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# Robust optimization : formulation, kriging and evolutionary approaches

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Rodolphe Le Riche. Robust optimization : formulation, kriging and evolutionary approaches. Doctoral. France. 2014. cel-01081293

**HAL Id: cel-01081293**

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Submitted on 7 Nov 2014

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# **Robust optimization : formulation, kriging and evolutionary approaches**

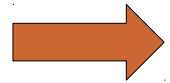
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CNRS and Ecole des Mines de Saint-Etienne

class given as part of the “Modeling and Numerical Methods for  
Uncertainty Quantification” French-German summer school, Porquerolles,  
Sept. 2014

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# Outline of the talk

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1. Motivations for robust optimization
2. Formulations of optimization problems with uncertainties
3. Kriging-based approaches (costly functions)
4. Evolutionary approaches (non costly functions)

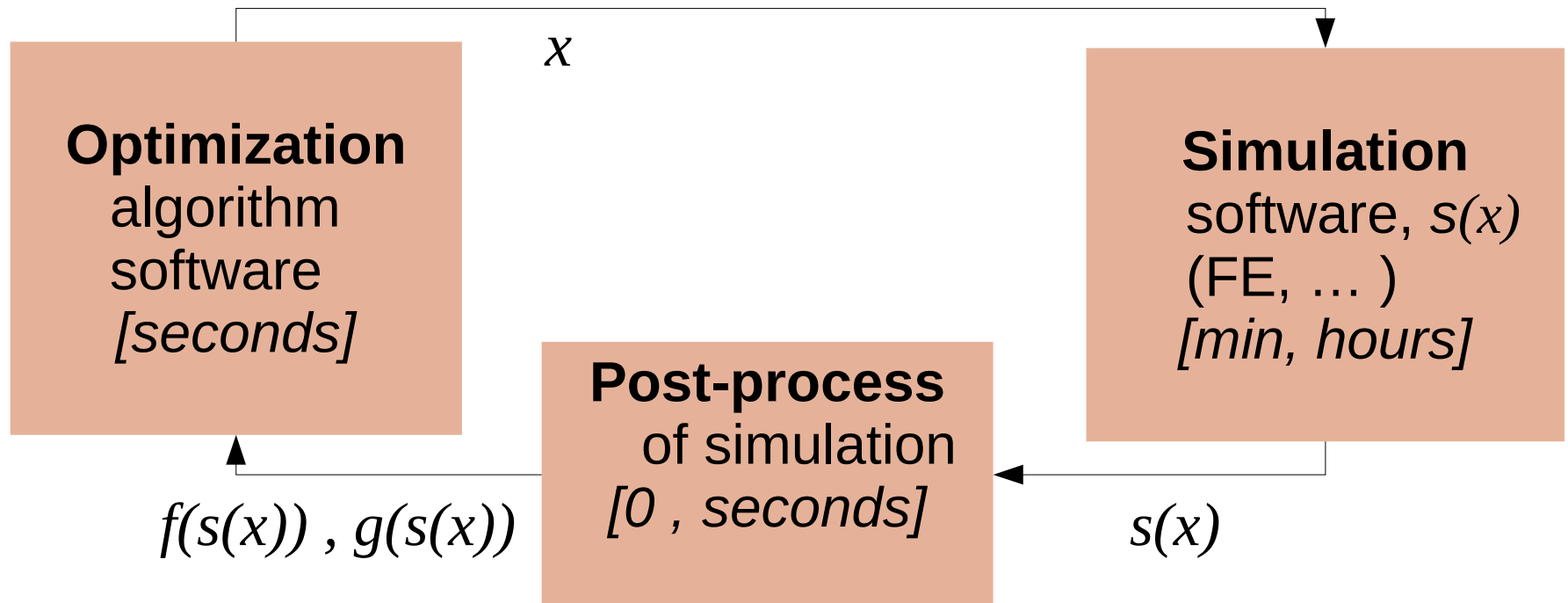
# Why do we optimize ?

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Optimization as a mathematical formulation for decision

$$\begin{aligned} \min_{x \in S} f(x) \\ g(x) \leq 0 \end{aligned}$$

followed by a numerical, approximate, resolution,



Communication between programs by file, pipe, messages, ...

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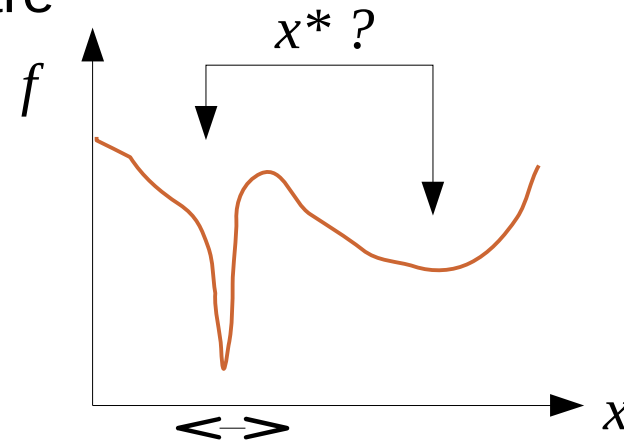
# Motivations for robust optimization

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What is the point – in practice – for deterministically solving an optimization problem when there are

- unstable optima
- aleatory model (  $s$  ) parameters
- model uncertainties
- dynamically changing model conditions (complex systems)

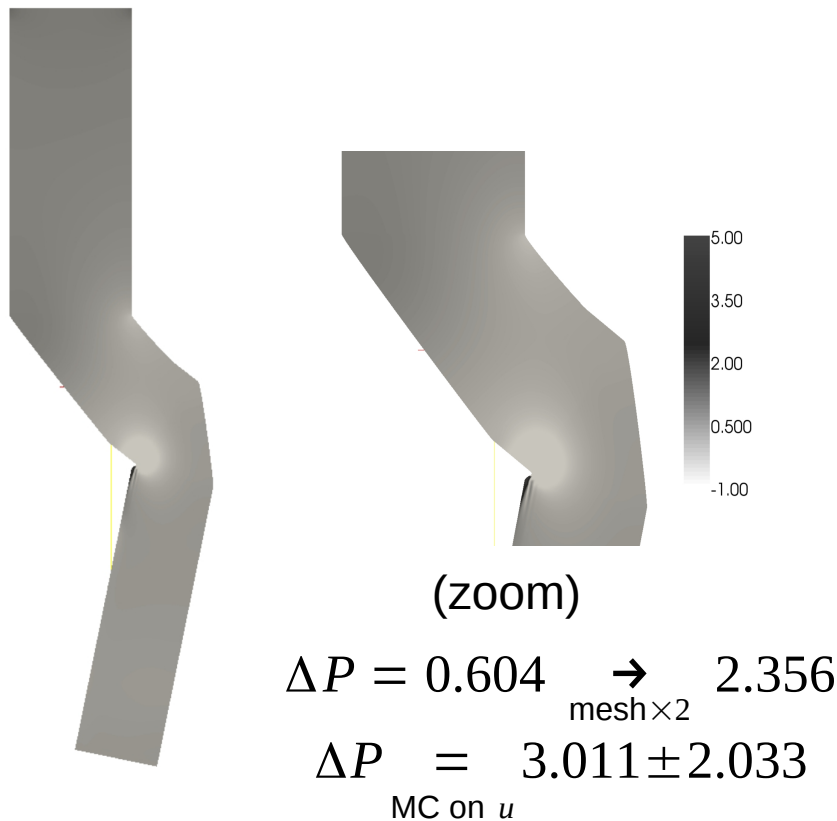
???



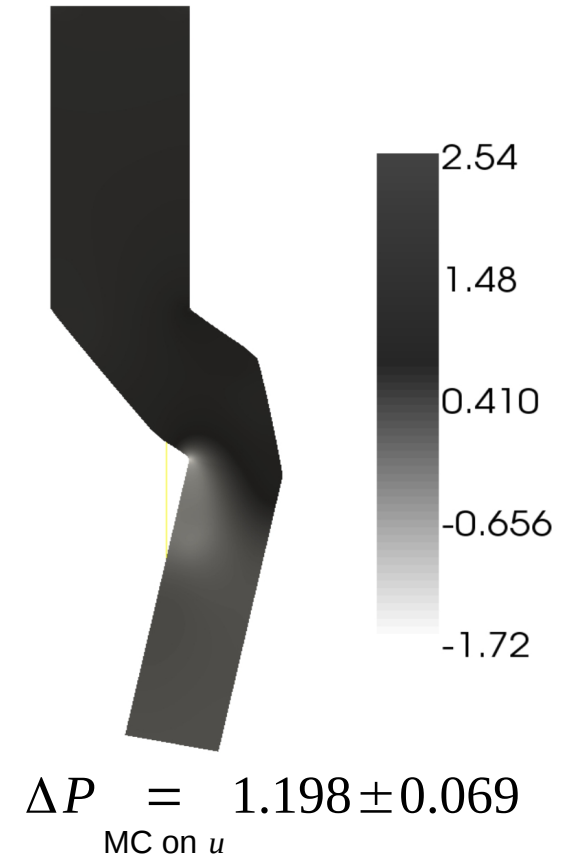
# Unstable deterministic optimum. Expl of an air duct.

Minimize pressure loss by changing the (parameterized) shape.

## deterministic design



## robust design

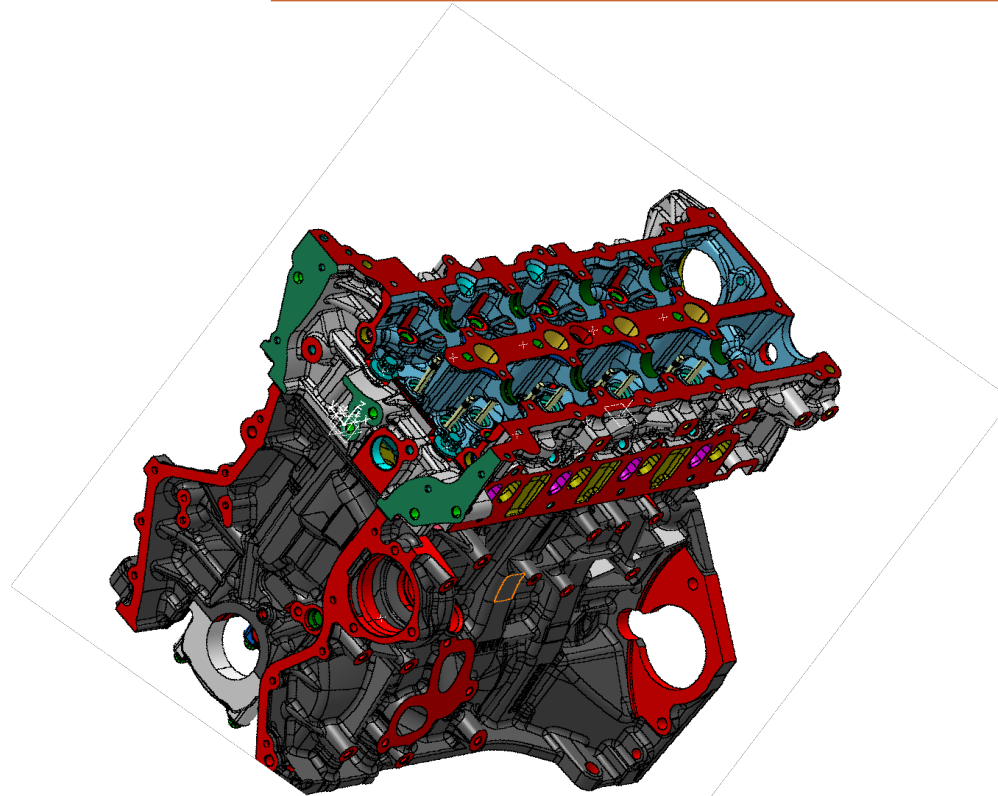


The optimization exploits meshing flaws.  
The result is not stable w.r.t. mesh or boundary conditions changes.

Cf. J. Janusevskis and R. Le Riche, *Robust optimization of a 2D air conditioning duct using kriging*, technical report hal-00566285, feb. 2011.

# Unstable deterministic optimum. Expl of a combustion engine.

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a +/- 1mm dispersion in the manufacturing of a car cylinder head can degrade its performance (g CO<sub>2</sub>/km) by -20% (worst case)

# Motivations for robust optimization

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What is the point – in practice – for deterministically solving an optimization problem when there are

- unstable optima
- aleatory model ( s ) parameters
- model uncertainties
- dynamically changing model conditions (complex systems)

???

→ **modify the problem statement, therefore also the optimization algorithms** → **robust optimization**



# Outline of the talk

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1. Motivations for robust optimization



2. Formulations of optimization problems with uncertainties

3. Kriging-based approaches (costly functions)

4. Evolutionary approaches (non costly functions)

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# Formulations of optimization problems under uncertainties

H.G. Beyer, B. Sendhoff, Robust Optimization – A comprehensive survey, Comput. Methods Appl. Mech. Engrg, 196, pp. 3190-3218, 2007.

G. Pujol, R. Le Riche, O. Roustant and X. Bay, *L'incertitude en conception: formalisation, estimation*, Chapter 3 of the book *Optimisation Multidisciplinaire en Mécaniques : réduction de modèles, robustesse, fiabilité, réalisations logicielles*, Hermes, 2009 (in French ;-( )

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## Formulation of optimization under uncertainty

# The double (x,U) parameterization

We introduce  $U$ , a vector of uncertain (random) parameters that affect the simulator  $s$ .

$x$  is a vector of deterministic optimization (controlled) variables.  $x$  in  $S$ , the search space.

(cf. Taguchi, 80's)

$s(x) \rightarrow s(x,U)$  , therefore  $f(x) \rightarrow f(s(x,U)) = f(x,U)$   
and  $g(x) \rightarrow g(s(x,U)) = g(x)$

$U$  used to describe

- noise (as in identification with measurement noise)
- model error (epistemic uncertainty)
- uncertainties on the values of some parameters of  $s$ .

# Formulation of optimization under uncertainty

## The $(x,U)$ parameterization is general

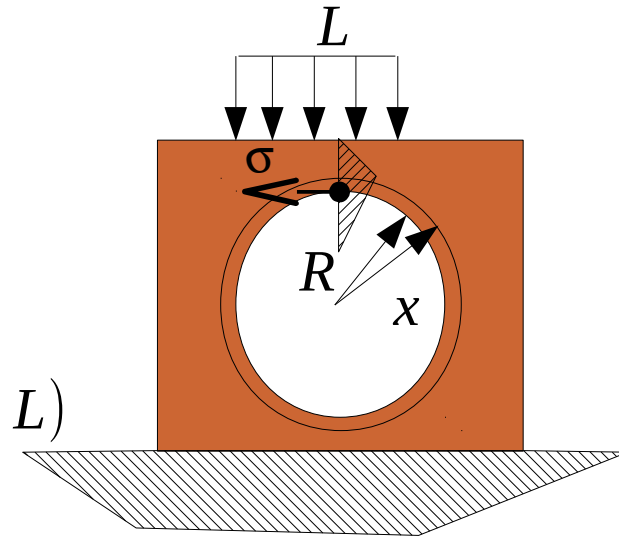
Three cases (which can be combined)

Expl :  $f(.) \equiv s(.) \equiv \sigma(R,L)$  (radial stress)

### 1. Noisy controlled variables

Expl : manufacturing tolerance,

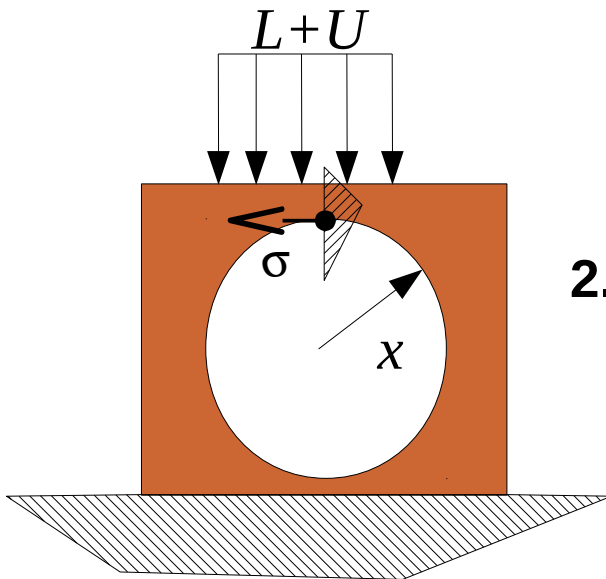
$$R \equiv x+U \quad , \quad f(x,U) \equiv \sigma(x+U,L)$$



### 2. Noise exogenous to the optimization variables

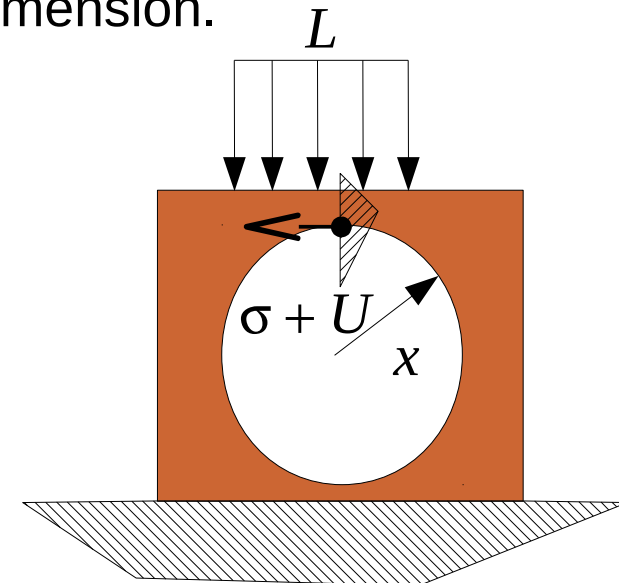
Expl : random load  $L+U$ ,  $x$  is a dimension.

$$f(x,U) \equiv \sigma(x,L+U)$$



### 3. Noise as an error model for the simulation

$$\text{Expl. : } f(x,U) \equiv \sigma(x,L)+U$$

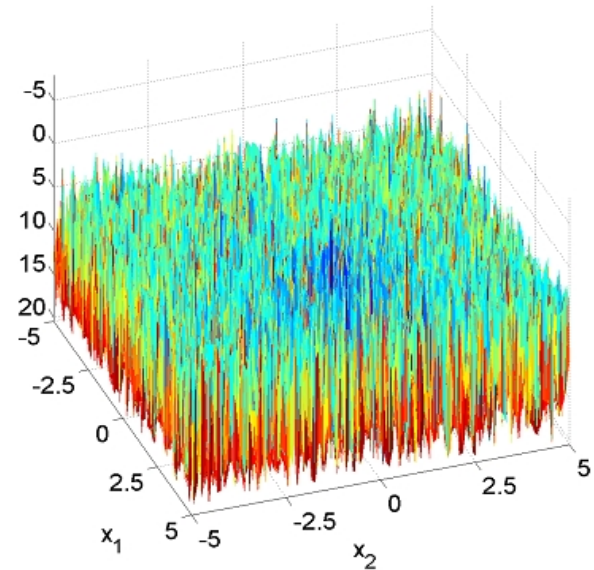


# Formulation of optimization under uncertainties (1) the noisy case

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Let's not do anything about the uncertainties, i.e., try to solve

$$\begin{aligned} \min_{x \in S \subset \mathbb{R}^d} \quad & f(x, U) \\ & g(x, U) \leq 0 \end{aligned}$$



It does not look good : gradients are not defined, what is the result of the optimization ?

But sometimes there is no other choice. Ex :  $y$  expensive with uncontrolled random numbers inside (like a Monte Carlo statistical estimation, numerical errors, measured input).

