# Optimization under uncertainties by composing sampling and optimization with Bayesian algorithms

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- Optimization under uncertainty is a huge field: 3690 articles have "optimization" and "uncertainty" in their title (google scholar).
- We focus on
  - uncertainties within an optimization problem.
  - for costly functions and constraints.
- There are two aspects:
  1. How to formulate the problem.
  2. How to solve it

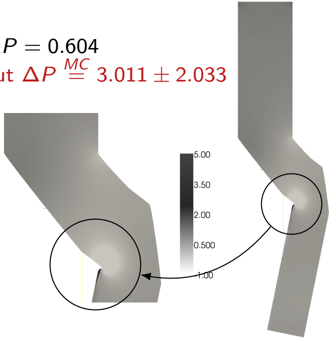
# A motivating example: robust air duct design

Minimize the pressure loss by changing the parameterized shape [Janusevskis and Le Riche, 2011]. Uncertain bottom position.

deterministic design

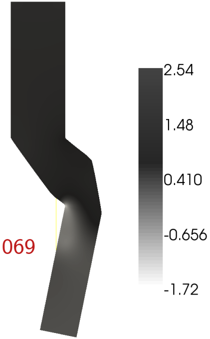
$\Delta P = 0.604$

but $\Delta P \overset{MC}{=} 3.011 \pm 2.033$



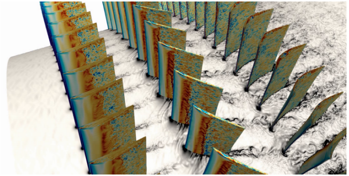

robust design

$\Delta P \overset{MC}{=} 1.198 \pm 0.069$

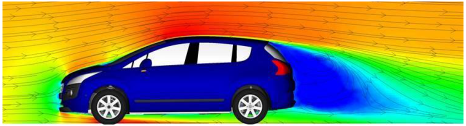



The deterministic optimization exploits mesh flaws. The robust optimization (mean of $\Delta P$) has two advantages: the final solution accounts for uncertainties and the numerical model flaws.

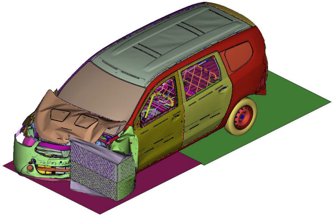
# Other examples of costly simulations & need for robust design



