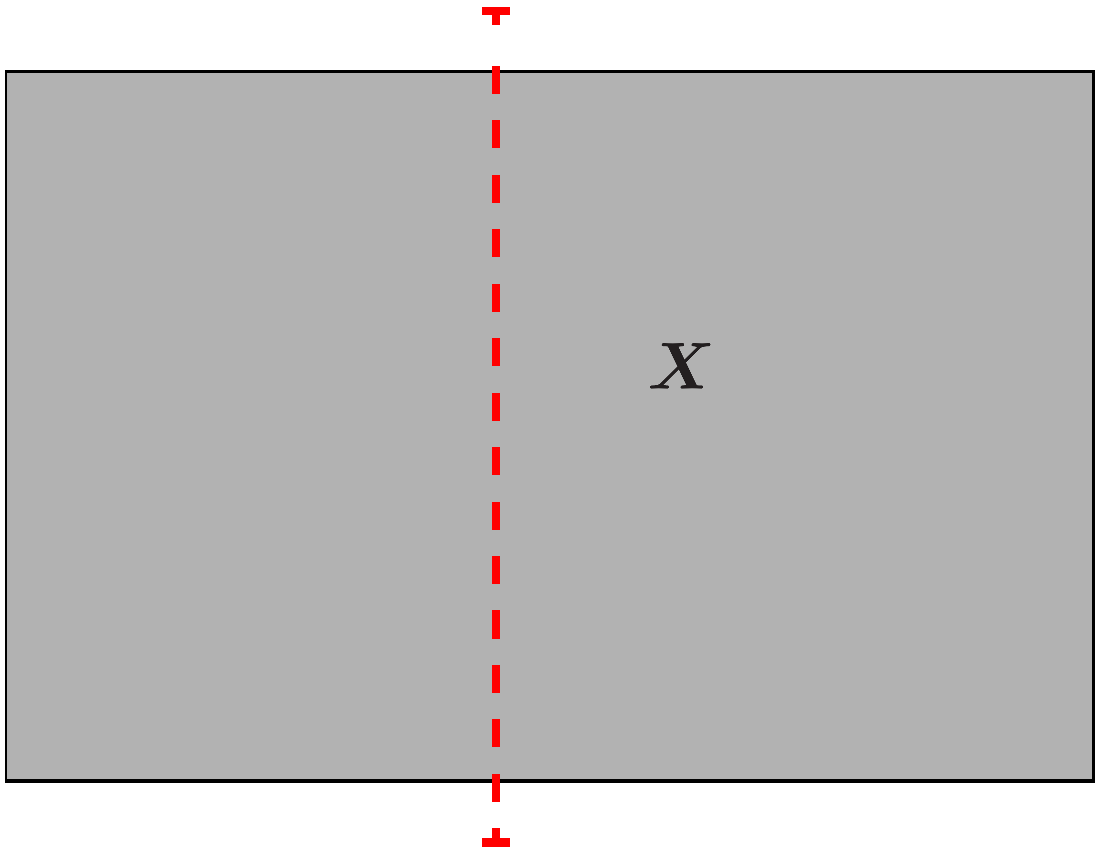
For centered forms,

$$\text{dist}\left(\, \boldsymbol{f}_{c}(\boldsymbol{x}, \tilde{x}), f(\boldsymbol{x})\,\right) \;\leq\; 2\,(\text{wid}\,\boldsymbol{g}(\boldsymbol{x}, \tilde{x}))^{\top}|\,\boldsymbol{x} - \tilde{x}\,|$$