## Formulation of optimization under uncertainties (2) an ideal series formulation

---

Replace the noisy optimization criteria by statistical measures

$G(x)$  is the random event "all constraints are satisfied" ,

$$G(x) = \bigcap_i \{g_i(x, U) \leq 0\}$$

$$\begin{aligned} \min_{x \in S} q_\alpha^c(x) \quad & \text{(conditional quantile)} \\ \text{such that } P(G(x)) & \geq 1 - \varepsilon \end{aligned}$$

where the conditional quantile is defined by

$$P(f(x, U) \leq q_\alpha^c(x) \mid G(x)) = \alpha$$

## Formulation of optimization under uncertainties

### (3) simplified formulations often seen in practice

---

For bad reasons (joint probabilities ignored) or good ones (simpler numerical methods – Gaussian pdf – , lack of data, organization issues), quantiles are often replaced by averages and variances, conditioning is neglected, constraints are handled independently :

$$\min_{x \in S} q_\alpha(x) \quad \text{or} \quad \min_{x \in S} E(f(x, U)) \quad \text{and / or} \quad \min_{x \in S} V(f(x, U))$$

$$\text{or} \quad \min_{x \in S} E(f(x, U)) + r \sqrt{V(f(x, U))}$$

$$\text{where} \quad P(f(x, U) \leq q_\alpha(x)) = \alpha \quad \text{and} \quad r > 0$$

$$\text{such that} \quad P(G(x)) \geq 1 - \varepsilon \quad \text{or} \quad P(g_i(x) \leq 0) \geq 1 - \varepsilon_i$$

where  $\varepsilon$  is the series system risk  
and  $\varepsilon_i$  is the  $i$ th failure mode risk

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# Formulation of optimization under uncertainties

## Direct approaches (1/4)

---

In practice, statistical performance measures are estimated

$$\hat{f}(x) = \left\{ \widehat{E}_U(f(x, U)) \text{ or } \widehat{E}_U(f(x, U)) + r \sqrt{\widehat{V}_U(f(x, U))} \text{ or } \widehat{E}_U q_\alpha(x) \right\}$$

Crude Monte Carlo expl :

$$\hat{f}(x) = \widehat{E}_U(f(x, U)) = \frac{1}{MC} \sum_{i=1}^{MC} f(x, u^i), \quad u^i \text{ i.i.d. } \sim U$$

$$\hat{f}(x) = \widehat{E}_U q_\alpha(x) = [MC \times \alpha]\text{-th lowest among } f(x, u^1), \dots, f(x, u^{MC})$$

$\hat{g}(x) = \dots$  (cf. reliability estimation classes)

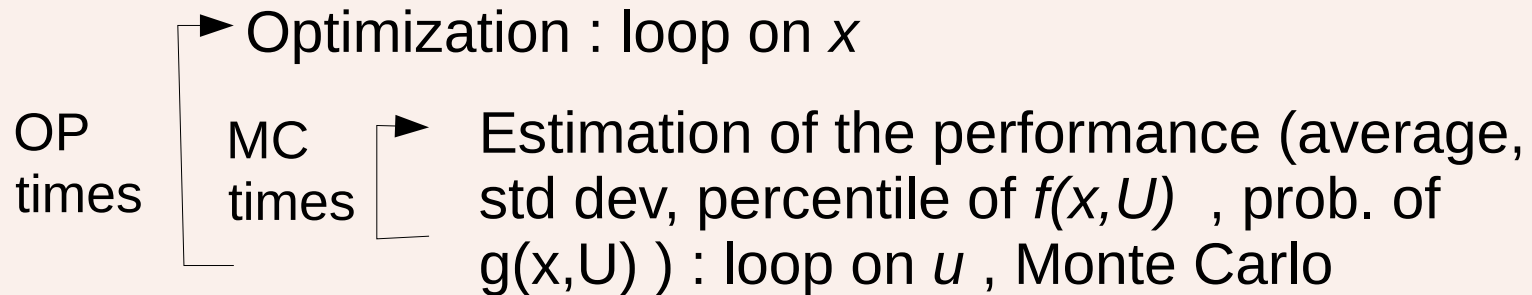


## Formulation of optimization under uncertainties

# Direct approaches (2/4)

---

Direct (naive) approaches to optimization with uncertainties have a **double loop** : propagate uncertainties on  $U$ , optimize on  $x$ .



Such a double loop is **very costly** : Total cost =  $OP \times MC$   
( calls to  $s$  )

# Formulation of optimization under uncertainties

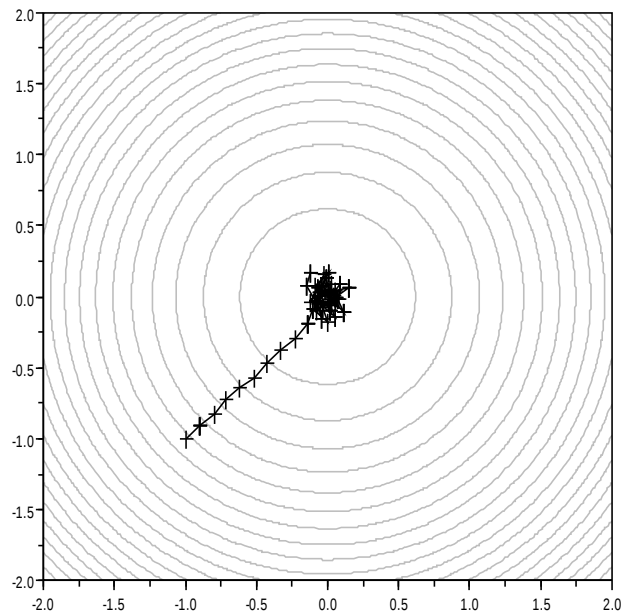
## Direct approaches (3/4)

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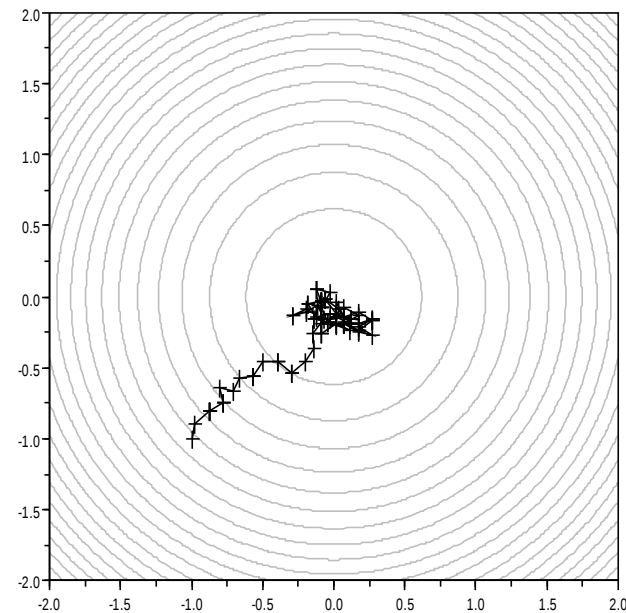
Most local (e.g., gradient based) optimizers will show poor convergence with noisy statistical estimators (e.g., crude Monte Carlo).

Ex : quasi-Newton method with finite differences

little noise



more noise



$$\hat{f}(x) = \frac{1}{100} \sum_{i=1}^{100} \|x + u_i\|^2$$

$$u_i \sim N(0, I_2)$$

$$\hat{f}(x) = \|x + u_i\|^2$$

# Formulation of optimization under uncertainties

## Direct approaches (4/4)

---

Avoid noisy statistical estimators with **common random numbers**

Expl :  $\hat{f}(x) = \frac{1}{MC} \sum_{i=1}^{MC} f(x, u^i)$  has same regularity as  $f$  for given  $u^i$ 's

see Bruno  
Tuffin's class on  
sampling (quasi  
Monte Carlo)

Sample  $\{u^1, \dots, u^{MC}\}$  according to  $U$

once for  
all before  
the loops

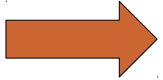
```
for i=1:OP
  optimizer(past x,  $\hat{f}(x)$ ) → new x
  for j=1:MC
     $\hat{f}(x) \leftarrow \hat{f}(x) + f(x, u^i)$ 
  end
   $\hat{f}(x) \leftarrow \hat{f}(x) / MC$ 
end
```

But,

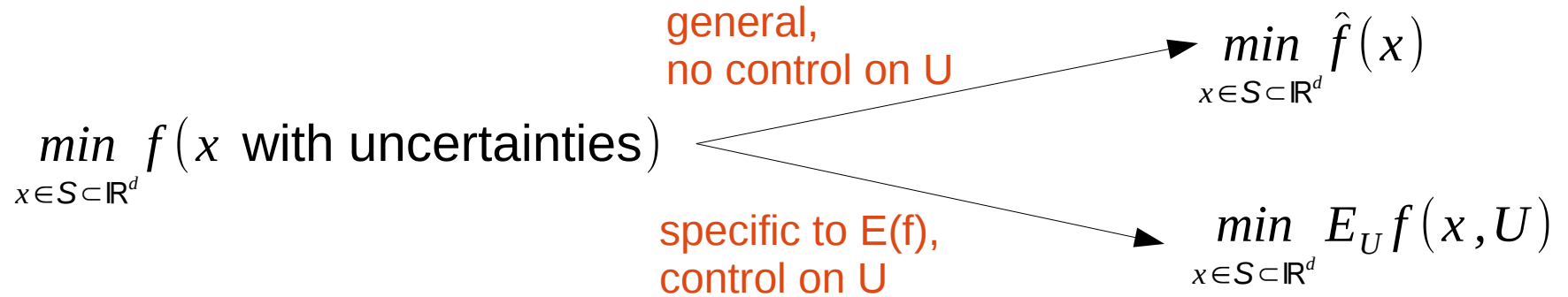
- does not solve the cost issue
- (less critically) the estimates  $\hat{f}(x^1), \dots, \hat{f}(x^{OP})$  depend on the choice of  $u^1, \dots, u^{MC}$

# Outline of the talk

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1. Motivations for robust optimization
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-  3. Kriging-based approaches (costly functions)
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## Unconstrained continuous optimization



[ Constraints,  $g(x) \leq 0$ , are not explicitly discussed in this talk. As a patch, you may assume that

$$\begin{array}{l}
 \min_{x \in S \subset \mathbb{R}^d} f(x) \\
 g(x) \leq 0
 \end{array}
 \rightarrow
 \min_{x \in S \subset \mathbb{R}^d} f(x) + p \times \max^2(0, g(x))$$

Constraints satisfaction problem : A. Chaudhuri, R. Le Riche and M. Meunier, *Estimating feasibility using multiple surrogates and ROC curves*, 54th AIAA SDM Conference, Boston, USA, 8-11 April 2013. ]

## Unconstrained continuous optimization **of costly functions**

~ 20 to 1000 calls possible,  $d = 1$  to 20

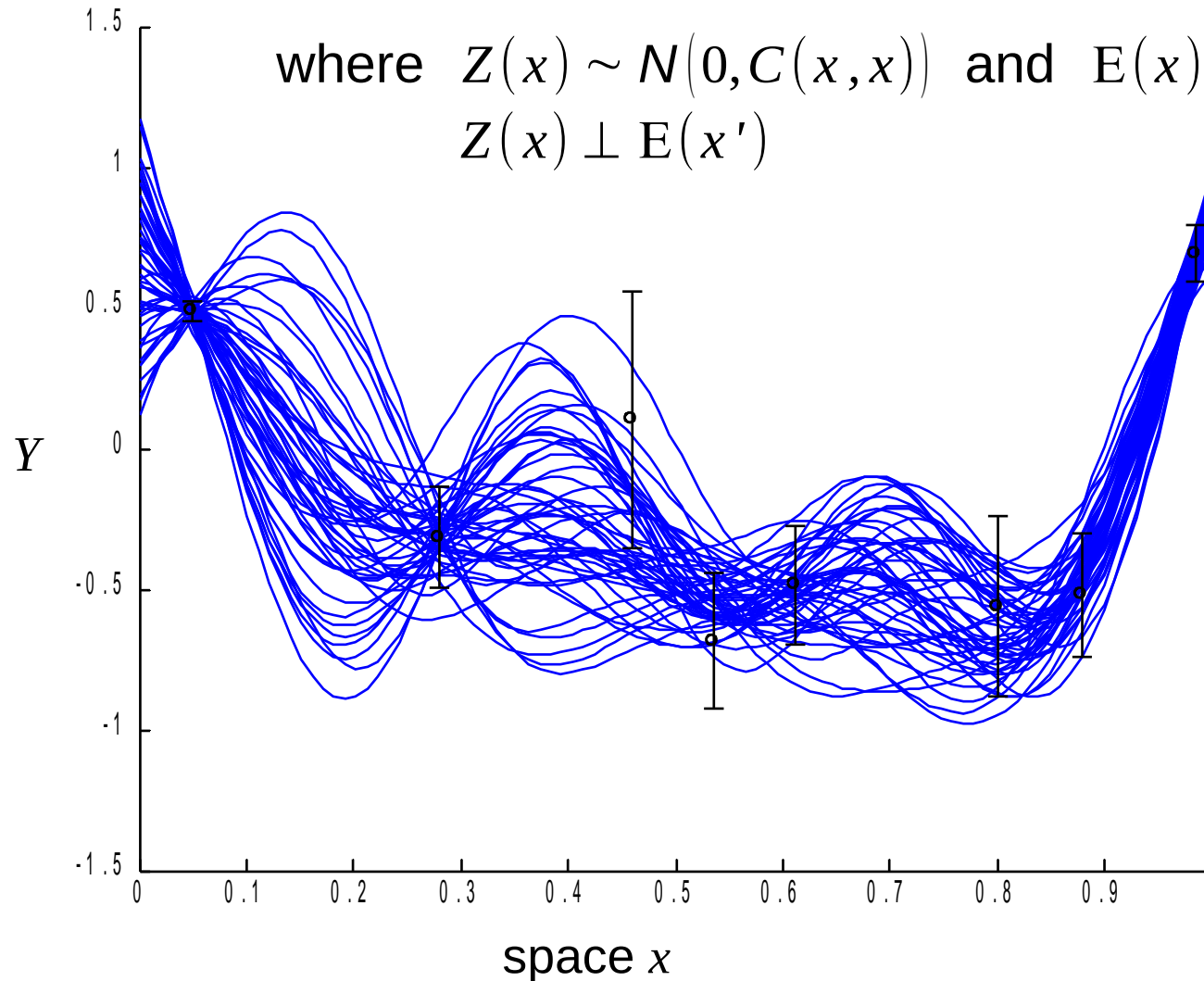
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# Kriging with noisy observations (1/5)

$$Y(x) = \mu(x) + Z(x) + E(x)$$

$\hat{f}(x)$   
here

where  $Z(x) \sim N(0, C(x, x))$  and  $E(x) \sim N(0, \tau_x^2)$   
 $Z(x) \perp E(x')$



kriging-based approaches

# Kriging with noisy observations (2/5)

---

Apply the conditioning result to the vector

$$\begin{bmatrix} Z(x^*) + \mu(x^*) \\ Y(x^1) \\ \vdots \\ Y(x^n) \end{bmatrix} = \begin{bmatrix} Z(x^*) + \mu(x^*) \\ \boldsymbol{\mu} + \mathbf{Z} + \mathbf{E} \end{bmatrix} \sim N \left( \begin{bmatrix} \mu(x^*) \\ \boldsymbol{\mu} \end{bmatrix}, \begin{bmatrix} \sigma^2 & C(x^*, \mathbf{X}) \\ C(x^*, \mathbf{X})^T & \mathbf{C} + \text{diag}(\boldsymbol{\tau}^2) \end{bmatrix} \right)$$

because  $\text{Cov}(Y(x^i), Y(x^j)) = E((\mu^i + Z^i + E^i - \mu^i)(\mu^j + Z^j + E^j - \mu^j)) = C_{ij} + \delta_{ij} \tau_i^2$

The only change w.r.t. the usual kriging formula is the addition of the observation variances on the covariance diagonal

$$(Z(x^*) + \mu(x^*)) | \mathbf{Y} = \mathbf{y} \sim N(m_{SK}(x^*), v_{SK}(x^*))$$

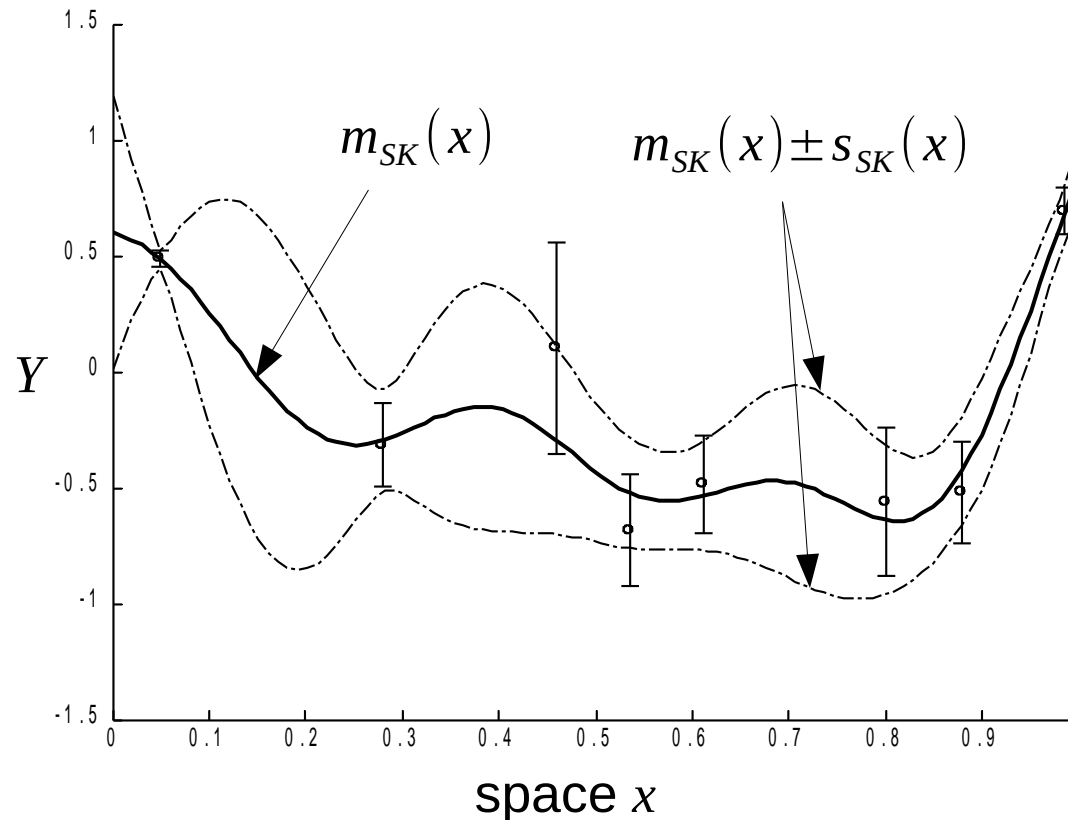
$$m_{SK}(x^*) = \mu(x^*) + C(x^*, \mathbf{X})(\mathbf{C} + \text{diag}(\boldsymbol{\tau}^2))^{-1}(\mathbf{y} - \boldsymbol{\mu})$$

$$v_{SK}(x^*) = \sigma^2 - C(x^*, \mathbf{X})(\mathbf{C} + \text{diag}(\boldsymbol{\tau}^2))^{-1}C(x^*, \mathbf{X})^T$$

# kriging-based approaches

## Kriging with noisy observations (3/5)

---



- **kriging no longer interpolating**
- **the kriging mean filters the noise**
- additive covariance diagonal terms called « nugget effect »
- often used as a regularization technique in non noisy situations
  
- kriging = our approach to link  $x$  and  $U$  spaces in optimization



# kriging-based approaches

## Kriging with noisy observations (4/5)

---

In the context of robust optimization with MC estimators, the observation noise can be set as

$$\tau_i^2 = \text{variance of performance estimate, } \hat{f}(\cdot), \text{ at } x^i$$

Expl.: mean estimate has variance

$$\tau_i^2 = V(\hat{f}(x^i)) = \frac{1}{MC(MC-1)} \sum_{j=1}^{MC} (f(x, u^j) - \hat{f}(x))^2$$

( Expl. with quantile estimate, cf. Le Riche et al., *Gears design with shape uncertainties using Monte Carlo simulations and kriging*, SDM, AIAA-2009-2257 )

# Kriging with noisy observations (5/5)

---

The hyperparameters can be tuned through max likelihood, 2 cases

## Known (from context) heterogeneous noise

$$\mathbf{C}_\tau \equiv \mathbf{C} + \text{diag}(\tau_1^2, \dots, \tau_n^2) \quad , \quad \mathbf{C}_\tau \equiv \sigma^2 \mathbf{R}_\tau$$

and do the usual MLE estimation (cf. ``intro. to kriging class")

replacing  $\mathbf{R}$  by  $\mathbf{R}_\tau \rightarrow \hat{\sigma} , \hat{\theta}_1 , \dots , \hat{\theta}_n$

## Unknown homogeneous noise

$$\mathbf{C}_\tau \equiv \mathbf{C} + \tau^2 \mathbf{I} \quad , \quad \mathbf{C}_\tau \equiv \sigma^2 \mathbf{R}_\tau$$

and do the usual MLE estimation replacing  $\mathbf{R}$  by  $\mathbf{R}_\tau$

(1 additional parameter in the concentrated likelihood,  $\tau$ )

$\rightarrow \hat{\tau} , \hat{\sigma} , \hat{\theta}_1 , \dots , \hat{\theta}_n$

# kriging-based approaches

---

We have seen

- how to formulate a robust optimization problem
- how to model noisy observations with kriging
- but how to optimize when a kriging metamodel is built ?