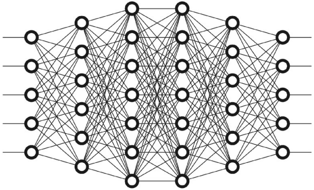
fan blades



design for drag

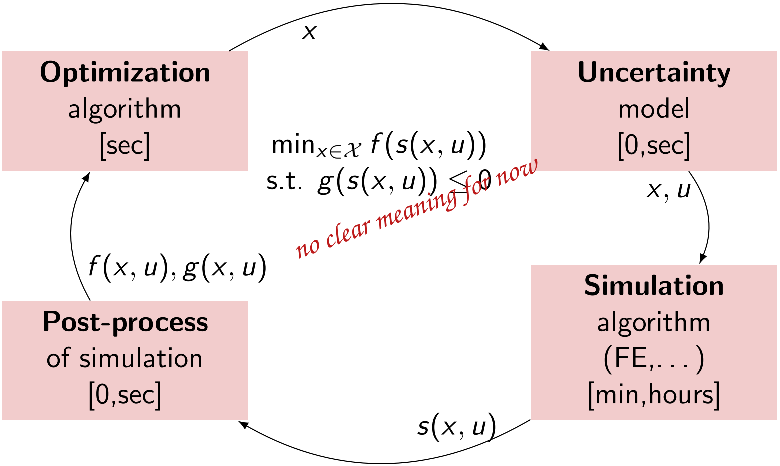


design for crash



hyper-parameter optimization in machine learning

# Computational context



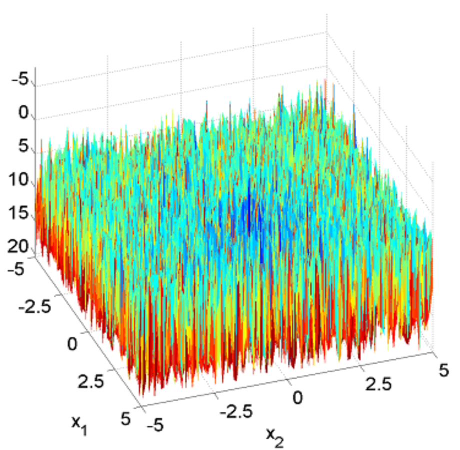
# The double $(x, U)$ parameterization

- $x \in \mathcal{X}$, vector of deterministic, controlled variables over which the optimization is carried out.
- $U : \Omega \to \mathcal{A}$, vector of random variables of pdf $p_{U|x}(.)$ (here, $p_U(.)$ for simplicity).
  $\Rightarrow s(x, U),\ f(x, U),\ g(x, U)$ are dependent random variables.
- This double parameterization, underlying Taguchi's methods in the 80's, is general. It is also called "augmented space" or "hybrid space". Cf. [Beyer and Sendhoff, 2007], [Pujol et al., 2009].

# Problem formulation: the noisy case

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

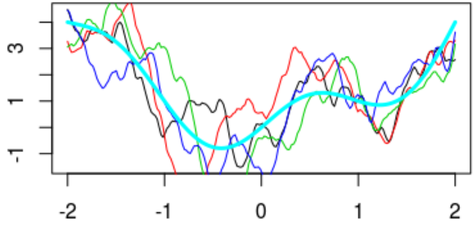
$$\min_{x \in \mathcal{X}} f(x, U)$$
$$\text{such that } g(x, U) \leq 0$$




It does not look good for local optimization ?
But sometimes (e.g., machine learning) one still wants to do it: $f()$ and $g()$ are inexpensive, their gradient known, large base of $u^i$'s available $\leftarrow$ scope of stochastic descent methods.
Not appropriate for costly functions.

# Problem formulation: statistical measures

Remove the uncertainty (mathematically) with statistical (risk) measures,




$f(x, u^i)$ in black, blue, red, green.

$\wp(x) = \mathbb{E} f(x, U)$ in thick light blue does not explicitely depend on the $u$'s (marginalized, implicit dependance through $p_U()$)

$$\min_x \wp\left(f(x, U), g(x, U)\right) \text{ s.t. } \wp^g(x) \leq 0$$

For example, an ideal formulation:

$$\min_{x \in \mathcal{X}} \mathbb{Q}_\alpha \left(f(x, U) \;\middle|\; g_i(x, U) \leq 0, i = 1, l\right)$$
$$\text{such that } 1 - \alpha' - \mathbb{P}(G(x)) \;\leq\; 0$$

# Today's formulations

- The choice of the measure changes the solution.
- First problem, robust optimization:

$$\min_x \mathbb{E}_U f(x, U)$$

- Second problem, RBDO with chance constraints:

$$x^* = \arg\min_x \; \mathbb{E}_U(f(x,U)) \;\text{ s.t. } \mathbb{P}(g_i(x,U) \le 0,\; i = 1,\ldots,l) \ge 1-\alpha \;.$$

cf. also [Park et al., 2006], [Baudoui, 2012]

# The double loop issue

1 Optimization loop: propose new $x$ based on past $[x, \rho(x)]$, $N$ times

$x$

2 Risk estimation loop: at a given $x$ loop on $u$'s to estimate $\rho(x)$.
For example, crude Monte Carlo and mean,
$u$
$\mathbb{E}f(x, U) \approx \frac{1}{M}\sum_{i=1}^{M} f(s(x, u^i))$

for a multiplicative cost of $N \times M \Rightarrow$ methods to avoid the double loop.

# Bibliographical hints

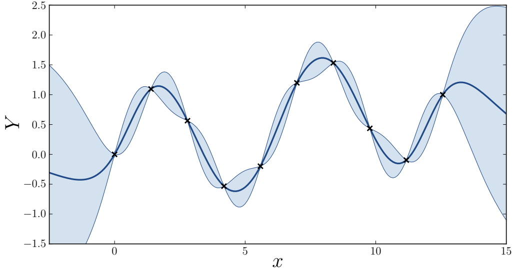
- The original reliability optimization problem (RBDO) is expressed in terms of reliability indices [Hasofer and Lind, 1974]: $\mathbb{P}(g(x, U) \leq 0) \approx \Phi(\beta(x))$. See [Valdebenito and Schuëller, 2010] for a review of FORM / SORM. Probabilistic interpretation is lost.
- Keep the noisy formulation: [Andrieu et al., 2011] for RBDO generalization of the Arrow-Hurwicz algorithm (stochastic gradient).