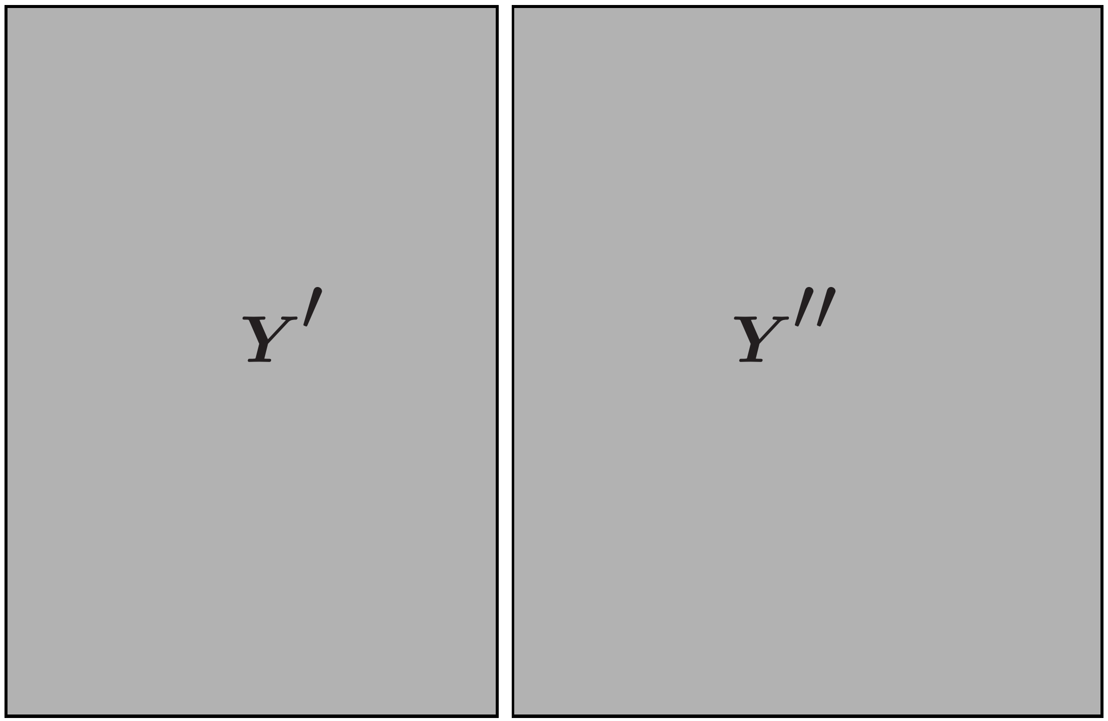
# Enforced subdivision



# Enforced subdivision

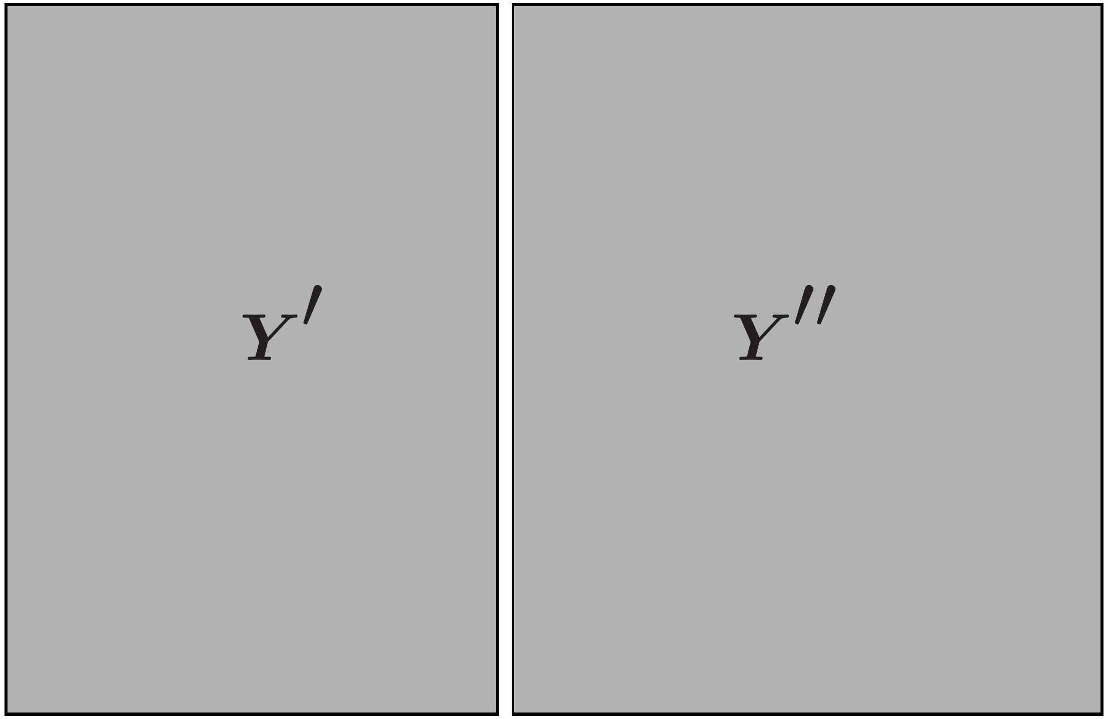


# Enforced subdivision



# Enforced subdivision

a new estimate of the minimum is min$\{ \underline{\boldsymbol{F}(\boldsymbol{Y}')}, \underline{\boldsymbol{F}(\boldsymbol{Y}'')} \}$



# “Branch-and-bound” strategy

- ♢ organize a list of the boxes $\boldsymbol{Y}$ emerging in the subdivision of the initial box $\boldsymbol{X}$, jointly with their estimates $\underline{\boldsymbol{F}(\boldsymbol{Y})}$;

- ♢ bisect only the box $\boldsymbol{Y}$ that provides the smallest estimate $\underline{\boldsymbol{F}(\boldsymbol{Y})}$ for $\min\limits_{x \in \boldsymbol{X}} F(x)$;

- ♢ the subdivided box is bisected along the widest interval component.

# Technical details

To keep and process all the subdomains, a *working list* $\mathcal{L}$ is maintained that consists of the records

$$\big(\ \boldsymbol{Y}\ ,\ \underline{\boldsymbol{F}(\boldsymbol{Y})}\ \big),$$

where $\boldsymbol{Y}$ is an interval $n$-box, $\boldsymbol{Y} \subseteq \boldsymbol{X}$.

The records in $\mathcal{L}$ are usually ordered so as the estimates $\underline{\boldsymbol{F}(\boldsymbol{Y})}$ increase.