# Kriging-based approaches

## Kriging prediction minimization

The simplest (naive) approach.

For  $t=1, t^{max}$  do,

Learn  $Y^t(x)$  ( $m_K$  and  $s_K^2$ ) from  $f(x^1), \dots, f(x^t)$

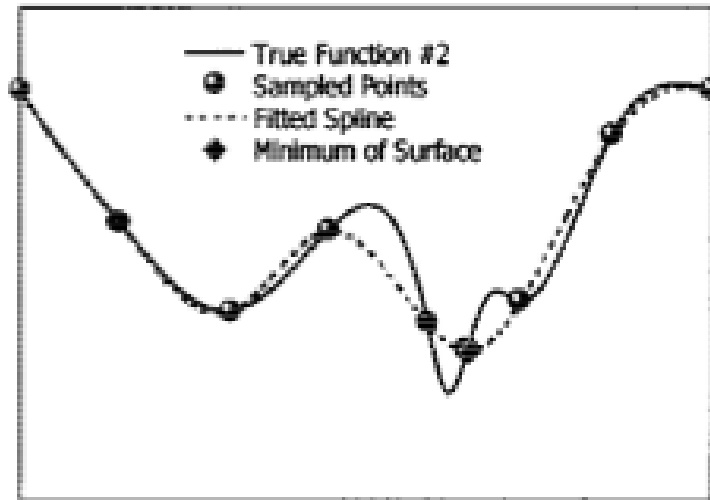
$x^{t+1} = \min_x m_K(x)$

Calculate  $f(x^{t+1})$

$t = t+1$

End For

e.g., using CMA-ES\*  
if multimodal  
\* Hansen et al., 2003



But it may fail if  $m_K(x^{t+1}) = f(x^{t+1})$  :  
the minimizer of  $m_K$  is at a data point  
which may not even be a local optimum.

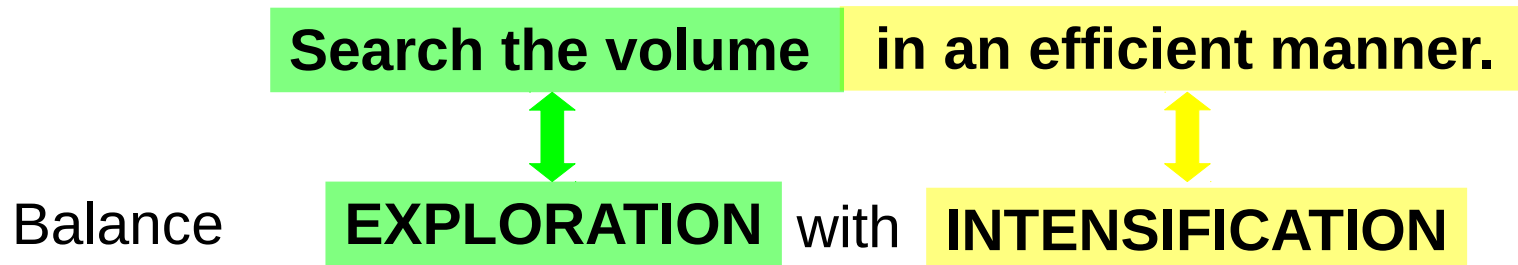
D. Jones, A taxonomy of global optimization methods  
based on response surfaces, JOGO, 2001.

Notation : this slide + the ones coming about EGO are general to any optimization,  
therefore  $\hat{f} \rightarrow f$

# kriging-based approaches

## Kriging and optimization

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- We will deterministically fill the design space in an efficient order.
  - Other global search principles
    - **Stochastic searches** : (pseudo)-randomly sample the design space  $S$ , use probabilities to intensify search in known high performance regions and sometimes explore unknown regions.
    - (pseudo-)Randomly restart local searches.
    - (and mix the above principles)
-

kriging-based approaches

# A state-of-the-art global optimization algorithm using metamodels : EGO

---

(D.R. Jones et al., JOGO, 1998)

EGO = Efficient Global Optimization = use a « kriging » metamodel to define the Expected Improvement (EI) criterion. Maximize EI to create new  $x$ 's to simulate.

EGO deterministically creates a series of design points that ultimately would fill  $S$ .

Some opensource implementations :

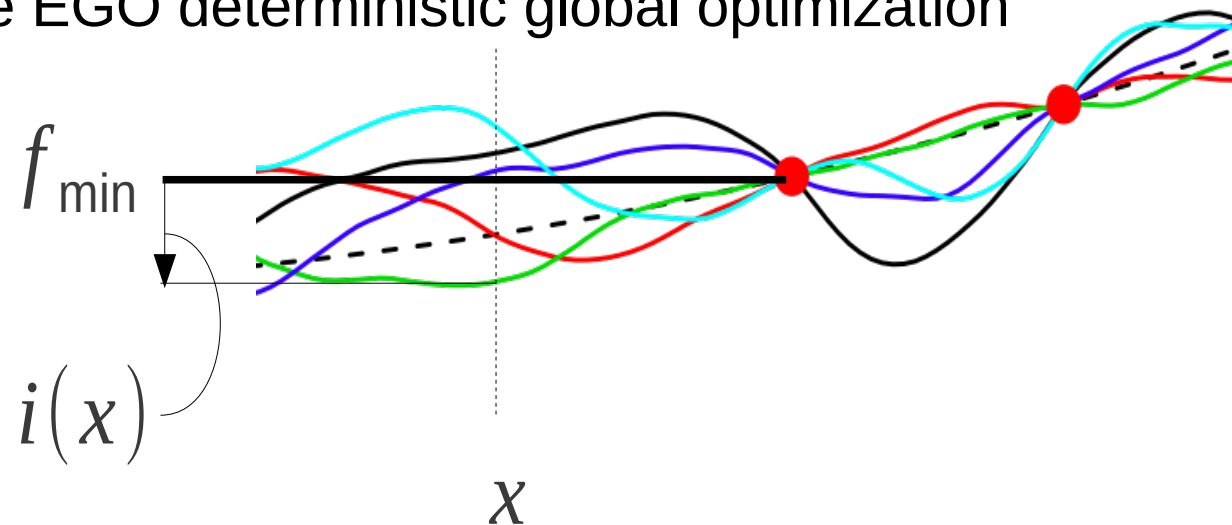
- DiceOptim in R (EMSE & Bern Univ.)
  - Krisp in Scilab (Riga Techn. Univ & EMSE)
  - STK: a Small (Matlab/GNU Octave) Toolbox for Kriging, (Supelec)
-

# kriging-based approaches (one point-) Expected improvement

A natural measure of progress : the improvement,

$$I(x) = [f_{\min} - F(x)]^+ \mid F(x) = f(x) \quad , \quad \text{where } [.]^+ \equiv \max(0, .)$$

- The expected improvement is known analytically.
- It is a parameter free measure of the exploration-intensification compromise.
- Its maximization defines the EGO deterministic global optimization algorithm.



$$EI(x) = \sqrt{v_K(x)} \times (u(x)\Phi(u(x)) + \varphi(u(x))) \quad , \quad \text{where } u(x) = \frac{f_{\min} - m_K(x)}{\sqrt{v_K(x)}}$$

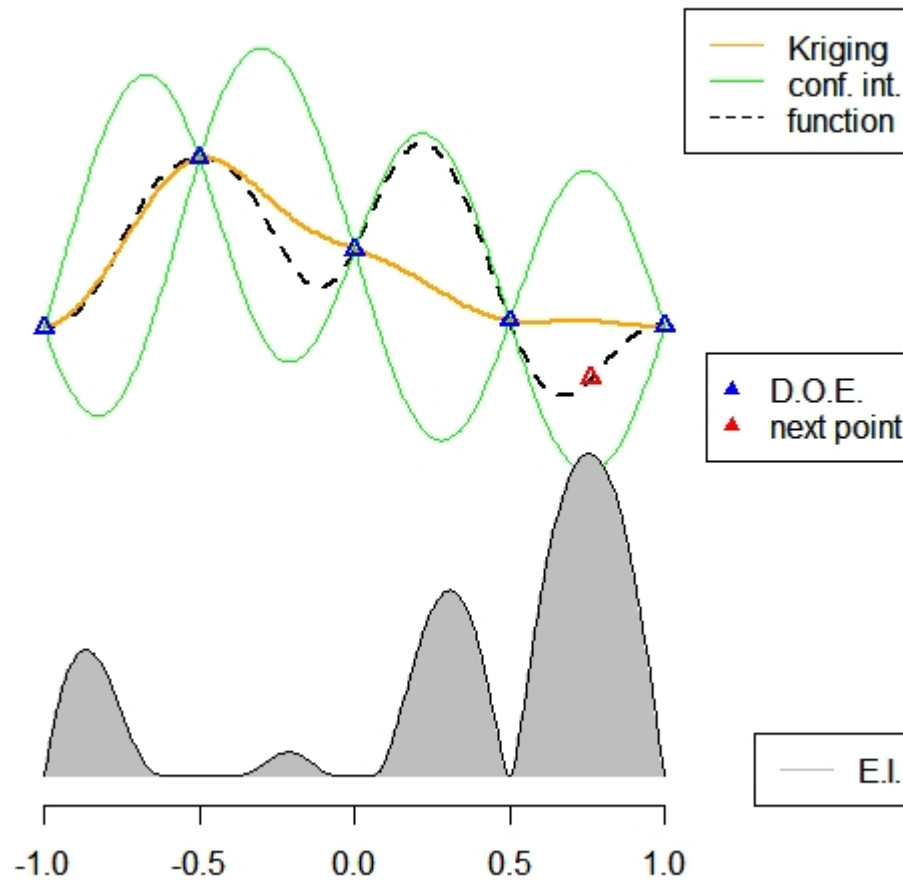
# kriging-based approaches

## One EGO iteration

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At each iteration, EGO adds to the  $t$  known points the one that maximizes EI,

$$x^{t+1} = \arg \max_x EI(x)$$



then, the kriging model is updated ...

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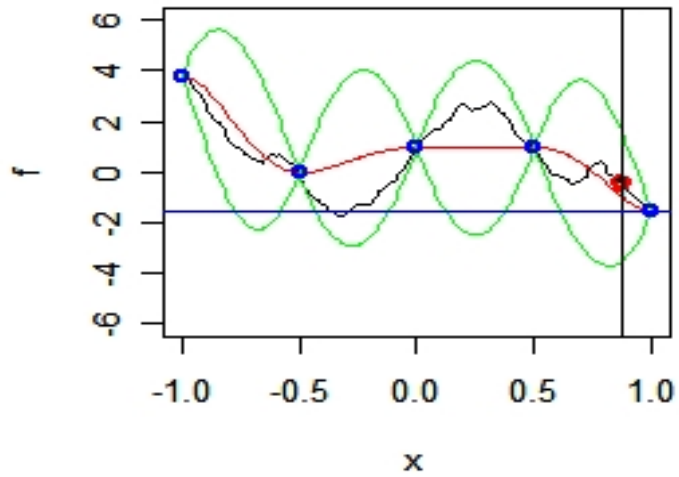


# kriging-based approaches

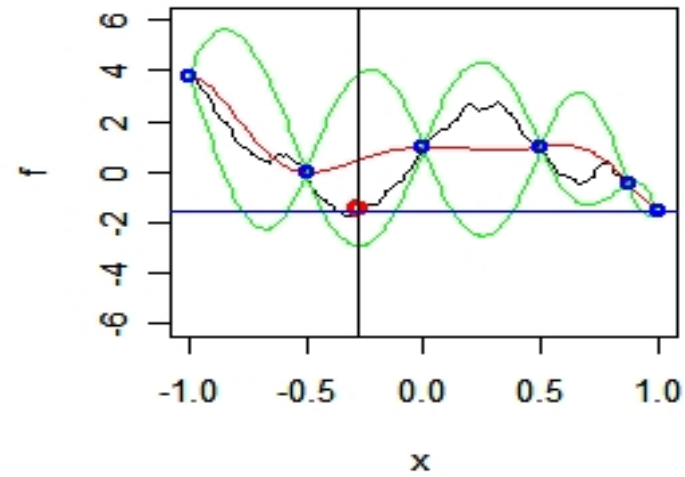
## EGO : example

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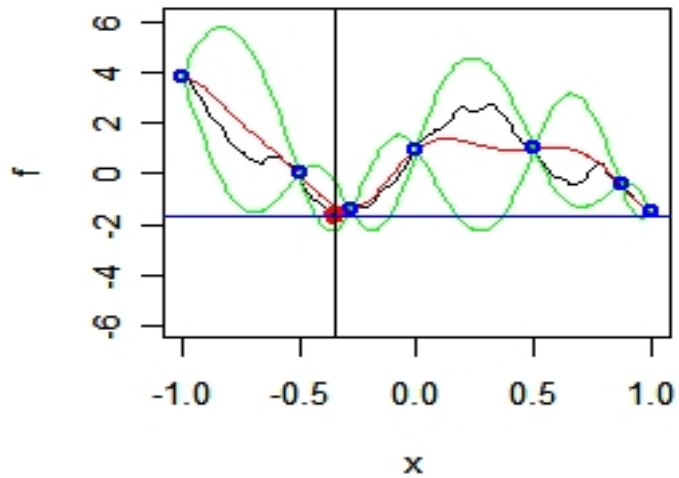
iteration  
1



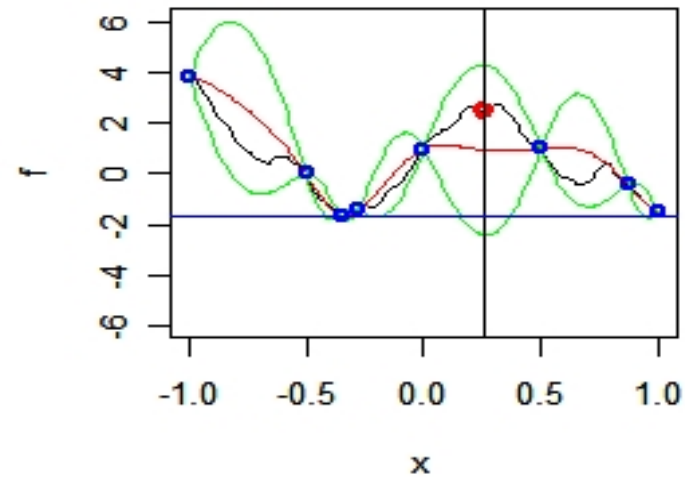
iteration  
2



iteration  
3



iteration  
4

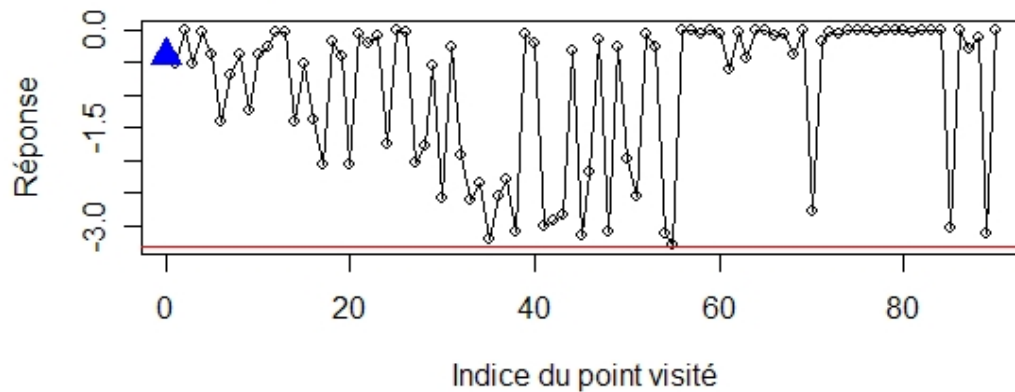


# kriging-based approaches

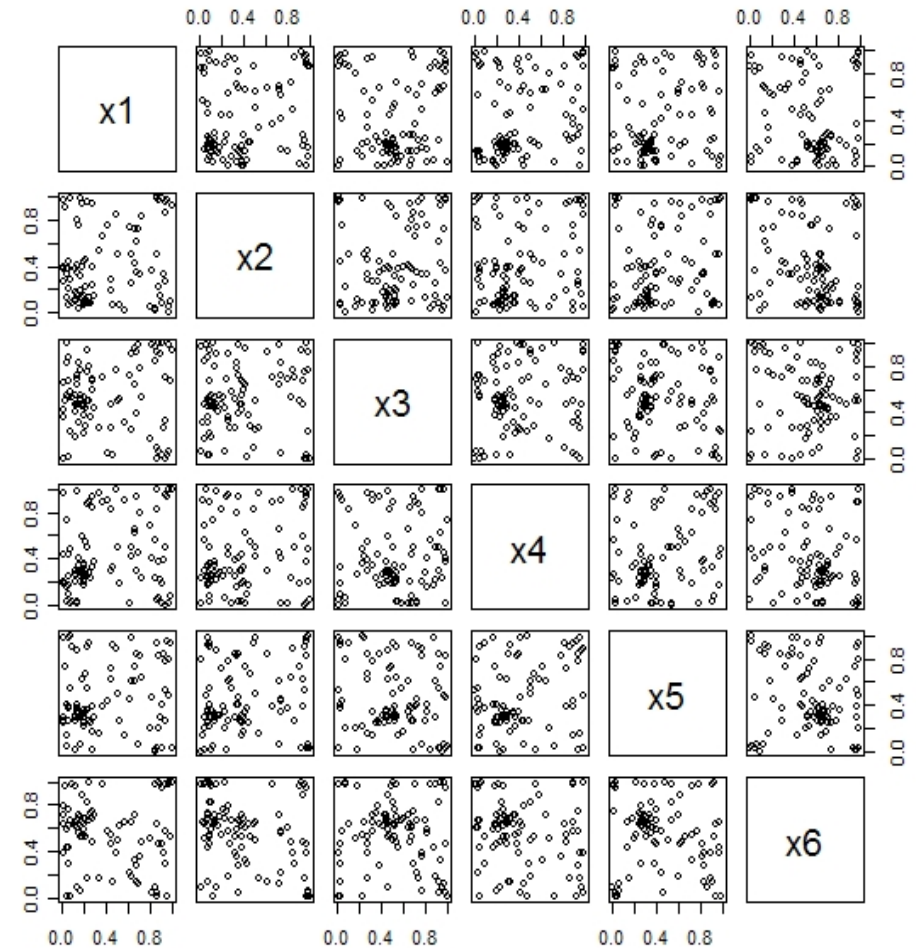
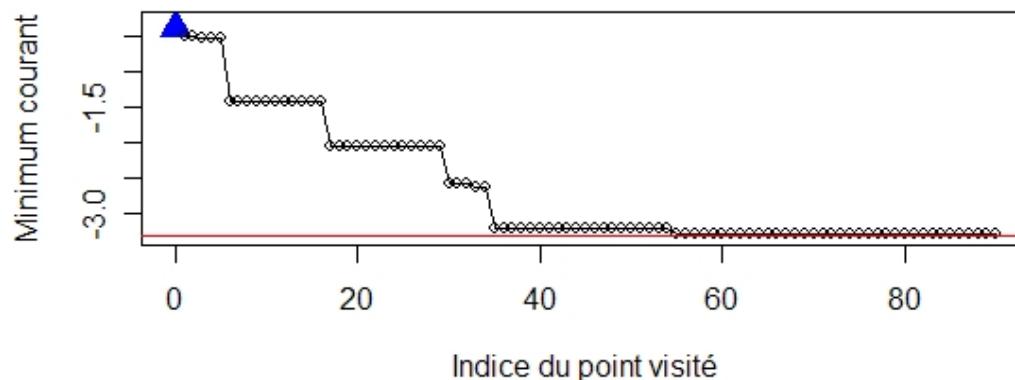
## EGO : 6D example

Hartman function,  $f(x^*) = -3.32$ , 10 points in initial DoE

Séquence des valeurs observées durant EGO




Séquence du minimum courant durant EGO



(DiceOptim, D. Ginsbourger, 2009)

# Outline of the talk

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1. Motivations for robust optimization
2. Formulations of optimization problems with uncertainties
3. Kriging-based approaches to robust optimization (costly functions)
  - Kriging noisy observations
  - Optimization and kriging
  -  Robust optimization, no control on U
  - Robust optimization, control on U
4. Evolutionary approaches (non costly functions)