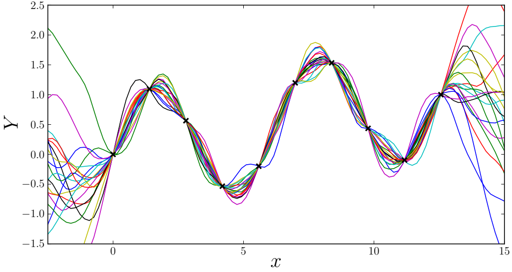
Rest of the talk: methods based on Gaussian processes approximations to $f$ and $g$.
Scope: costly, non-convex functions whose gradients if any are not known, 20 dimensions or less.
Start without uncertainties.

# Content

**Bayesian optimization under uncertainties**

# Gaussian Process Regression (kriging)




$Y(x)|Y(X){=}F$ is $\mathcal{N}(m(.), c(.,.))$ with

$$m(x) = \mathbb{E}[Y(x)|Y(X){=}F] = k(x,X)k(X,X)^{-1}F$$
$$c(x,x') = \mathrm{Cov}[Y(x), Y(x')|Y(X){=}F] = k(x,x') - k(x,X)k(X,X)^{-1}k(X,x')$$

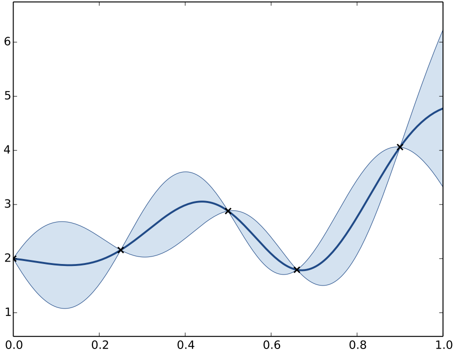
idem with the constraints (independent GPs).

# First, $\min_x f(x)$

**Global optimization** methods are a trade-off between

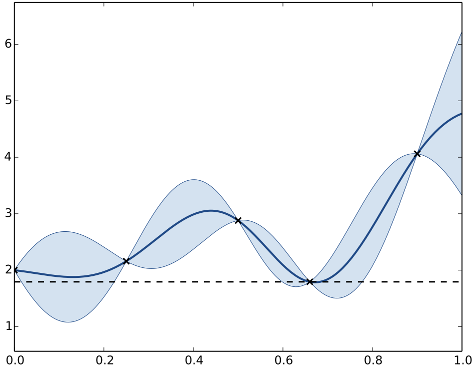
- Intensification in known good regions
- Exploration of new regions

**How can kriging models be helpful?**




(EGO figures from [Durrande and Le Riche, 2017])

In our example, the best observed value is 1.79

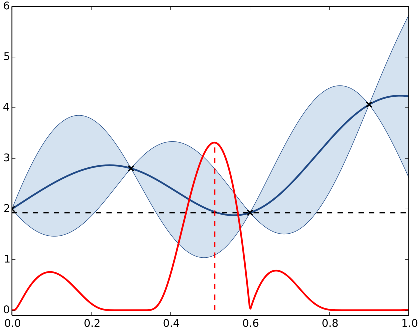



We need a criterion that uses the GP and seeks a compromise between exploration and intensification: the expected improvement . . .

# The Expected Improvement

Measure of progress: the improvement, $I(x) = \max\left(0, (\min(F) - Y(x))\right)$.
Acquisition criterion:
$\text{EI}(x) = \int_{-\infty}^{+\infty} I(x)\ dy(x) = \cdots = \sqrt{c(x,x)}\left[w(x)\text{cdf}_{\mathcal{N}}(w(x)) + \text{pdf}_{\mathcal{N}}(w(x))\right]$

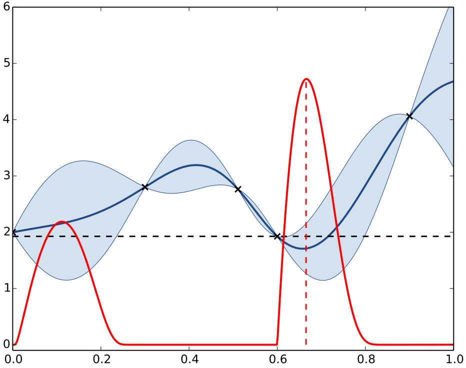
with $w(x) = \frac{\min(F) - m(x)}{\sqrt{(c(x,x))}}$.