The first record of the list, the corresponding box $\boldsymbol{Y}$ and the estimate $\underline{\boldsymbol{F}(\boldsymbol{Y})}$ are called *leading* at the current step.

# The simplest interval global optimization algorithm

## Input

Interval extension $\boldsymbol{F} : \mathbb{I}\boldsymbol{X} \to \mathbb{IR}$ of the objective function $F$.

A prescribed accuracy $\epsilon > 0$.

## Output

An estimate for the global minimum $F^*$ for the function $F$ over $\boldsymbol{X}$.

## Algorithm

$\boldsymbol{Y} \leftarrow \boldsymbol{X}$ ;

compute $\boldsymbol{F}(\boldsymbol{Y})$ and initialize the list $\mathcal{L} := \left\{ (\boldsymbol{Y}, \underline{\boldsymbol{F}(\boldsymbol{Y})}) \right\}$;

**DO WHILE** $\Big($ wid $(\boldsymbol{F}(\boldsymbol{Y})) \geq \epsilon$ $\Big)$

choose the component $l$ along which the box $\boldsymbol{Y}$ has
the largest width, i. e. wid $\boldsymbol{Y}_l = \max_i$ wid $\boldsymbol{Y}_i$ ;

bisect the $l$-th component in $\boldsymbol{Y}$ to produce the subboxes $\boldsymbol{Y}'$ и $\boldsymbol{Y}''$ ;

compute $\boldsymbol{F}(\boldsymbol{Y}')$ and $\boldsymbol{F}(\boldsymbol{Y}'')$ ;