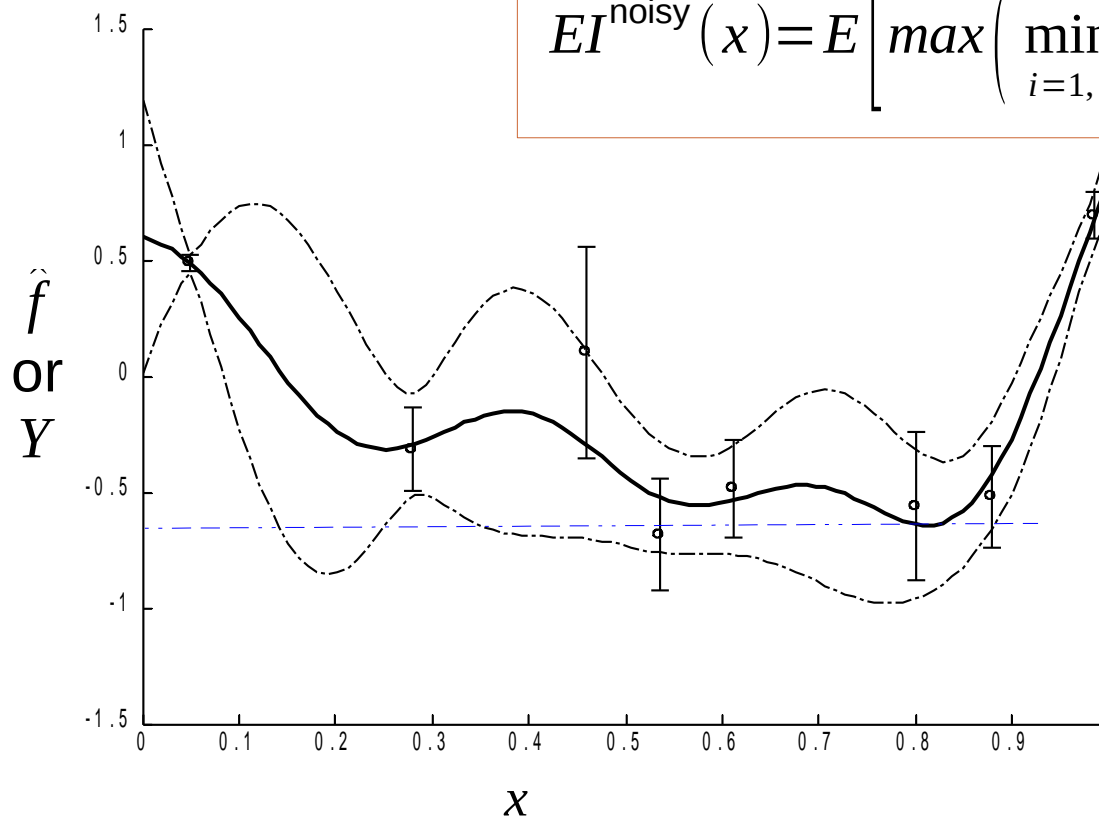
# Kriging-based robust optimization, no control on U

## EI for noisy functions

**EI should not be used for noisy observations** because  $\hat{f}_{min} \equiv y_{min}$  is noisy ! (a low  $y_{min}$  would mislead EGO for a long time)

**Solution 1** : Add nugget effect and replace  $y_{min}$  by the best observed mean (filters out noise in already sampled regions) :

$$EI^{noisy}(x) = E \left[ \max \left( \min_{i=1,t} m_K(x^i) - (Z(x) + \mu(x)), 0 \right) \right]$$



known analytically  
replace  $f_{min}$  by  
 $\min_{i=1,t} m_K(x^i)$   
in *EI* formula

# Kriging-based robust optimization, no control on U

## Expected Quantile Improvement

V. Picheny, D. Ginsbourger, Y. Richet, *Optimization of noisy computer experiments with tunable precision*, Technometrics, 2011.

Solution 2 : Add nugget effect and use the expected quantile improvement.

$$EQI(x) = E \left[ \max \left( q_{min} - Q^{t+1}(x), 0 \right) \right]$$

$$q_{min} = \min_{i=1,t} m_K(x^i) + \alpha s_K(x^i)$$

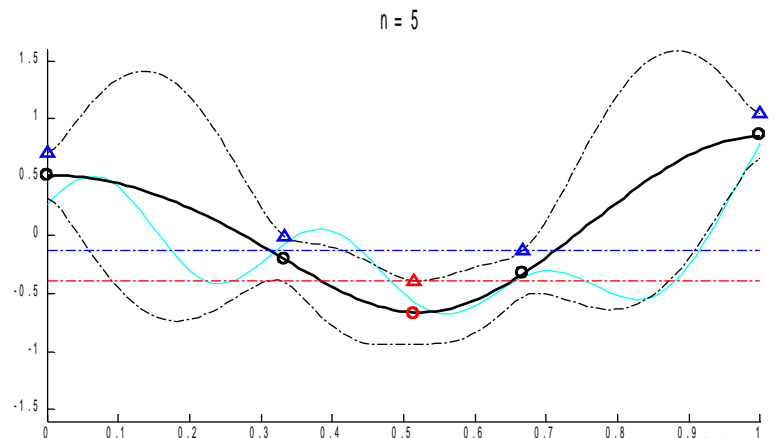
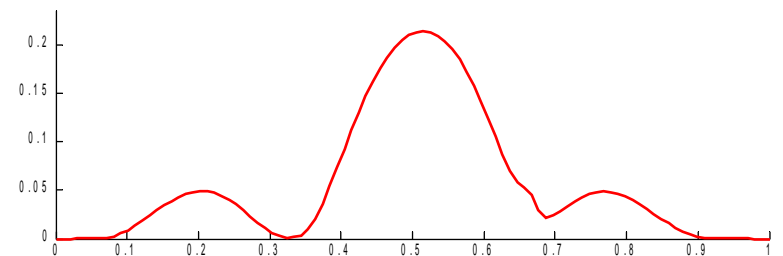
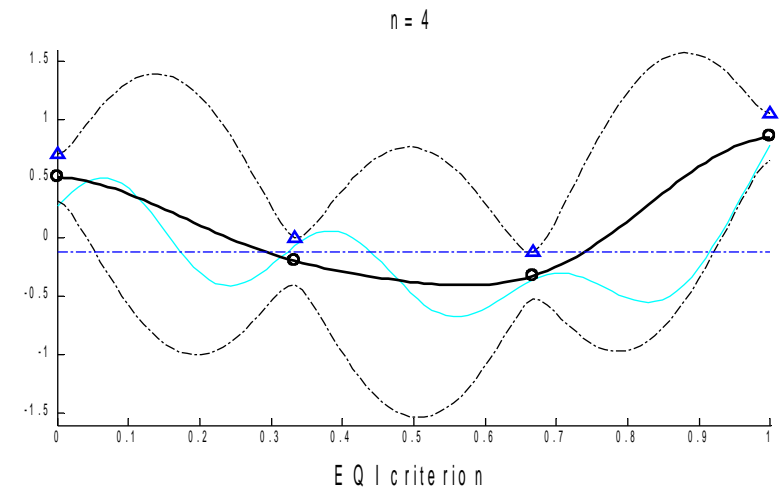
$$Q^{t+1}(x) = M_K^{t+1}(x) + \alpha s_K^{t+1}(x)$$

$M_K^{t+1}(x)$  is a linear function of  $Y(x)$

$\Rightarrow EQI(x)$  is known analytically


A conservative criterion (noise and spatial uncertainties are seen as risk rather than opportunities).

Better for assigning resources to reduce noise on a given DoE  $X^t$  obtained by Solution 1.



# Outline of the talk

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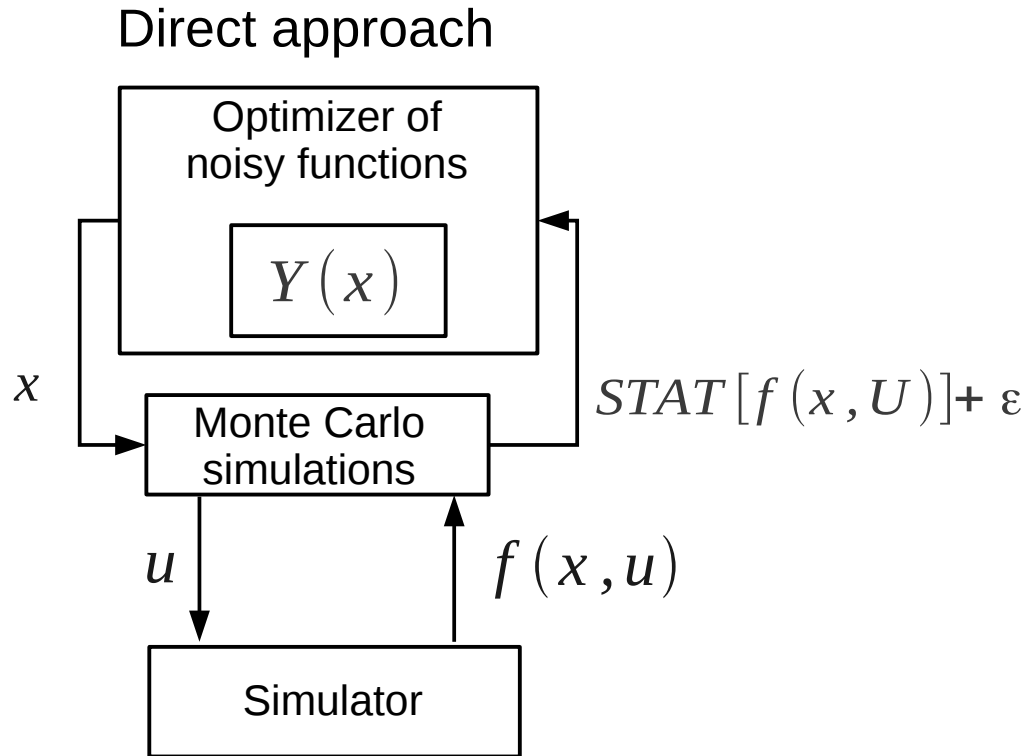
1. Motivations for robust optimization
2. Formulations of optimization problems with uncertainties
3. Kriging-based approaches to robust optimization (costly functions)
  - Kriging noisy observations
  - Optimization and kriging
  - Robust optimization, no control on  $U$
  -  Robust optimization, control on  $U$
4. Evolutionary approaches (non costly functions)

# Kriging based optimization with uncertainties, $U$ controlled $(x,u)$ surrogate based approach

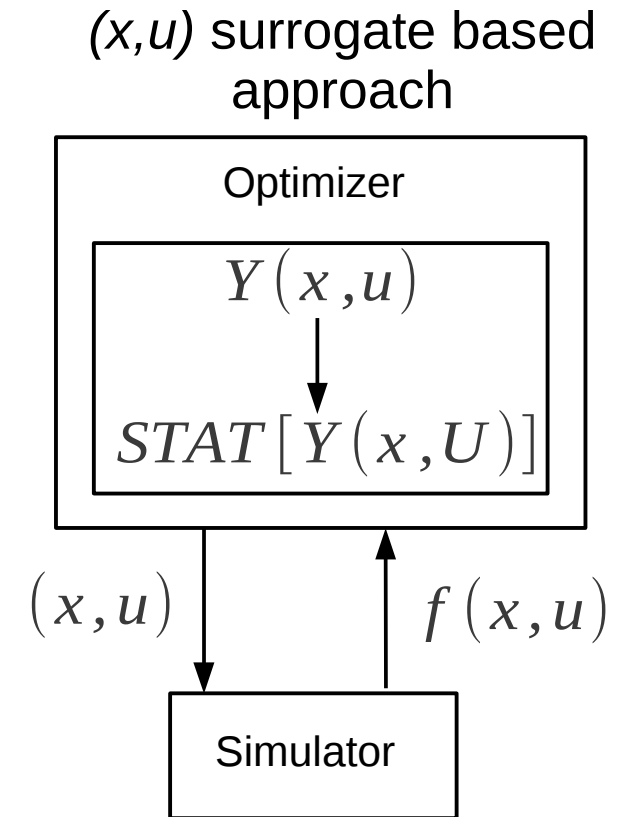
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Assumptions :  $x$  and  $U$  controlled

$Y$  : surrogate model



Multiplicative cost of two loops involving  $f$



Only one loop of  $f$

# Kriging based optimization with uncertainties, U controlled

## A general Monte Carlo - kriging algorithm

Hereafter is an example of a typical surrogate-based (here kriging) algorithm for optimizing any statistical measure of  $f(x,u)$  (here the average).

Create initial DOE  $(X^t, U^t)$  and evaluate  $f$  there ;  
While stopping criterion is not met:

MC – kriging algorithm

- Create kriging approximation  $Y^t$  in the joint  $(x,u)$  space from  $f(X^t, U^t)$
- Estimate the value of the statistical objective function from Monte Carlo simulations on the kriging average  $m_Y^t$ .

$$\text{Expl : } \hat{f}(x^i) = \frac{1}{S} \sum_{k=1}^S m_K^t(x^i, u^k) \quad , \quad \text{where } u^k \text{ i.i.d. from pdf of } U$$

- Create kriging approximation  $Z^t$  in  $x$  space from  $(x^i, \hat{f}(x^i))_{i=1,t}$
- Maximize  $EI_Z^{\text{noisy}}(x)$  to obtain the next simulation point  $\rightarrow x^{t+1}$   
 $u^{t+1}$  sampled from pdf of  $U$
- Calculate simulator response at the next point,  $f(x^{t+1}, u^{t+1})$ .  
Update DOE and  $t$

only call to f !

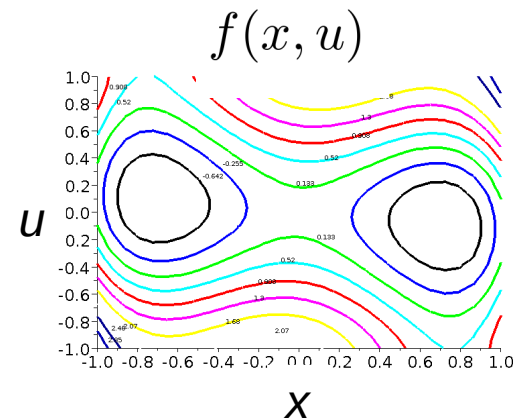


# Kriging based optimization with uncertainties, U controlled Simultaneous optimization and sampling

---

**Objective :**  $\min_x \mathbb{E}_U [f(x, U)]$

Principle : work in the joint (x,u) space.



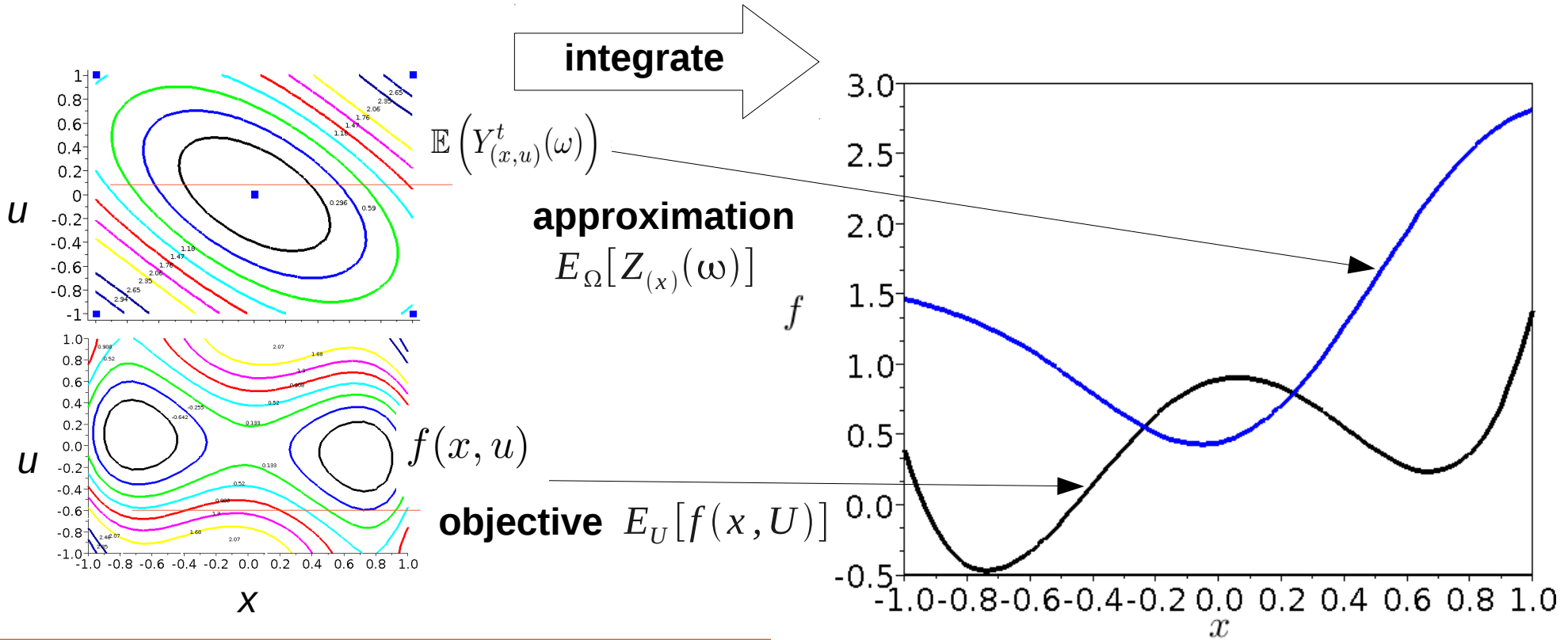
Cf. J. Janusevskis and R. Le Riche, *Simultaneous kriging-based estimation and optimization of mean response*, Journal of Global Optimization, Springer, 2012

# Kriging based optimization with uncertainties, U controlled Integrated kriging (1)

$$\min_x \mathbb{E}_U [f(x, U)] : \text{objective}$$

$$Y_{(x,u)}^t(\omega) : \text{kriging approximation to deterministic } f(x, u)$$

$$Z_{(x)}^t(\omega) = \mathbb{E}_U [Y_{(x,U)}^t(\omega)] : \text{integrated process approximation to } \mathbb{E}_U [f(x, U)]$$



# Kriging based optimization with uncertainties, U controlled Integrated kriging (2)

---

The integrated process over  $U$  is defined as

$$Z_{(x)}(\omega) = \mathbb{E}_U [Y_{(x,U)}^t(\omega)] = \int_{\mathbb{R}^m} Y_{(x,u)}^t(\omega) d\mu(u)$$

$d\mu(u)$ -probability measure on  $U$

Because it is a linear transformation of a Gaussian process, it is Gaussian, and fully described by its mean and covariance

$$m_Z(x) = \int_{\mathbb{R}^m} m_Y(x, u) d\mu(u)$$

$$\text{cov}_Z(x; x') = \int_{\mathbb{R}^m} \int_{\mathbb{R}^m} \text{cov}_Y(x, u; x' u') d\mu(u) d\mu(u')$$

Analytical expressions of  $m_Z$  and  $\text{cov}_Z$  for Gaussian  $U$ 's are given in

J. Janusevskis and R. Le Riche, *Simultaneous kriging-based estimation and optimization of mean response*, Journal of Global Optimization, Springer, 2012