# Expected Improvement

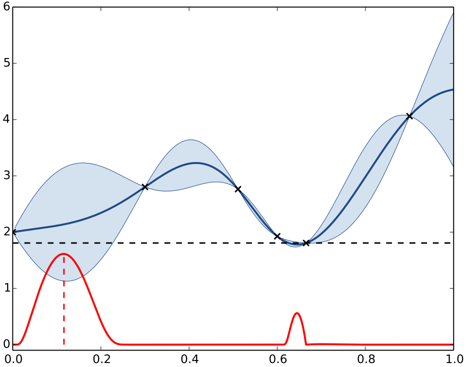
$$x^{t+1} = \arg\max_{x \in \mathcal{X}} \mathrm{EI}(x)$$

Let's see how it works... iteration 1



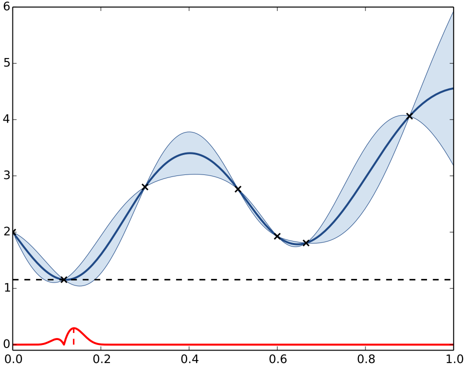
# Expected Improvement

$x^{t+1} = \arg\max_{x \in \mathcal{X}} \mathrm{EI}(x)$... iteration 2



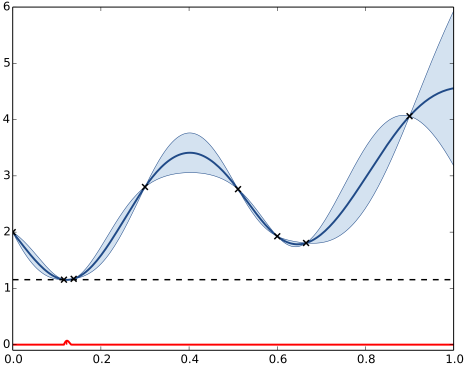
# Expected Improvement

$x^{t+1} = \arg\max_{x \in \mathcal{X}} \mathrm{EI}(x)$... iteration 3



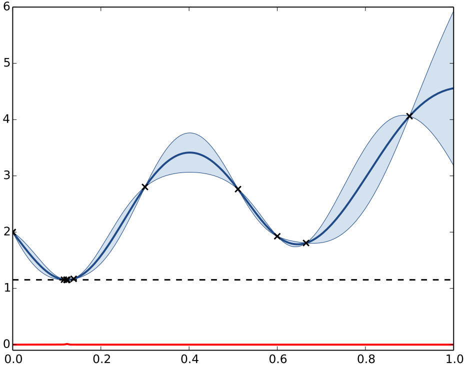
# Expected Improvement

$x^{t+1} = \arg\max_{x \in \mathcal{X}} \mathrm{EI}(x)$... iteration 4



# Expected Improvement

$x^{t+1} = \arg\max_{x \in \mathcal{X}} \mathrm{EI}(x)$... iteration 5



This algorithm is called **Efficient Global Optimization** (EGO, [Jones et al., 1998]):

1. make an initial design of experiments $X$ and calculate the associated $F$, $t = \texttt{length}(F)$
2. built a GP from $(X, F)$ (max. log-likelihood on $\sigma$ and $\theta_i$'s)
3. $x^{t+1} = \arg\max_x \mathrm{EI}(x)$ (with another optimizer, e.g. CMA-ES [Hansen and Ostermeier, 2001])
4. calculate $F_{t+1} = f(X_{t+1})$, increment $t$
5. stop ($t > t^{\max}$) or go to 2.

State-of-the-art for costly functions.