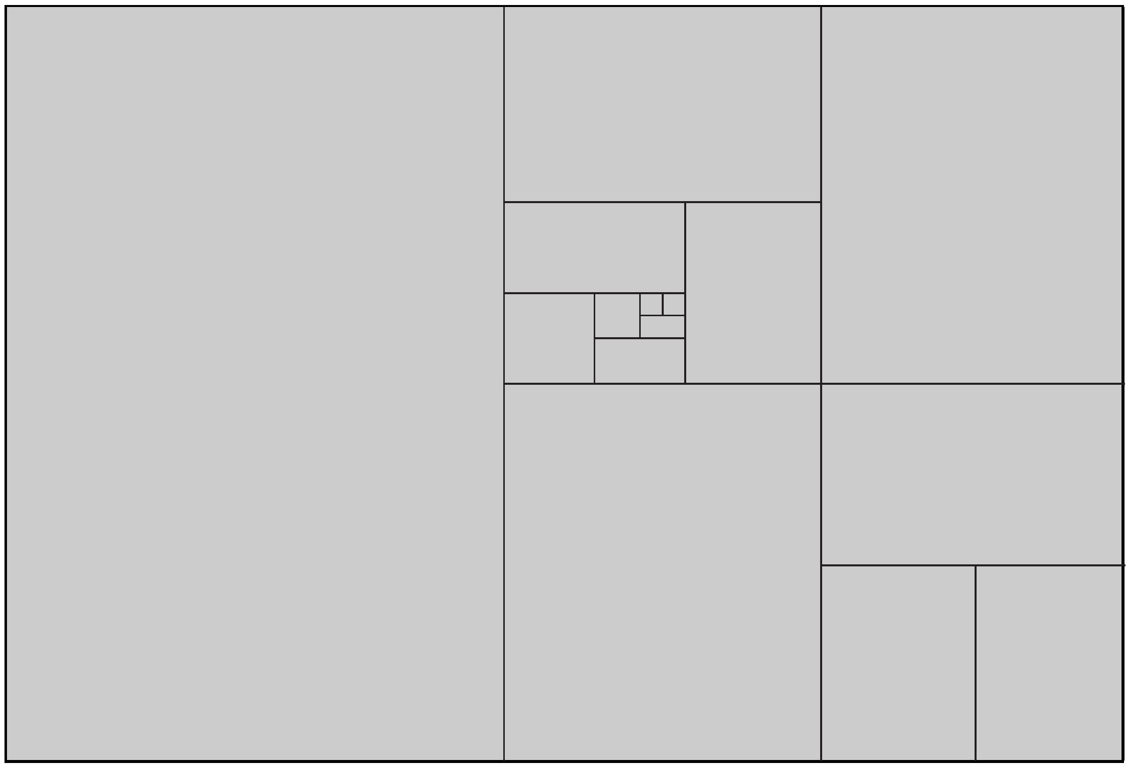
delete the record $(\boldsymbol{Y}, \underline{\boldsymbol{F}(\boldsymbol{Y})})$ from the list $\mathcal{L}$ ;

put the records $(\boldsymbol{Y}', \underline{\boldsymbol{F}(\boldsymbol{Y}')})$ and $(\boldsymbol{Y}'', \underline{\boldsymbol{F}(\boldsymbol{Y}'')})$ into the list $\mathcal{L}$
so that the second fields of the records from $\mathcal{L}$ icrease ;

denote the leading record of $\mathcal{L}$ as $(\boldsymbol{Y}, \underline{\boldsymbol{F}(\boldsymbol{Y})})$ ;

**END DO**

$F^* \leftarrow \underline{\boldsymbol{F}(\boldsymbol{Y})}$ ;



— domain configuration

resulted from the work of the algorithm

# Modifications

- Monotonicity of the objective function
- More accurate interval evaluation.
- Local optimization procedures.
- Upper bound of the global minimum.
- ... ...

Works well

for problems of the small

and moderate dimension. . .