# Kriging based optimization with uncertainties, U controlled EI on the integrated process (1)

---

$Z$  is a process approximating the objective function  $\mathbb{E}_U[f(x, U)]$

Optimize with an Expected Improvement criterion,

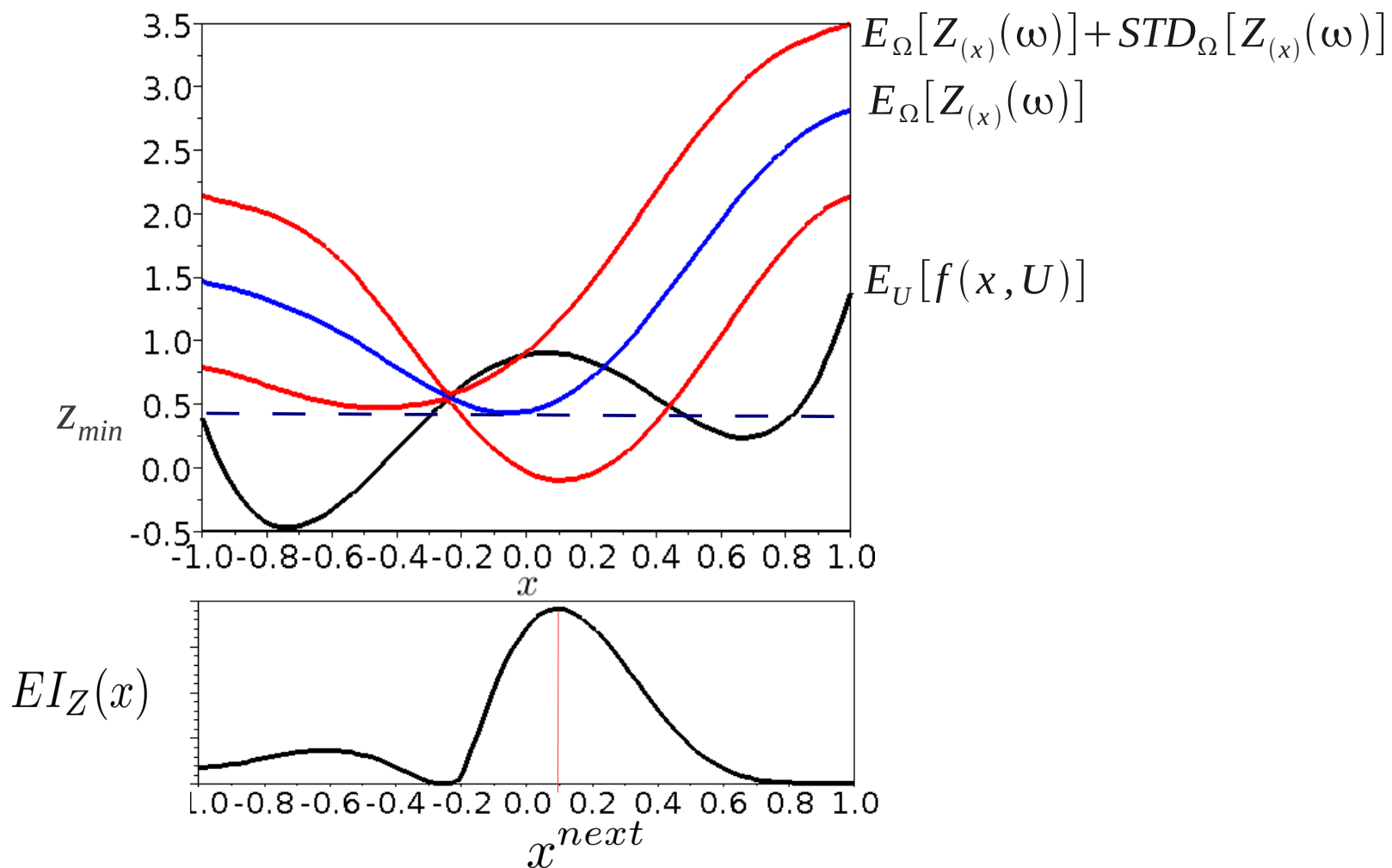
$$x^{next} = \arg \max_x EI_Z(x)$$

Optimize with an Expected Improvement criterion,

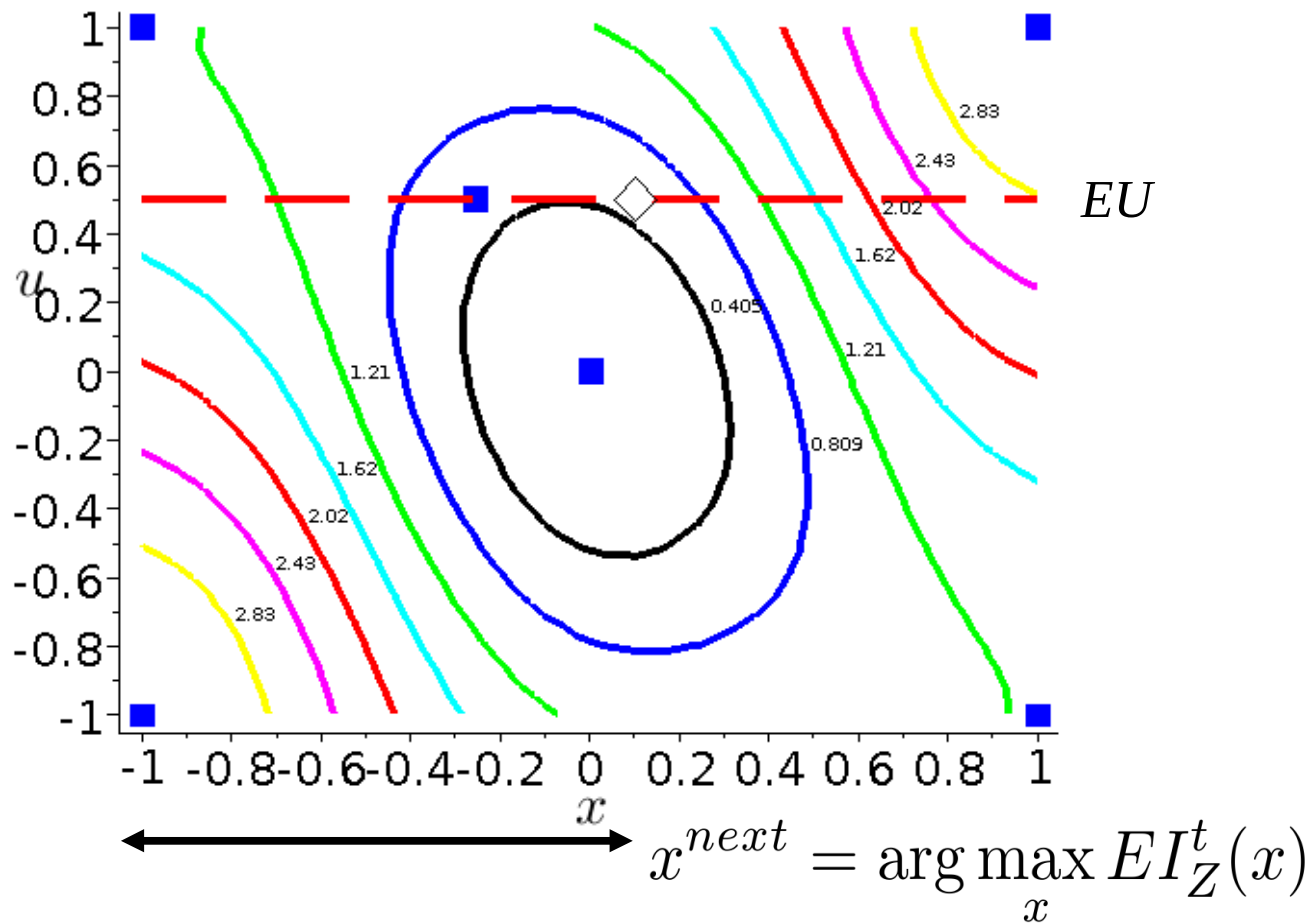
$I_Z(x) = \max(z_{min} - Z(x), 0)$  , but  $z_{min}$  not observed (in integrated space).  
 $\Rightarrow$  Define  $z_{min} = \min_{x^1, \dots, x^t} E(Z(x))$

# Kriging based optimization with uncertainties, U controlled EI on the integrated process (2)

---



# Kriging based optimization with uncertainties, U controlled EI on the integrated process (3)



$x$  ok. What about  $u$  ? (which we need to call the simulator)

# Kriging based optimization with uncertainties, U controlled Simultaneous optimization and sampling : method

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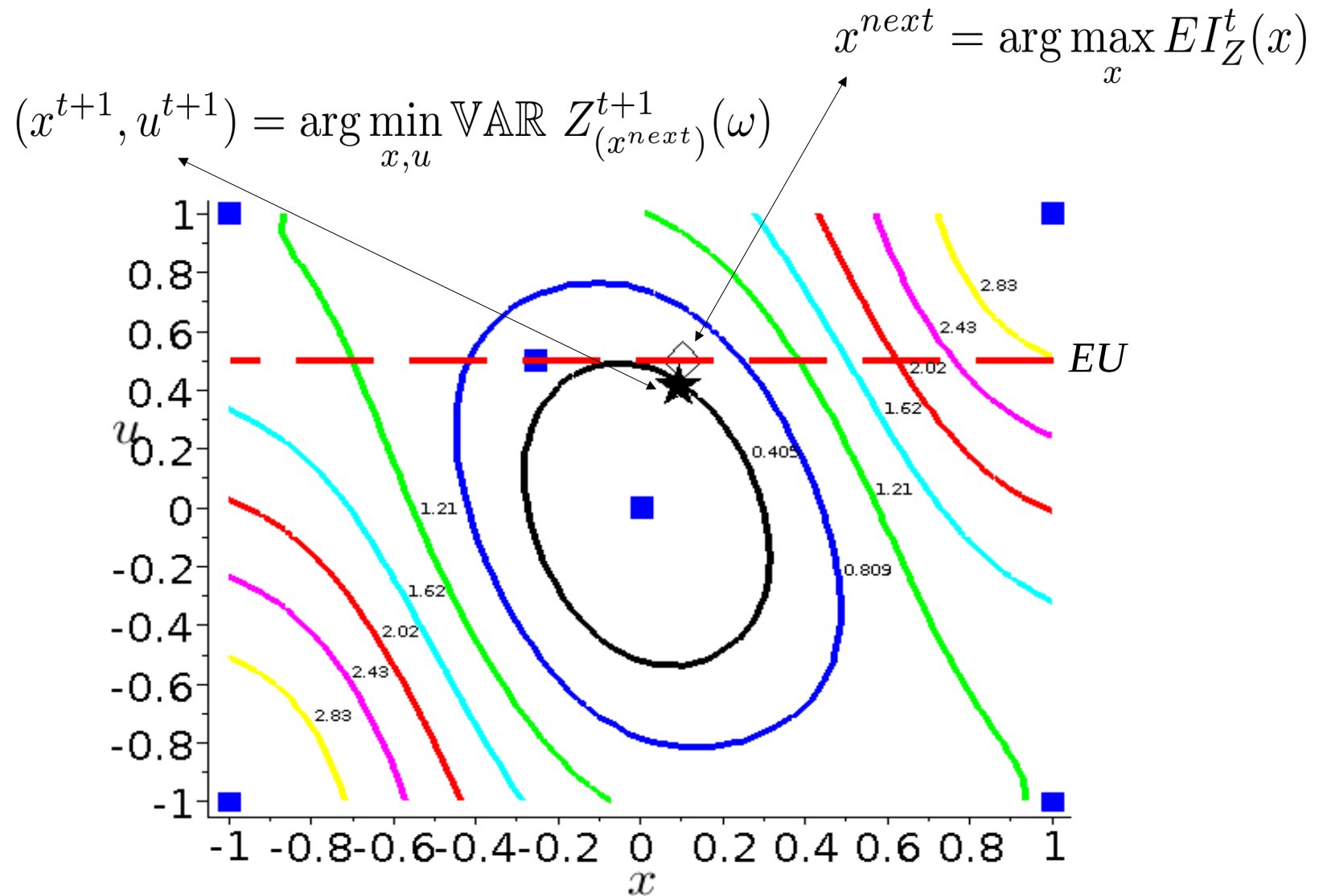
$x^{next}$  gives a region of interest from an optimization of the expected  $f$  point of view.

One simulation will be run to improve our knowledge of this region of interest → one choice of  $(x,u)$ .

Choose  $(x^{t+1}, u^{t+1})$  that provides the most information, i.e., which minimizes the variance of the integrated process at  $x^{next}$

$$(x^{t+1}, u^{t+1}) = \arg \min_{x,u} \text{VAR} Z_{(x^{next})}^{t+1}(\omega)$$

# Kriging based optimization with uncertainties, U controlled Simultaneous optimization and sampling : expl.





# Kriging based optimization with uncertainties, U controlled Simultaneous optimization and sampling : algo

---

Create initial DOE in  $(x,u)$  space;

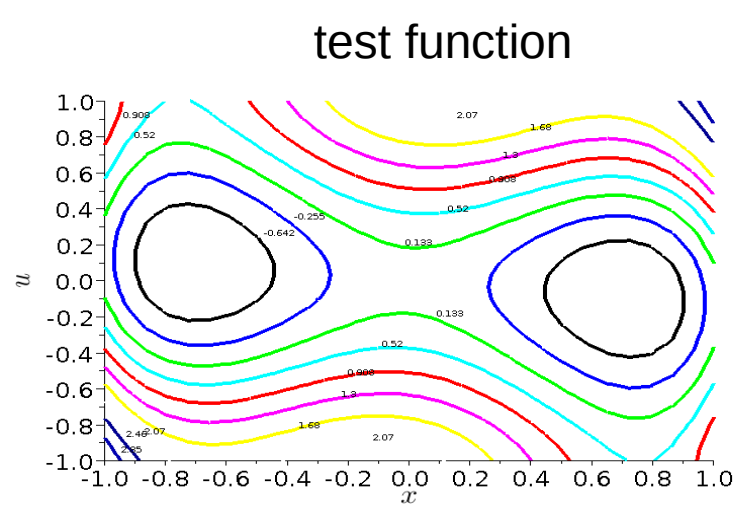
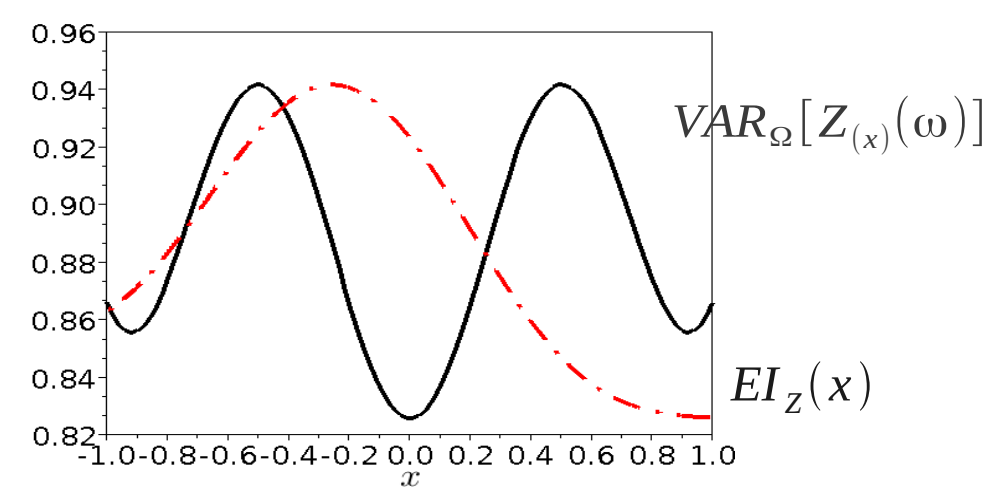
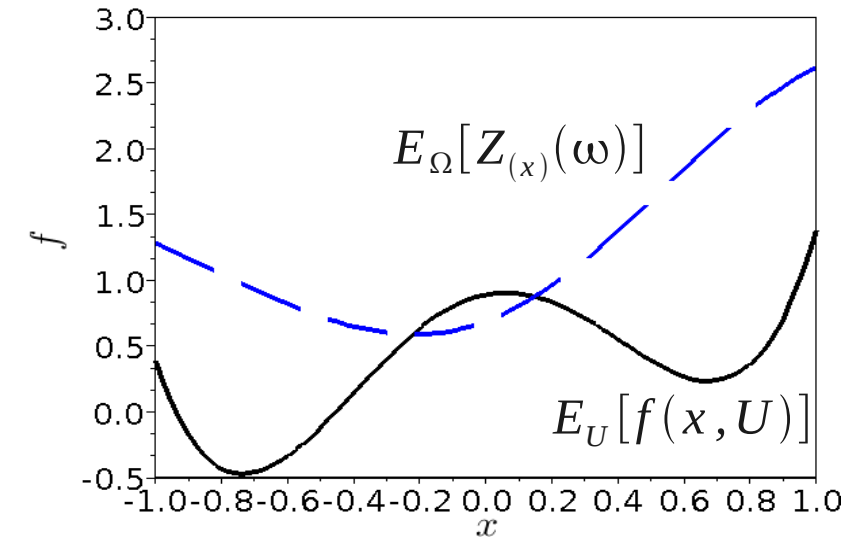
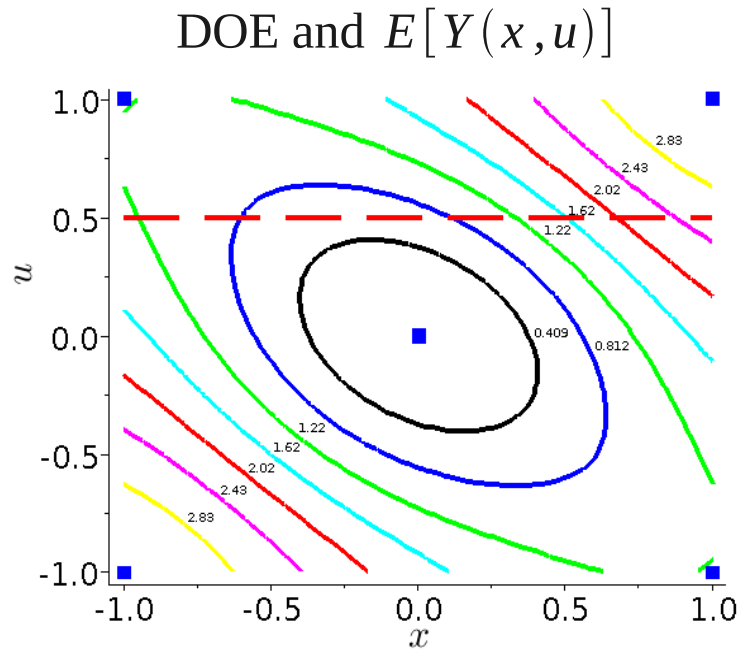
While stopping criterion is not met:

- Create kriging approximation  $Y$  in the joint space  $(x,u)$
- Using covariance information of  $Y$  to obtain approximation  $Z$  of the objective in the deterministic space  $(x)$
- Use EI of  $Z$  to choose  $(x^{next})$
- Minimize  $VAR(Z(x^{next}))$  to obtain the next point  $(x^{t+1}, u^{t+1})$  for simulation
- Calculate simulator response at the next point  $f(x^{t+1}, u^{t+1})$

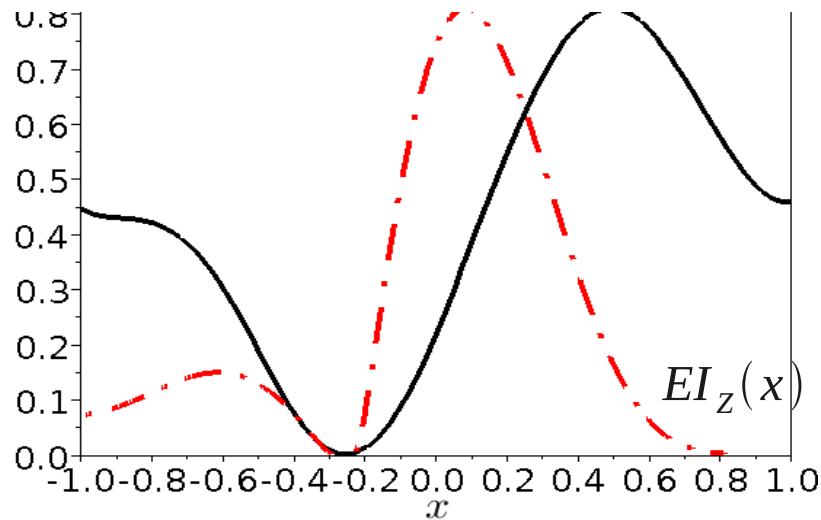
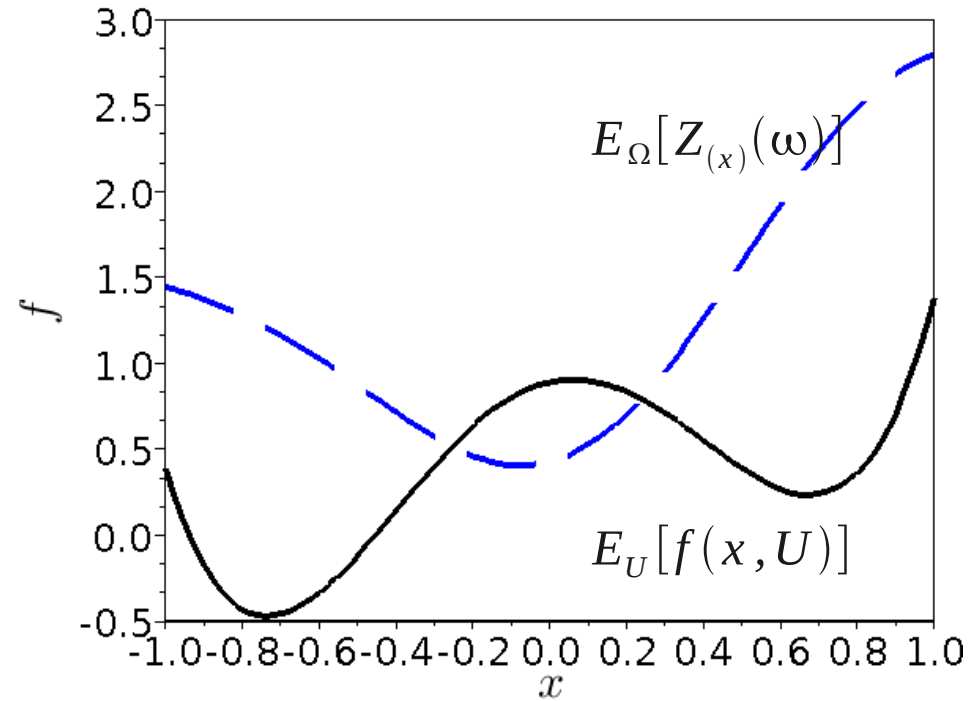
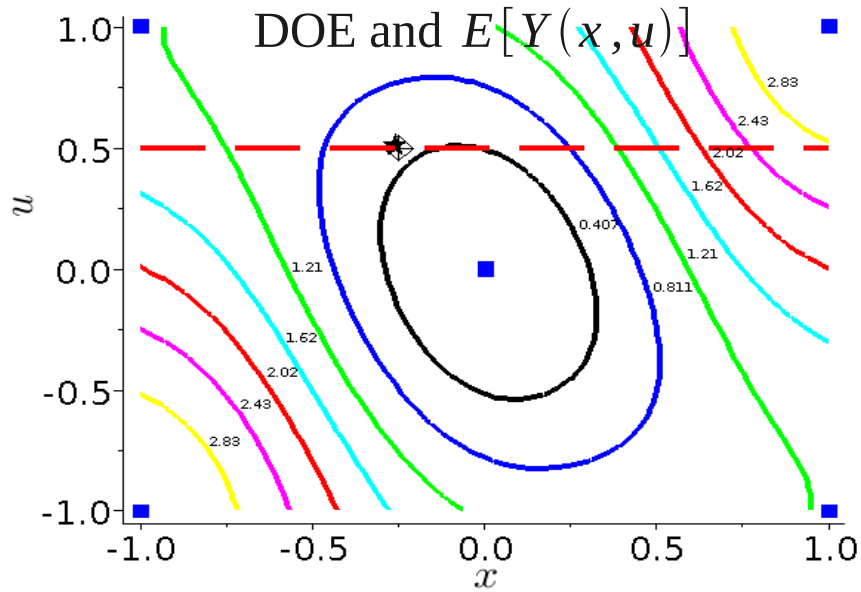
( 4 sub-optimizations, solved with CMA-ES )

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# Kriging based optimization with uncertainties, U controlled 2D Expl, simultaneous optimization and sampling



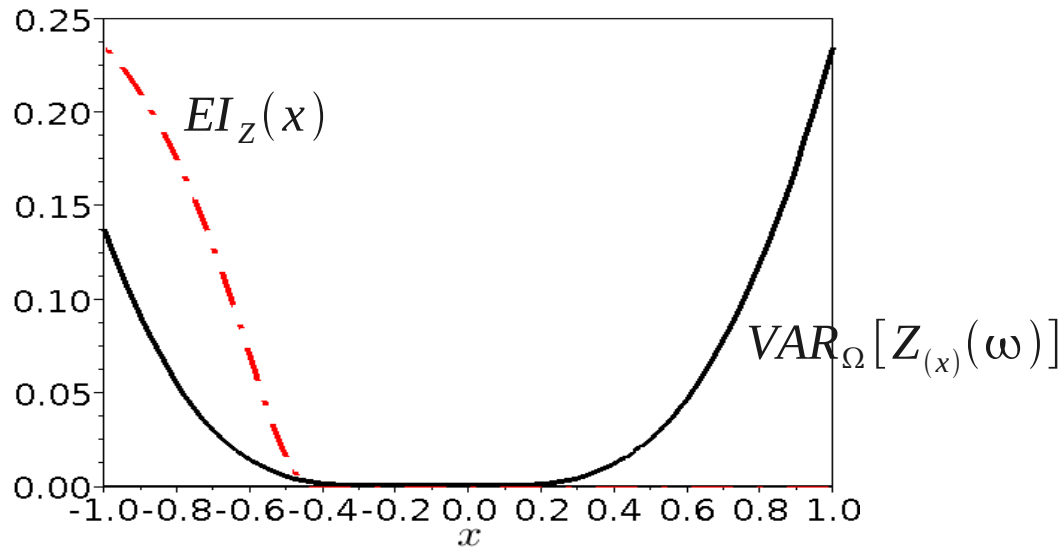
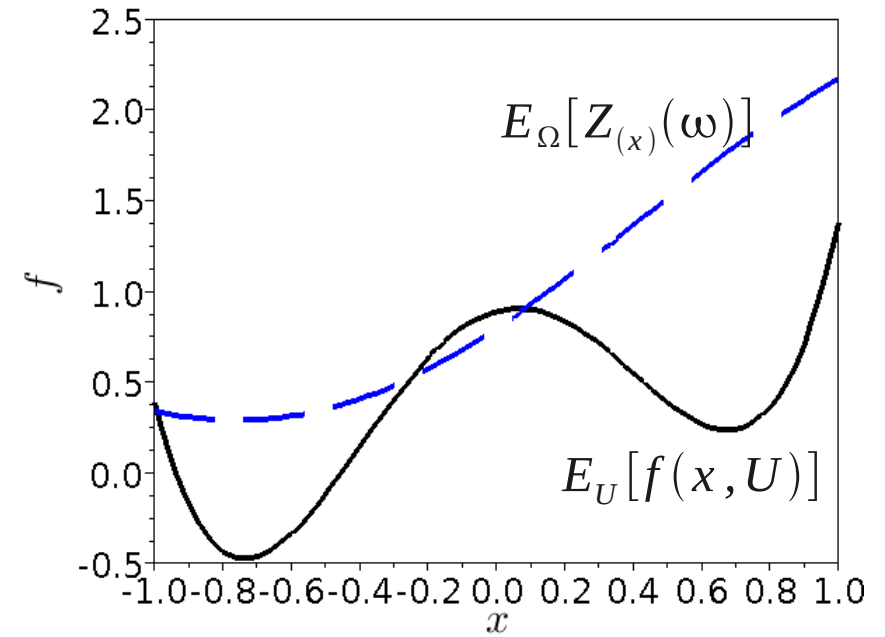
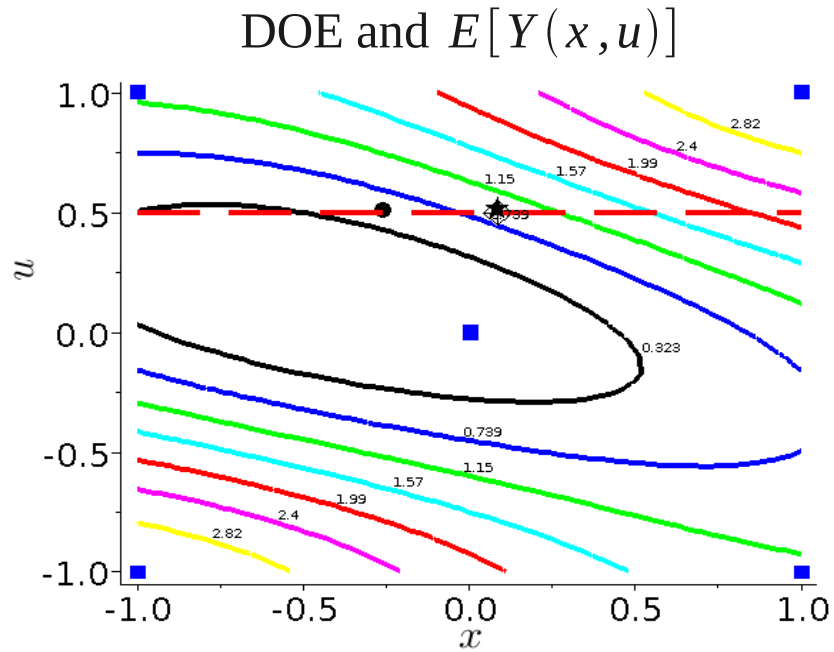
# Kriging based optimization with uncertainties, U controlled 1st iteration



$$VAR_\Omega[Z_{(x)}(\omega)]$$

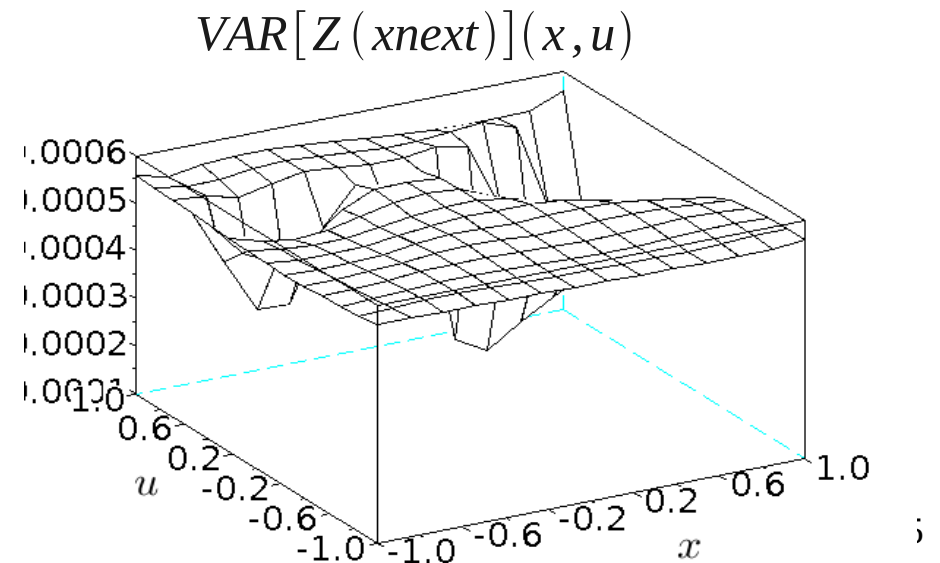
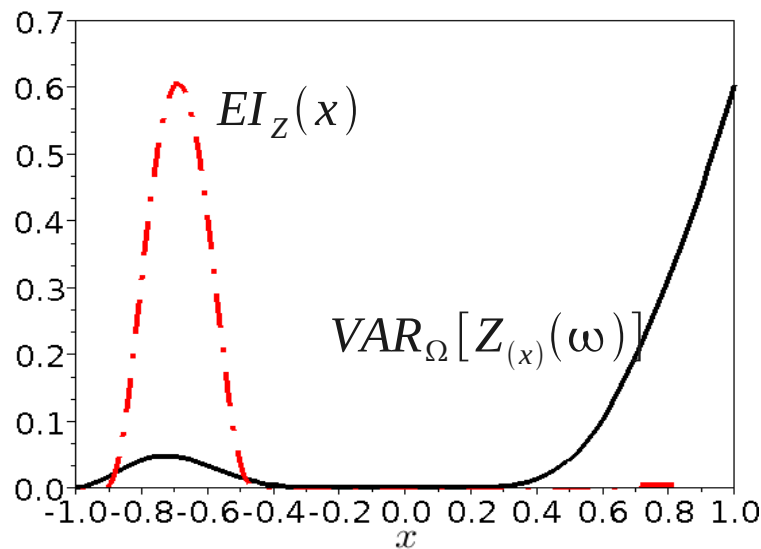
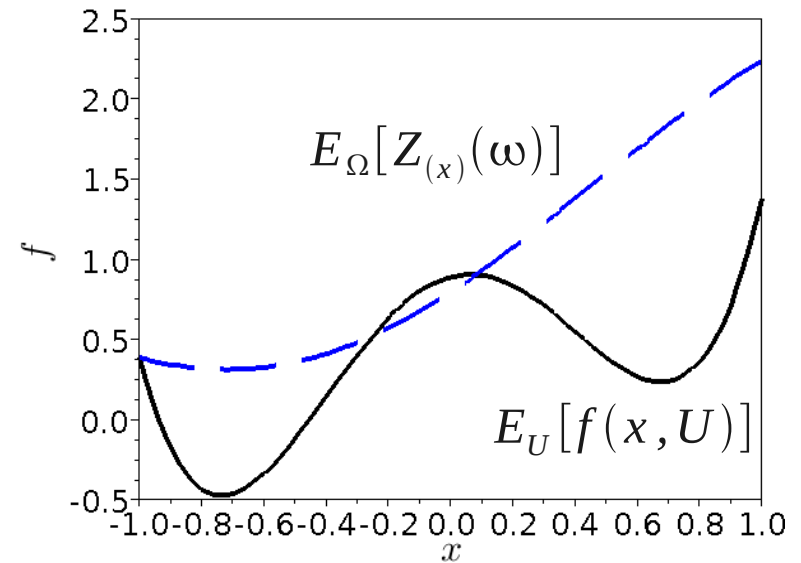
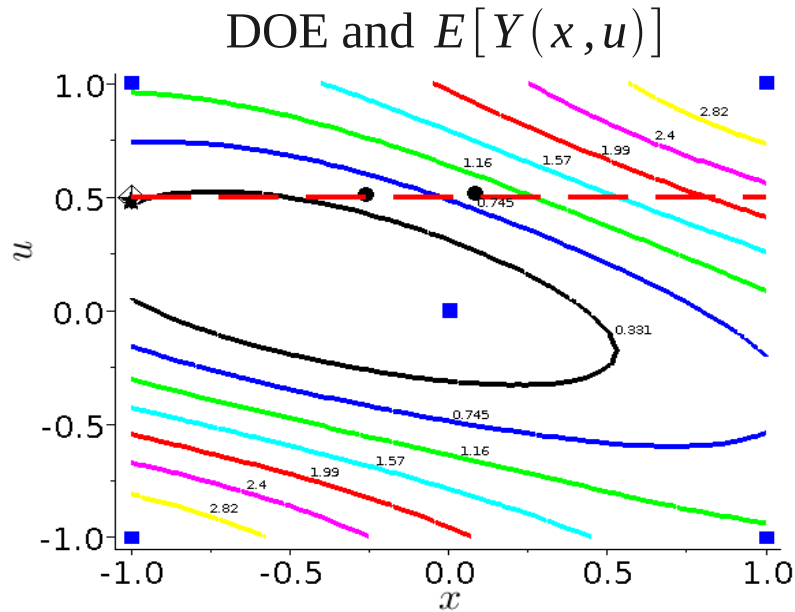
- $\diamond$  —  $(x^{next}, \mu)$
- $\star$  —  $(x^{t+1}, u^{t+1})$

# Kriging based optimization with uncertainties, U controlled 2nd iteration

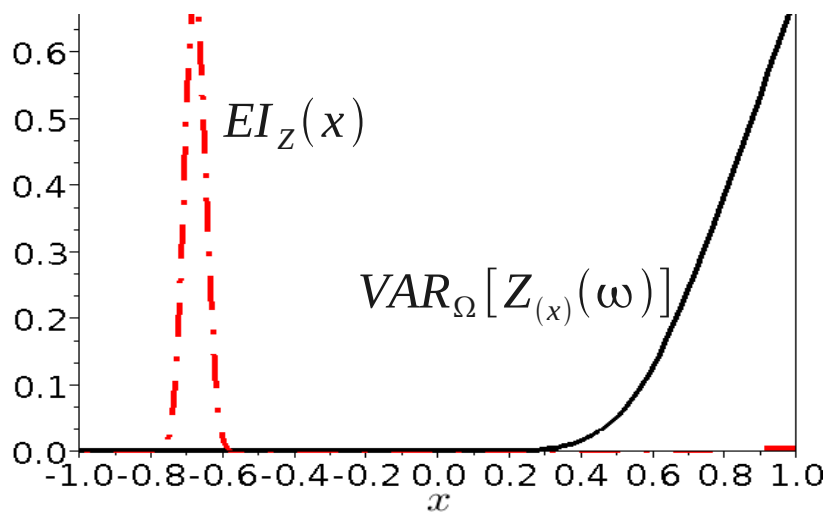
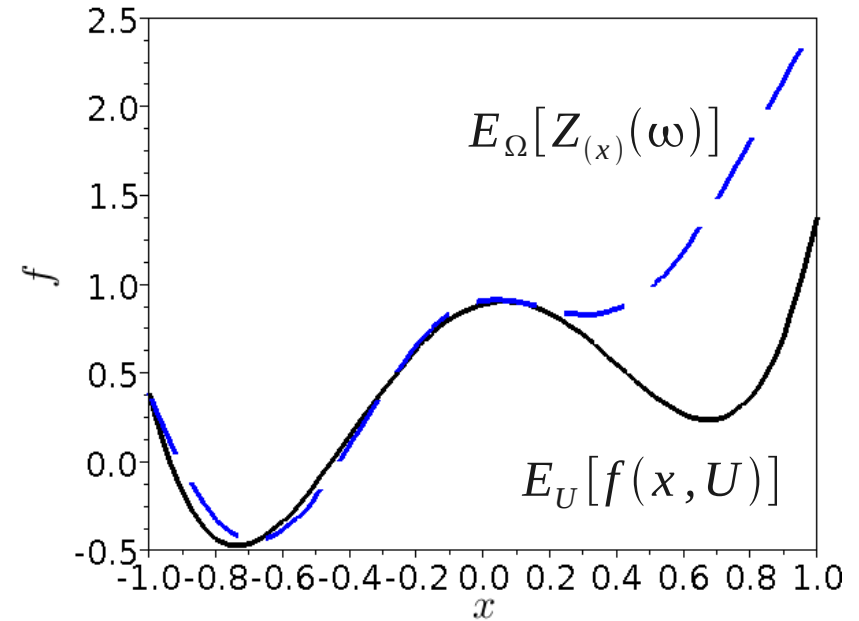
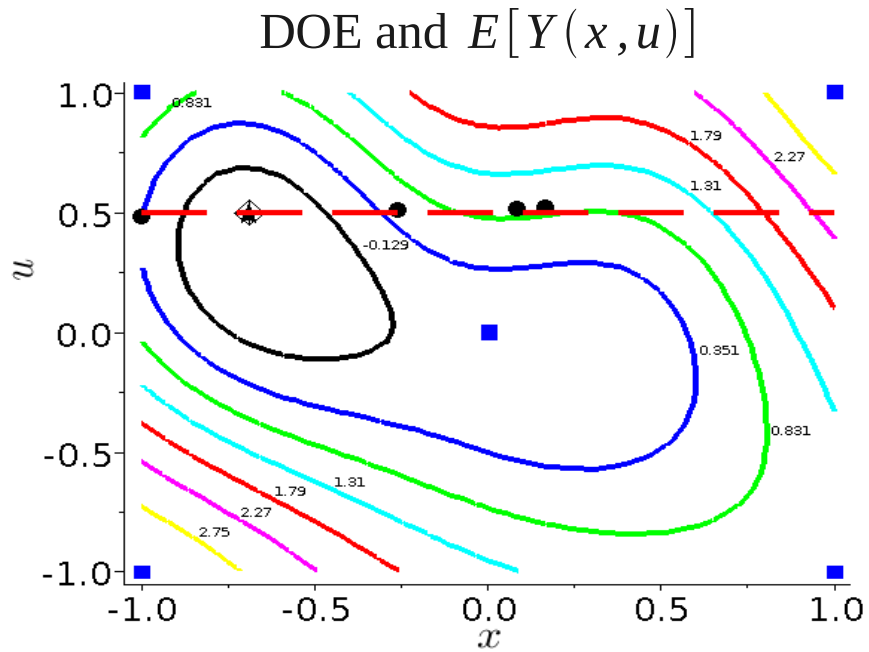