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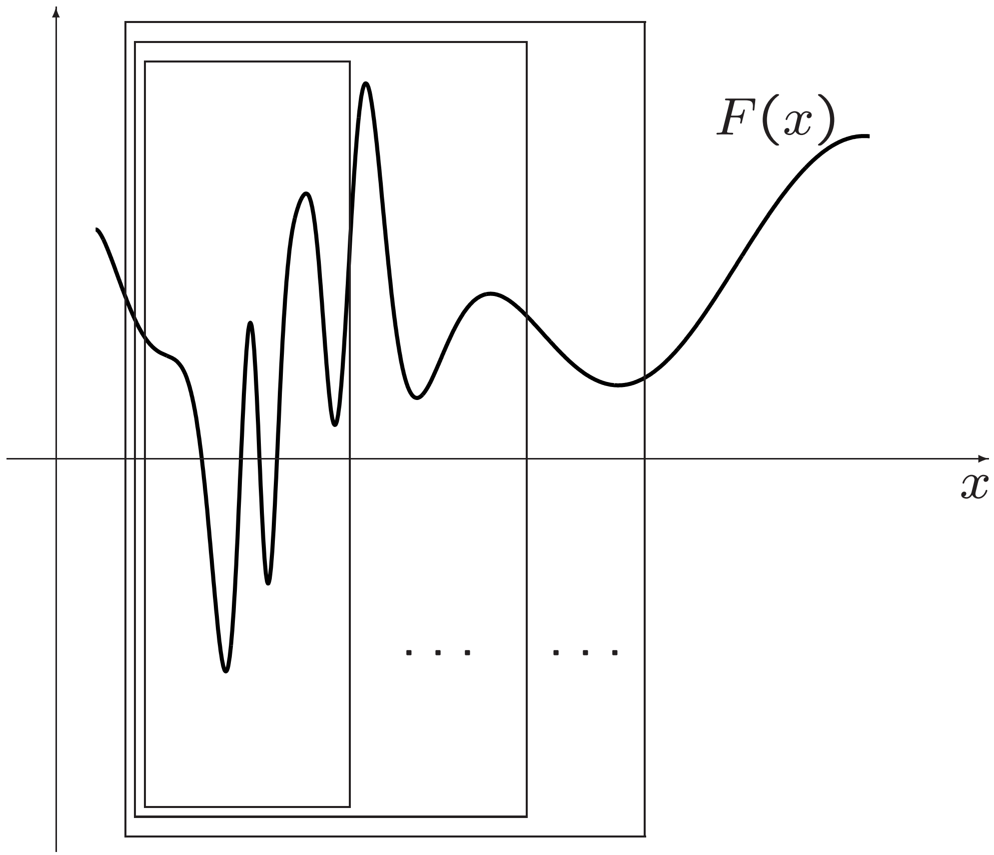
and moderate dimension . . .

And what for large dimensions?

# “Stagnation” of interval evaluation




— considerable decrease in the width of the box
results in a small increase of the enclosure sharpness

The deterministic “branch-and-bound”

turns out to be irrelevant . . .

The deterministic “branch-and-bound”

turns out to be irrelevant . . .

Randomization? . . .

# Randomization

= introducing

random transitions

of the control

into an algorithm

# “Simulated annealing”

choose a starting approximation $y = x_0 \in \boldsymbol{X}$ ;

set the starting “temperature” $T = T_0 > 0$ ;

set $N_T$, the number of trials per one temperature level ;

**DO WHILE** $( T > T_{fin} )$

**DO FOR** $k = 1$ **TO** $N_T$

randomly choose a new point $z \in \boldsymbol{X}$ according to the rule $\mathcal{S}(y)$ ;

accept $z$, i. e. $y \leftarrow z$, with probability $\mathrm{P}_T(y, z)$ ;

**END DO**

decrease the temperature $T \leftarrow \alpha T$ ;