- $\blacklozenge$  —  $(x^{next}, \mu)$
- $\star$  —  $(x^{t+1}, u^{t+1})$

# Kriging based optimization with uncertainties, U controlled 3rd iteration



# Kriging based optimization with uncertainties, U controlled 5th iteration

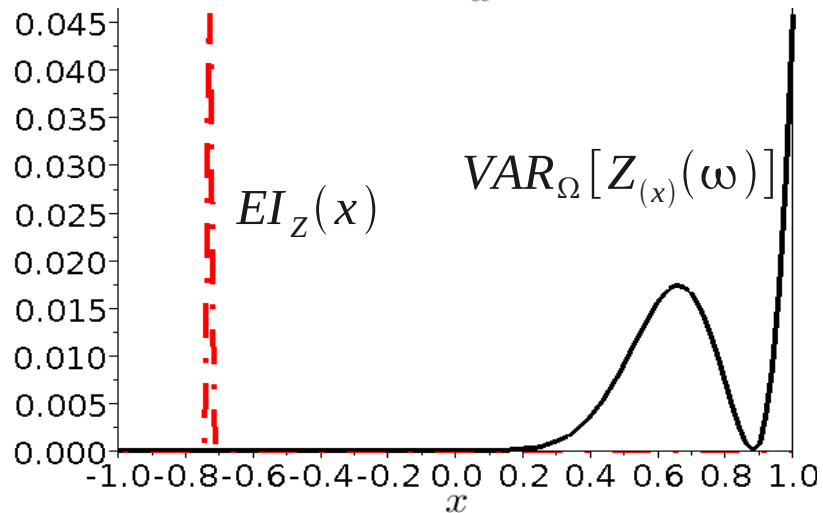
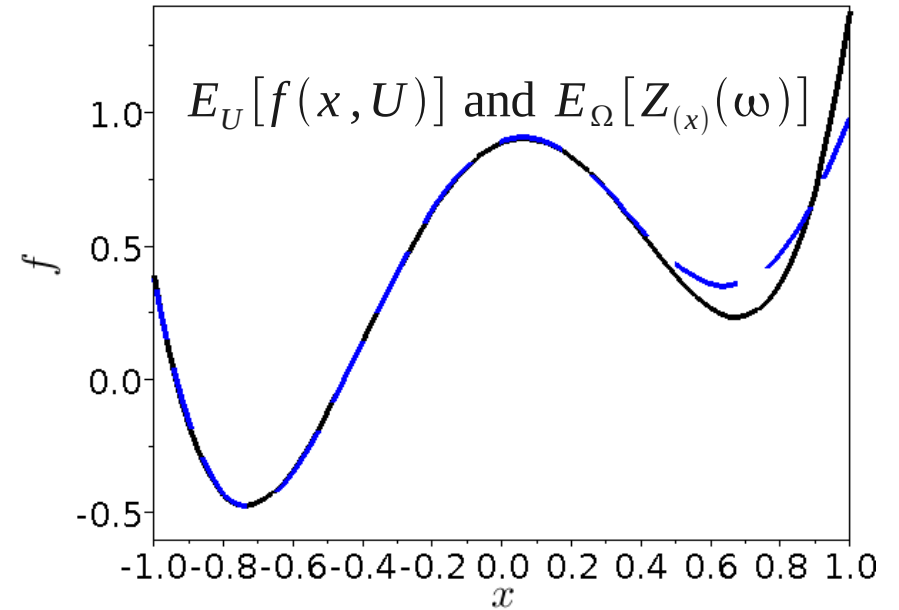
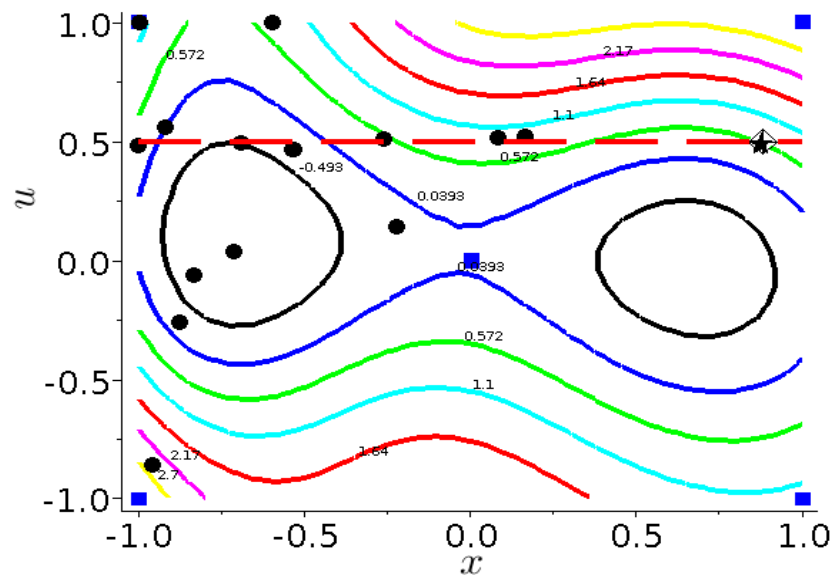


- $\diamond$  —  $(x^{next}, \mu)$
- $\star$  —  $(x^{t+1}, u^{t+1})$

# Kriging based optimization with uncertainties, U controlled

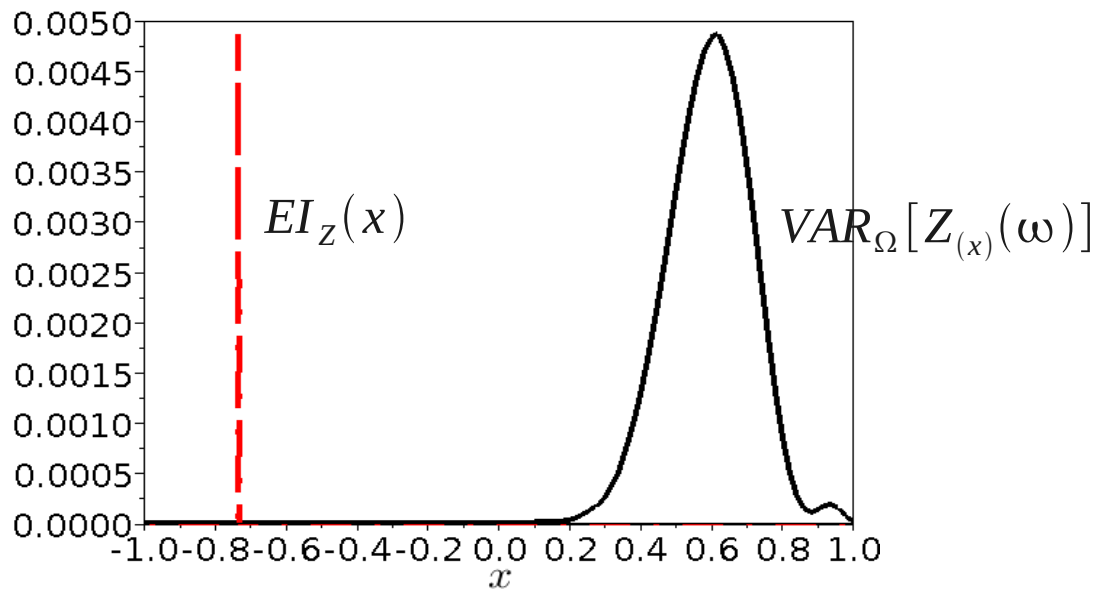
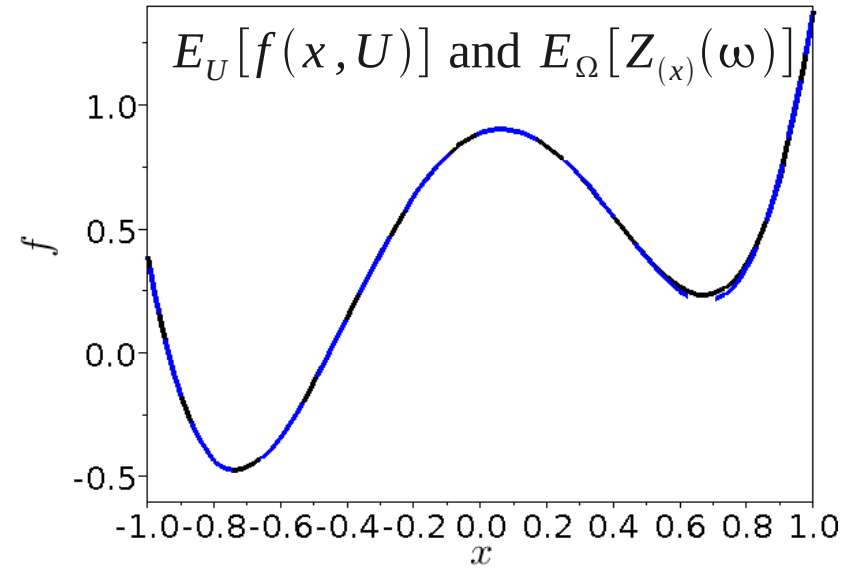
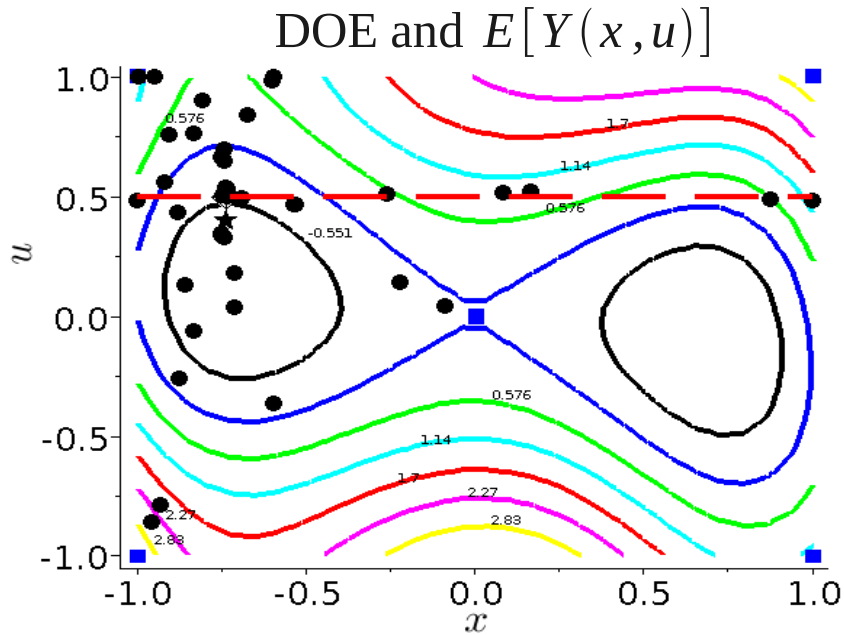
## 17th iteration

DOE and  $E[Y(x,u)]$



# Kriging based optimization with uncertainties, U controlled

## 50th iteration





# Kriging based optimization with uncertainties, U controlled

## Comparison tests

---

Compare « simultaneous opt and sampling » method to

1. A direct MC based approach :  
EGO based on MC simulations in  $f$  with fixed number of runs,  $s$ .  
Kriging with homogenous nugget to filter noise.
2. An MC-surrogate based approach :  
the MC-kriging algorithm.

# Kriging based optimization with uncertainties, U controlled

## Test functions

Test cases based on Michalewicz function

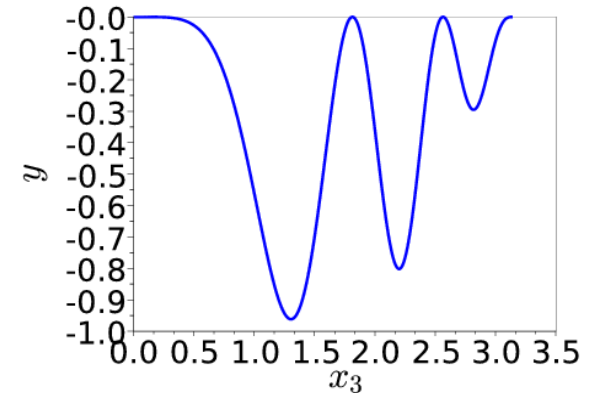
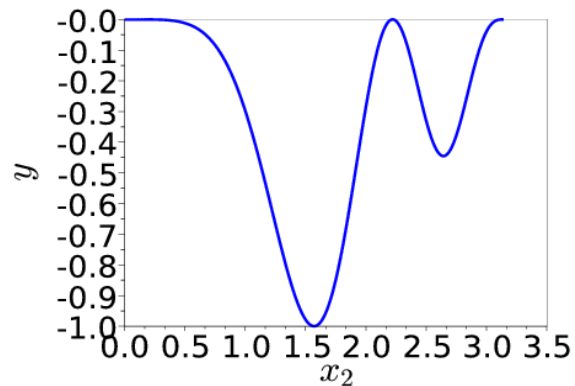
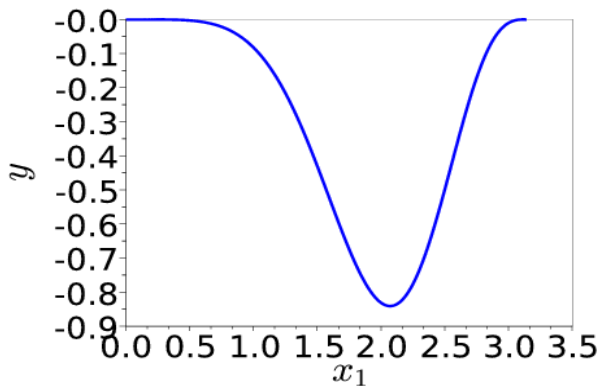
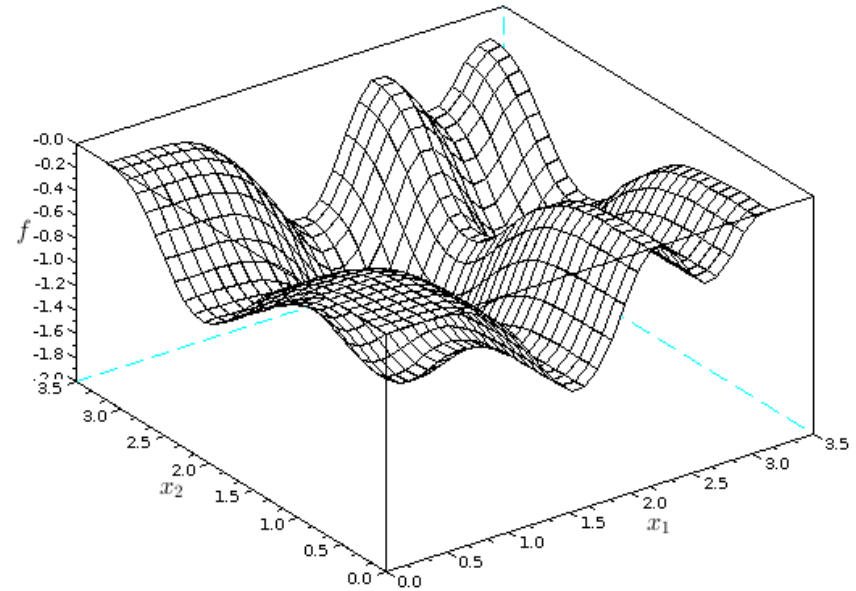
$$f(x) = -\sum_{i=1}^n \sin(x_i) [\sin(ix_i^2/\pi)]^2$$

$$f(x, u) = f(x) + f(u)$$

2D:  $n_x=1$   $n_u=1$   $\mu=1.5$   $\sigma=0.2$

4D:  $n_x=2$   $n_u=2$   $\mu=[1.5, 2.1]$   $\sigma=[0.2, 0.2]$

6D:  $n_x=3$   $n_u=3$   $\mu=[1.5, 2.1, 2]$   $\sigma=[0.2, 0.2, 0.3]$



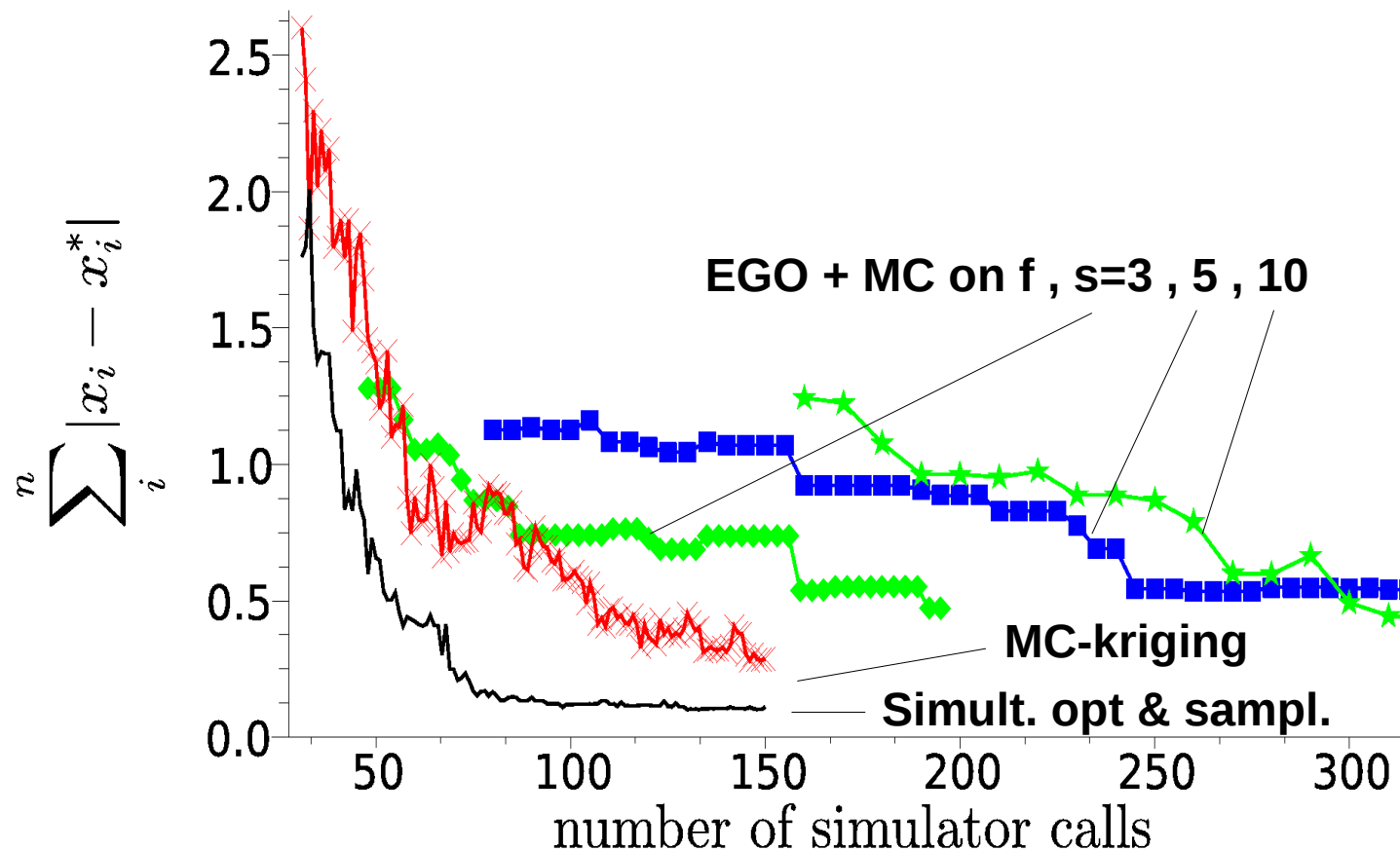
# Kriging based optimization with uncertainties, U controlled

## Test results

6D Michalewicz test case,  $n_{x=3} = 3$ ,  $n_U = 3$ .

Initial DOE: RLHS,  $m = (n_x + n_U) * 5 = (3 + 3) * 5 = 30$ ;

10 runs for every method.



# Partial conclusion

---

- $\min_x f(x, U)$

We have discussed spatial statistics to filter the noise → kriging based approaches.

- Limitation : number of dimensions ,  $\dim(x) + \dim(U) < 20$

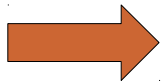
Beyond this, if the function  $f$  is not too costly, use stochastic evolutionary optimizers, which can be relatively robust to noise if properly tuned.

- Useful for optimizing statistical estimators which are noisy.
- No control over the  $U$ 's
- No spatial statistics (i.e. in  $S$  or  $S \times U$  spaces), pointwise approaches only.

# Outline of the talk

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1. Motivations for robust optimization
2. Formulations of optimization problems with uncertainties
3. Kriging-based approaches (costly functions)
  - No control on  $U$
  - With control on  $U$
4. Evolutionary approaches (non costly functions)
  - The general CMA-ES
  - Improvements for noisy functions :
    - Mirrored sampling and sequential selection
    - ~~Adding confidence to an ES~~



# Noisy optimization

## Evolutionary algorithms

---

Taking search decisions in probability is a way to handle the noise corrupting observed  $f$  values

→ use a stochastic optimizer, an evolution strategy (ES).