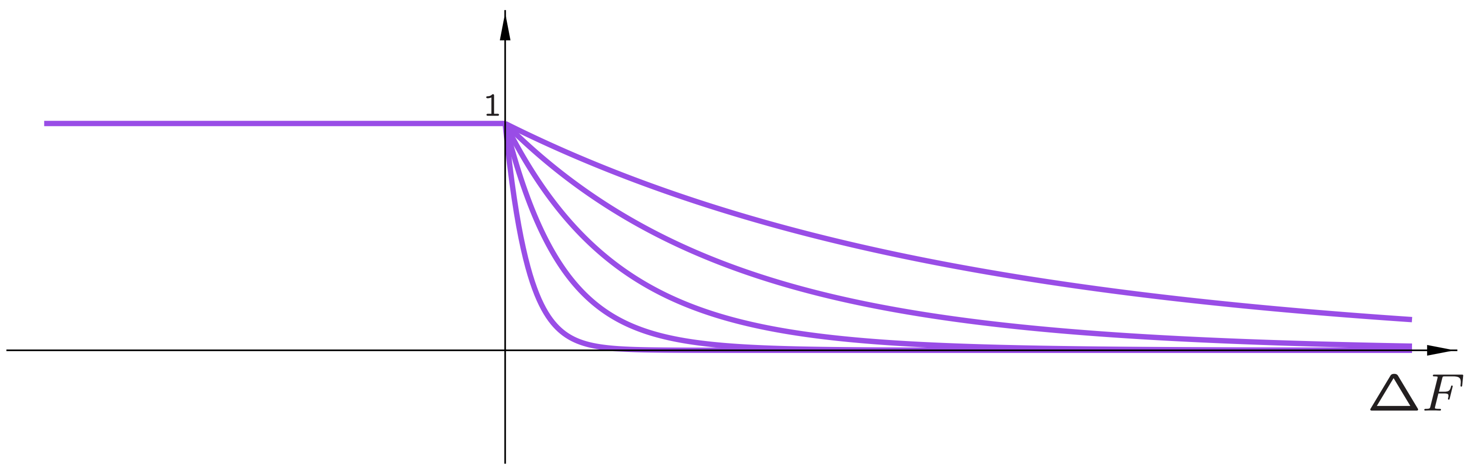
**END DO**

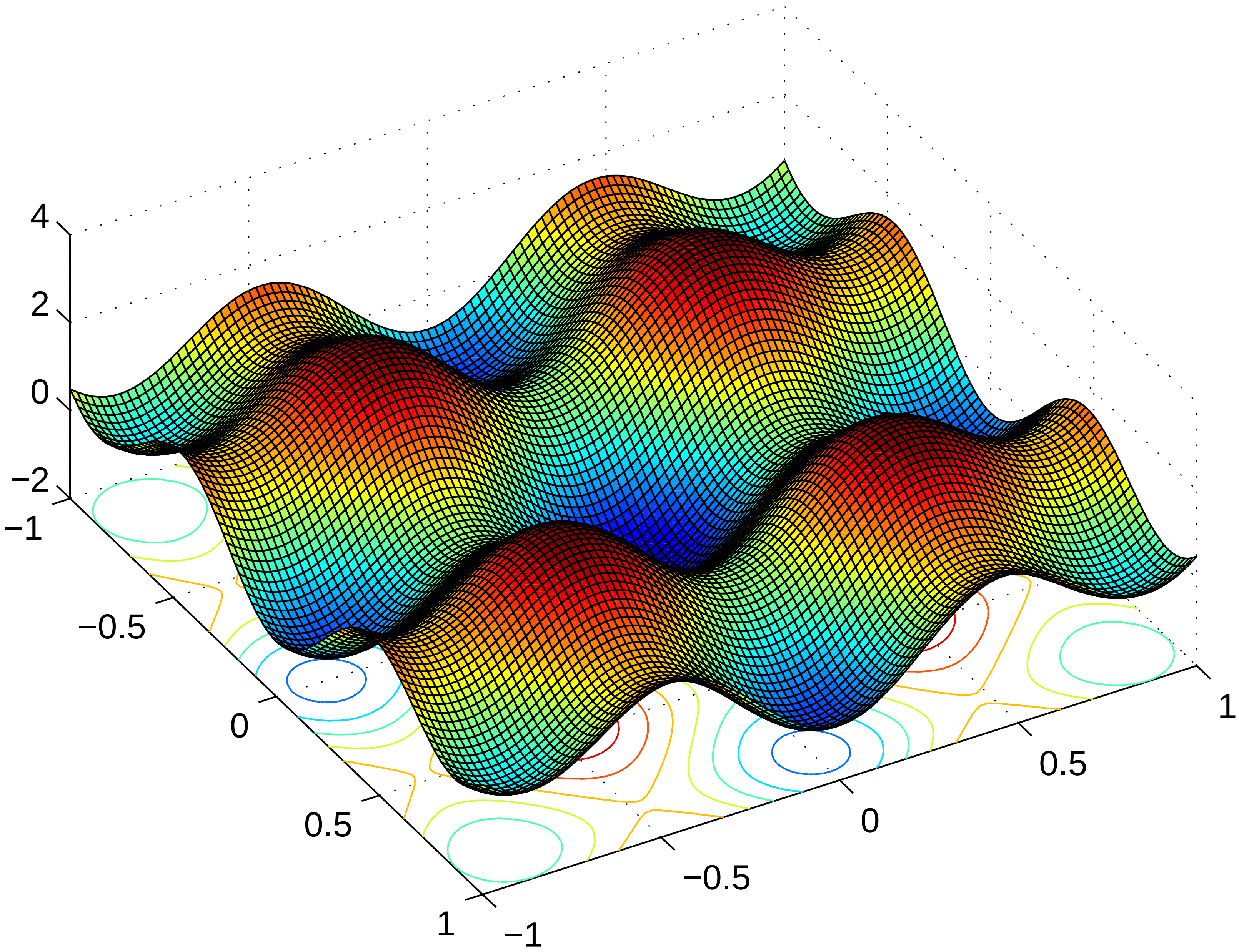
# Probability of accepting the new estimate $x'$