« elitism »

A simple (1 $\oplus$ 1)-ES

Initializations :  $x, f(x), m, C, t_{max}$ .

While  $t < t_{max}$  do,

Sample  $N(m, C) \rightarrow x'$

Calculate  $f(x'), t = t + 1$

▶ If  $f(x') < f(x)$ ,  $x = x', f(x) = f(x')$  Endif

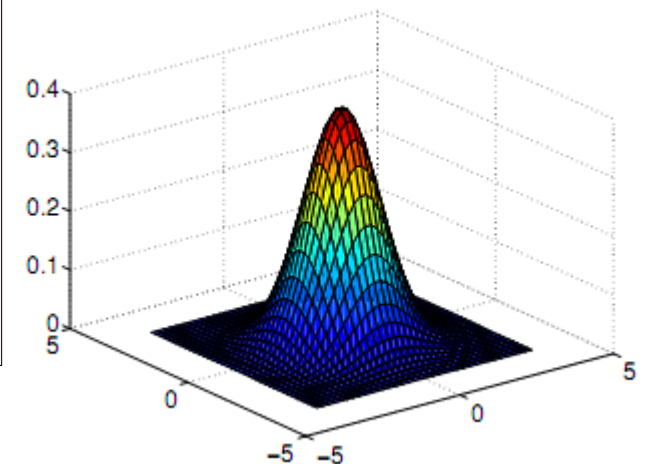
Update  $m$  (e.g.,  $m = x$ ) and  $C$

End while

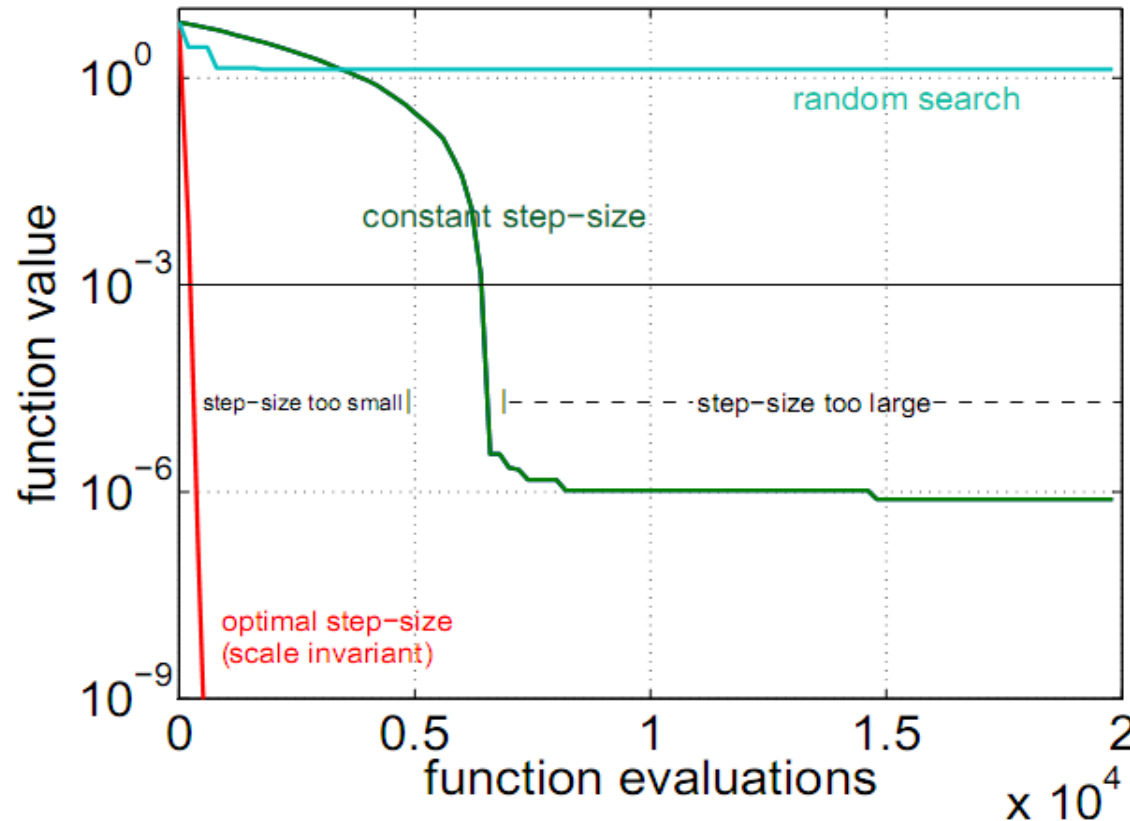
%(Scilab code)

$x = m + \text{grand}(1, 'mn', 0, C)$

2-D Normal Distribution



# Noisy optimization Adapting the step size ( $C^2$ ) is important



$$f(x) = \sum_{i=1}^n x_i^2$$

in  $[-0.2, 0.8]^n$   
for  $n = 10$

(A. Auger et N.  
Hansen, 2008)

Above isotropic ES(1+1) :  $C = \sigma^2 I$  ,  $\sigma$  is the step size.

With an optimal step size ( $\approx \|x\|/d$ ) on the sphere function, log linear speed that degrades only in  $O(d)$ .

# The population based CMA-ES

---

(N. Hansen et al., since 1996, now with A. Auger)

CMA-ES = *Covariance Matrix Adaptation Evolution Strategy* = optimization through sampling and updating of a multi-normal distribution.

A fully populated covariance matrix is build : pairwise variables interactions learned. Can adapt the step in any direction.

The state-of-the-art evolutionary / genetic optimizer for continuous variables.



## Noisy optimization flow-chart of CMA-ES

---

CMA-ES is an evolution strategy  $ES-(\mu, \lambda)$  :

Initializations :  $m, C, t_{max}, \mu, \lambda$

While  $t < t_{max}$  do,

Sample  $N(m, C) \rightarrow x^1, \dots, x^\lambda$

Calculate  $f(x^1), \dots, f(x^\lambda)$ ,  $t = t + \lambda$

Rank :  $f(x^{1:\lambda}), \dots, f(x^{\lambda:\lambda})$

Update  $m$  and  $C$  with the  $\mu$  bests,  
 $x^{1:\lambda}, \dots, x^{\mu:\lambda}$

End while

$m$  et  $C$  are updated with

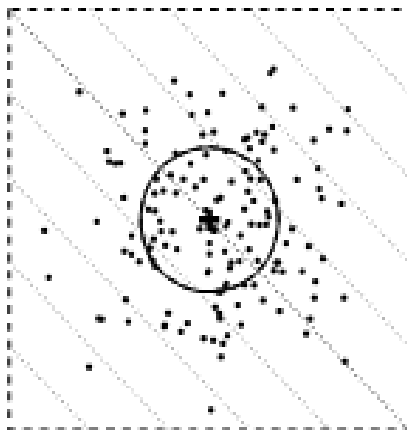
- the best **steps** (as opposed to points),
- a **time cumulation** of these best steps.

# Noisy optimization

## CMA-ES : adapting $C^2$ with good steps

(A. Auger et N. Hansen, 2008)

Initialization :  $m \in S$  ,  $C = I$  ,  $c_{cov} \approx 2/n^2$



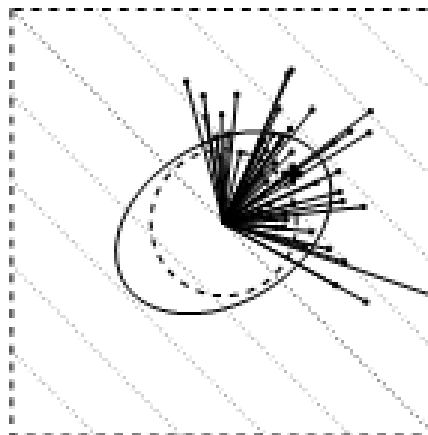
sampling

$$x^i = m + y^i$$

$$y^i \propto N(0, C)$$

$$i = 1, \dots, \lambda$$

calculate  $f$

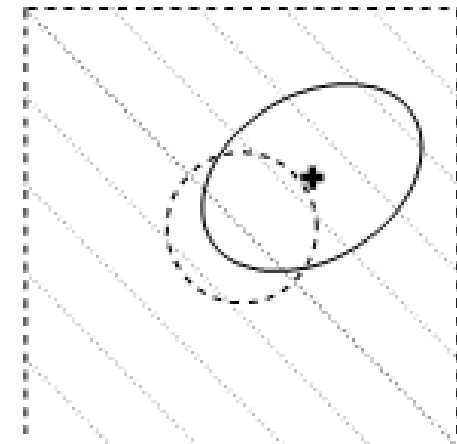


selection

$$y_w = \frac{1}{\mu} \sum_{i=1}^{\mu} y^{i:\lambda}$$

rank 1  $C$  update

$$C \leftarrow (1 - c_{cov})C + c_{cov} \mu y_w y_w^T$$



update  $m$

$$m \leftarrow m + y_w$$

## Noisy optimization

# The state-of-the-art CMA-ES

---

(A. Auger and N. Hansen, *A restart CMA evolution strategy with increasing population size*, 2005)

### Additional features :

- Steps weighting,  $y_w = \sum_{i=1}^{\mu} w_i y^{i:\lambda}$
- Time cumulation of the steps.
- Simultaneous rank 1 and  $\mu$  covariance adaptations.
- Use of a global scale factor,  $C \rightarrow \sigma^2 C$ .
- Restarts with increasing population sizes (unless it is the 2010 version with mirrored sampling and sequential selection, see later)

Has been used up to  $d \sim 1000$  continuous variables.

---

## Noisy optimization

- The general CMA-ES
- Improvements for noisy functions :  
Mirrored sampling and sequential selection



# Resampling, noise and evolutionary algorithms

---

$CMA-ES(\mu, \lambda)$  can optimize many noisy functions because

1. it is not elitist

2. the choice of the next iteration average

$$m^{t+1} = m^t + \frac{1}{\mu} \sum_{i=1}^{\mu} y^{i:\lambda}$$

averages out errors (spatial sampling as a proxy for  $U$  sampling)

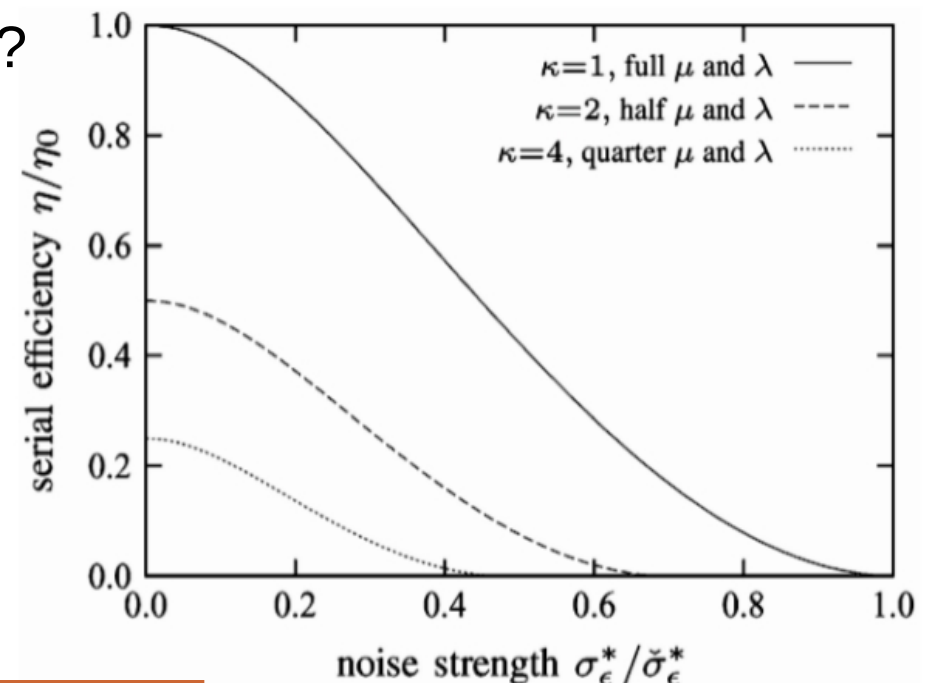
To improve convergence on noisy function, is it preferable

1. to resample  $\hat{f}(x) = \frac{1}{K} \sum_{i=1}^K \hat{f}^{(i)}(x)$

2. or to increase the population size ?

(for an equivalent increase in computation)

→ it is better to increase the population size. [Beyer and Sendhoff 2007, Arnold and Beyer 2006]



But one can still do better ...

---

# Noisy optimization, improved optimizers

## Mirrored sampling and sequential selection (1)

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D. Brockhoff, A. Auger, N. Hansen, D. V. Arnold, and T. Hohm. *Mirrored Sampling and Sequential Selection for Evolution Strategies*, PPSN XI, 2010

A. Auger, D. Brockhoff, N. Hansen, *Analysing the impact of mirrored sampling and sequential selection in elitist Evolution Strategies*, FOGA 2011

(1+1)-CMA-ES with restarts surprisingly good on some functions (including multimodal functions with local optima)  
← small population advantage.

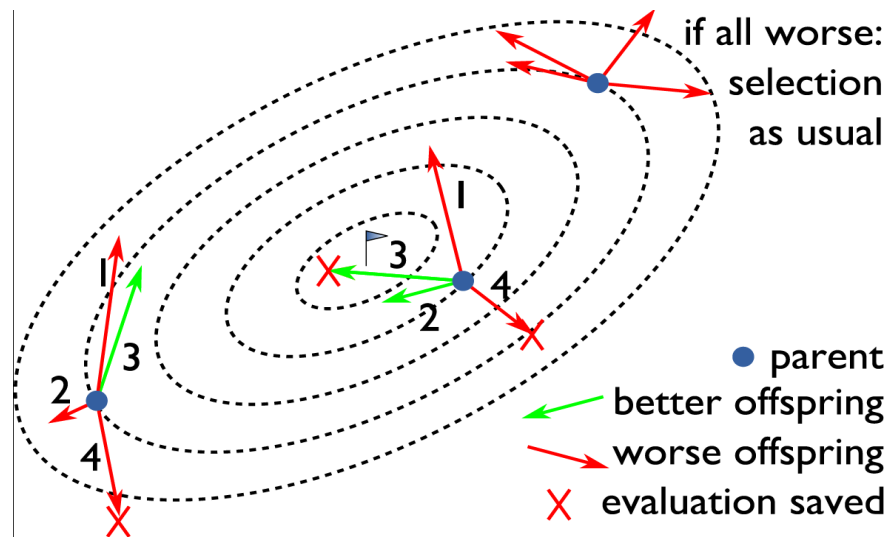
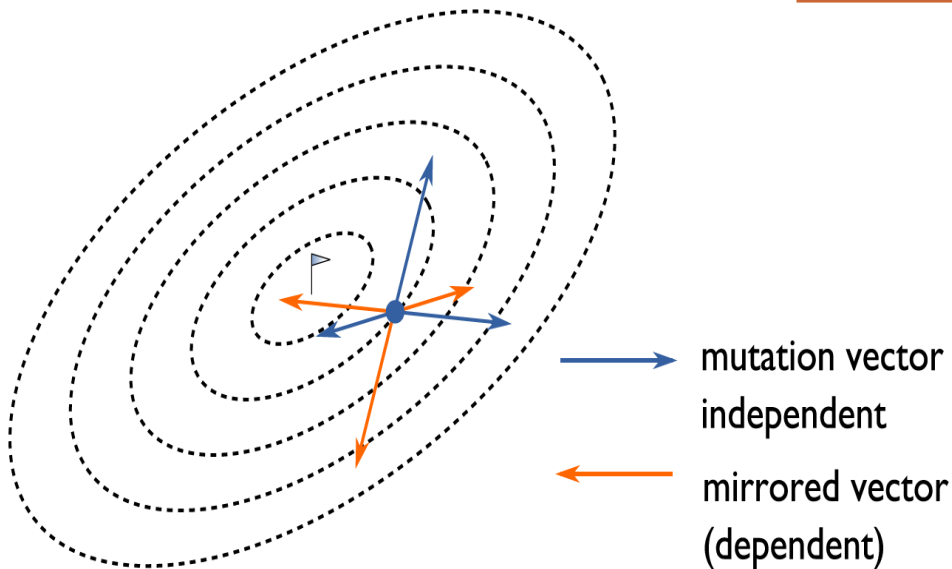
But « elitism » of (1+1)-ES bad for noisy functions : a lucky sample attracts the optimizer in a non-optimal region of the search space.

Question : how to design a fast local non-elitist ES ?

# Noisy optimization, improved optimizers

## Mirrored sampling and sequential selection (2)

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Derandomization via mirrored sampling : one random vector generates two offsprings. Often good and bad in opposite directions.

Sequential selection : stop evaluation of new offsprings as soon as a solution better than the parent is found.

Combine the two ideas : when an offspring is better than its parent, its symmetrical is worse (on convex level sets), and vice versa → evaluate in order  $m+y^1$  ,  $m-y^1$  ,  $m+y^2$  ,  $m-y^2$  , ... .

## Mirrored sampling and sequential selection (3)

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### Results :

small population, no elitism

(1,4)-ES with mirroring and sequential selection faster than (1+1)-ES on sphere function.

Theoretical result: Convergence Rate\* ES (1+1)=0.202 ,  
Convergence Rate (1,4ms)=0.223 .

[ Brockhoff et al., Mirrored sampling and sequential selection for evolution strategies, 2010. ]

Implementation within CMA-ES, tested in BBOB'2010\*\* (Black Box Optimization Benchmarking)

*Best performance among all algorithms tested so far on some functions of noisy testbed*

\* convergence rate  $\equiv -\lim_{t \rightarrow \infty} \frac{\ln(\text{distance to optimum})}{t}$  ,

cf. slope line of  $(\log(f), \text{time})$  earlier

\*\* <http://coco.gforge.inria.fr/bbob2010-downloads>



# Concluding remarks (1)

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## Today's story was :

- Optimization → difficult in the presence of noise → formulation of optimization in the presence of uncertainties → noisy functions
- → do spatial stats (kriging) [optimizer without U control → optimizer with U control]
- → stochastic optimizers directly applied to noisy functions.

## Each method has its application domain :

- Stochastic optimizers robust to noise cannot be directly applied to an expensive (simulation based) objective function. An intermediate surrogate is needed.
- Vice versa, kriging based method involve large side calculations : they are interesting only for expensive  $f$ 's.

## Concluding remarks (2)

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Many (most) methods were not discussed :

- Method of moments (Taylor expansions of the opt. criteria),
- FORM/SORM (local constraints approximations about probable points),
- Chance constraints and convex programming (worst U cases) ... .

A lot still to be done :

- effect of the a priori uncertainty model (law of random parameters),
- optimize quantiles,
- statistically joined criteria,
- kriging like approaches (spatial stats) in high dimension,
- ...

# Bibliography

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## Related books :

- A. Ben-Tal, L. El Ghaoui, A. Nemirovski, *Robust Optimization*, Princeton Univ. Press, 2009.
- R. E. Melchers, *Structural Reliability Analysis and Prediction*, Wiley, 1999.
- M. Lemaire, A. Chateauneuf, J.-C. Mitteau, *Structural Reliability*, Wiley, 2009.
- J. C. Spall, *Introduction to Stochastic Search and Optimization*, Wiley, 2003.
- *Multidisciplinary Design Optimization in Computational Mechanics*, P. Breitkopf and R. Filomeno Coehlo Eds., Wiley/ISTE, 2010.

## Articles :

- H.G. Beyer, B. Sendhoff, *Robust Optimization – A comprehensive survey*, Comput. Methods Appl. Mech. Engrg, 196, pp. 3190-3218, 2007.
- J. Janusevskis and R. Le Riche, *Simultaneous kriging-based estimation and optimization of mean response*, Journal of Global Optimization, Springer, 2012
- G. Pujol, R. Le Riche, O. Roustant and X. Bay, *L'incertitude en conception: formalisation, estimation*, Chapter 3 of the book *Optimisation Multidisciplinaire en Mécaniques : réduction de modèles, robustesse, fiabilité, réalisations logicielles*, Hermes, 2009 (in French)
- D. Salazar, R. Le Riche, G. Pujol and X. Bay, *An empirical study of the use of confidence levels in RBDO with Monte Carlo simulations*, in *Multidisciplinary Design Optimization in Computational Mechanics*, Wiley/ISTE Pub., 2010.