$$\mathsf{P}_T(y,z) \;=\; \begin{cases} 1, & \text{if} \quad \Delta F \le 0, \\ \exp\left(-\dfrac{\Delta F}{kT}\right), & \text{if} \quad \Delta F \ge 0, \end{cases}$$

where

$$\Delta F \;:=\; F(z) - F(y)$$

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# Interval simulated annealing

Input

Interval extension $\boldsymbol{F} : \mathbb{IX} \to \mathbb{IR}$ of the objective function $F$.

A prescribed accuracy $\epsilon > 0$.

Output

An estimate of the global minimum $F^*$ over $\boldsymbol{X}$ from below.

Algorithm

$\boldsymbol{Y} \leftarrow \boldsymbol{X}$ ;

set a starting "temperature" $T = T_0 > 0$ ;

set $N_T$, the number of trials per one temperature level ;

compute $\boldsymbol{F}(\boldsymbol{Y})$ and initialize the list $\mathcal{L} := \{ (\boldsymbol{Y}, \underline{\boldsymbol{F}(\boldsymbol{Y})}) \}$;

**DO WHILE** $\Big($ wid $(\boldsymbol{F}(\boldsymbol{Y})) \geq \epsilon$ $\Big)$

  **DO FOR** $k = 1$ **TO** $N_T$

    randomly choose, from the list $\mathcal{L}$, a record $(\boldsymbol{Z}, \underline{\boldsymbol{F}(\boldsymbol{Z})})$

      according to the rule $\mathcal{S}(\boldsymbol{Y})$ ;

    **DO** $\Big($ with probability $\mathsf{P}_T(\boldsymbol{Y}, \boldsymbol{Z})$ $\Big)$

      bisect $\boldsymbol{Z}$ along the widest component

        to produce the boxes $\boldsymbol{Z}'$ and $\boldsymbol{Z}''$ ;

      compute $\boldsymbol{F}(\boldsymbol{Z}')$ and $\boldsymbol{F}(\boldsymbol{Z}'')$ ;

      delete the record $(\boldsymbol{Z}, \underline{\boldsymbol{F}(\boldsymbol{Z})})$ from the list $\mathcal{L}$ ;

      put the records $(\boldsymbol{Z}', \underline{\boldsymbol{F}(\boldsymbol{Z}')})$ and $(\boldsymbol{Z}'', \underline{\boldsymbol{F}(\boldsymbol{Z}'')})$ into $\mathcal{L}$

        in increasing order of the second field ;

    **END DO**

    denote the leading record of the list $\mathcal{L}$ as $(\boldsymbol{Y}, \underline{\boldsymbol{F}(\boldsymbol{Y})})$ ;

  **END DO**

  decrease the temperature value $T \leftarrow \alpha T$ ;

**END DO**

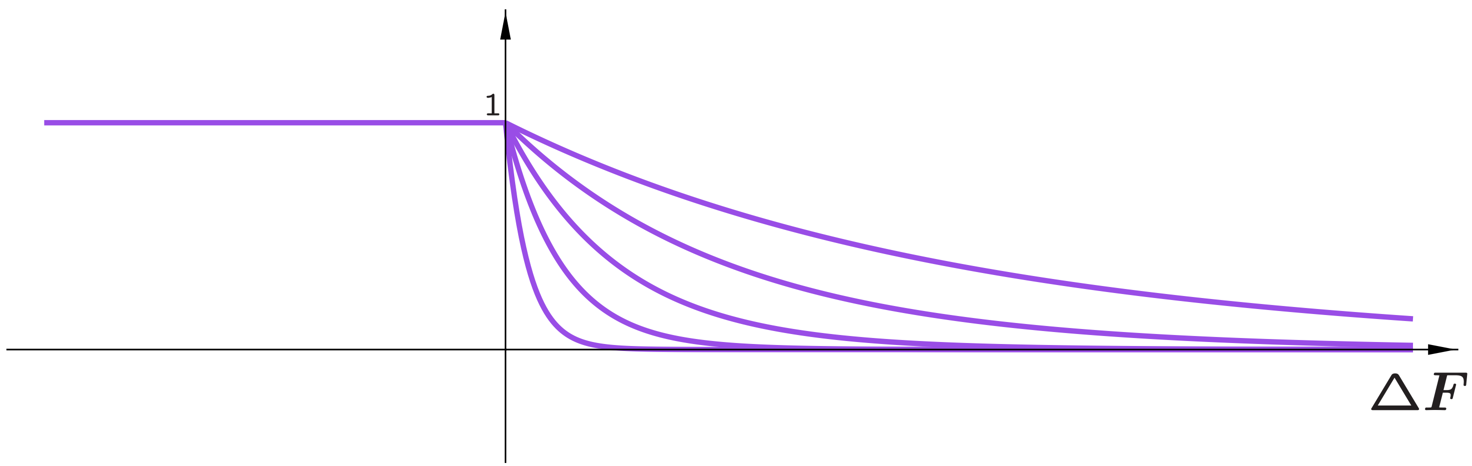
$F^* \leftarrow \underline{\boldsymbol{F}(\boldsymbol{Y})}$ ;

# Subdivision probability for the box $Z$

$$\mathsf{P}_T(\boldsymbol{Y},\boldsymbol{Z}) \;=\; \begin{cases} 1, & \text{for} \quad \Delta\boldsymbol{F} \le 0, \\ \exp\left(-\dfrac{\Delta\boldsymbol{F}}{kT}\right), & \text{for} \quad \Delta\boldsymbol{F} \ge 0, \end{cases}$$

where

$$\Delta\boldsymbol{F} \;:=\; \underline{\boldsymbol{F}(\boldsymbol{Z})} - \underline{\boldsymbol{F}(\boldsymbol{Y})}$$



# Interval simulated annealing

S.P. Shary
Randomized algorithms in interval global optimization
*Numerical Analysis and Applications*, Vol. 1 (2008),
No. 4, pp. 376–389.

# Interval genetic algorithm ?

# Interval genetic algorithm

N.V. Panov
Joining stochastic and interval approaches for the solution of problems of global optimization of functions
*Computational Technologies*, 2009, vol. 14, No. 5, pp. 49–65.

N.V. Panov, S.P. Shary
Interval evolutionary algorithm for searching global optimum
*Proceedings of Altai State University*, 2011, No. (69), vol. 2, pp. 108–113.

*in Russian for the time being*

# Summary

1) Global optimization is a fruitful applications area
of the interval methods

2) "Interval simulated annealing" is a new global optimization procedure in which randomization can be combined with verification of the results.

3) Next on this way are interval genetic algorithms, etc.

**Thanks for your attention!**