# Content

## Bayesian optimization under uncertainties

# Bayesian Optimization (BO) under uncertainties

Same as before, in the augmented space, other acquisition/sampling criteria

1. Create an initial Design of Experiments (DoE), $(x^i, u^i, f \text{ or } g(x^i, u^i))$ and use it to initialize 1/many Gaussian Processes (GPs) (in $\mathcal{X}$ or in augmented $\mathcal{X}, \mathcal{A}$).

   Then, there are 2 steps
2. Use the GP(s) to choose the next $x^{t+1}$
3. Use the GP(s) to choose the next $u^{t+1}$ knowing $x^{t+1}$ (2&3 may be simultaneous)
4. Evaluate $f(x^{t+1}, u^{t+1})$ and $g(x^{t+1}, u^{t+1})$ (i.e., $s(x^{t+1}, u^{t+1})$), update the GPs, stop or return to 2.

The acquisition/sampling criteria depend on the problem (// stat. measure and its estimator)

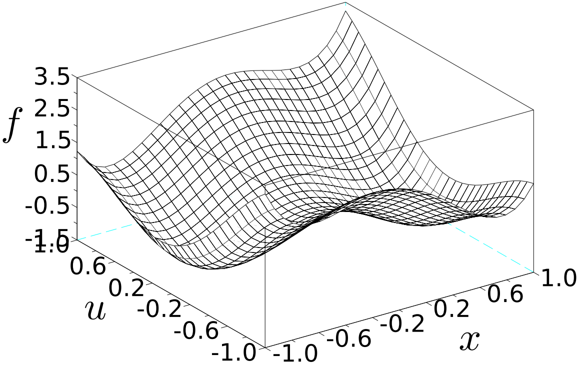
# Minimizing the mean

Objective

$$\min_{x \in \mathcal{X}} \mathbb{E} f(x, U)$$

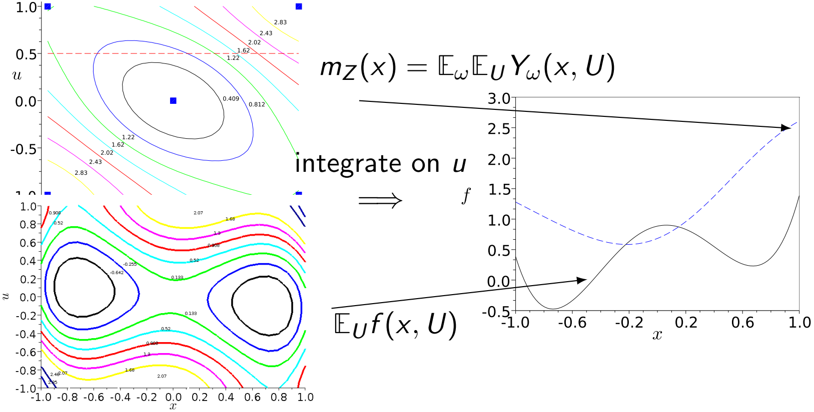
Cf. [Janusevskis and Le Riche, 2012]

GP built in the augmented space of $(x, u)$ variables.




Example: Camelback function, $U \sim \mathcal{N}(0.5, 0.01)$

- $f(x, u)$ is approximated by $Y_\omega^t(x, u)$
  $Y_\omega^t(x, u)$ the GP conditioned by the DoE at time $t$
- $\mathbb{E}_U f(x, U)$ is approximated by $Z_\omega^t(x) := \mathbb{E}_U Y_\omega^t(x, U)$
  $Z_\omega^t(x)$ the integrated process.



The integrated process

$$Z_\omega^t(x) := \mathbb{E}_U Y_\omega^t(x, U) = \int_{\mathcal{A}} Y_\omega^t(x, u) p_U(u) du$$

is a linear transformation of the Gaussian process $Y^t(,) \Rightarrow$ it is Gaussian and fully defined by its mean and covariance

$$m_Z(x) = \int_{\mathcal{A}} m(x, u) p_U(u) du$$
$$c_Z(x, x') = \int_{\mathcal{A}} \int_{\mathcal{A}} c((x, u), (x', u')) p_U(u) p_U(u') du du'$$

(analytical expressions given in [Janusevskis and Le Riche, 2012] for $U$ Gaussian, otherwise the integrations needs to be done numerically)

$Z^t_\omega(x)$ is just anoter GP so, back to the minimization of the average, the next $x$ can be found by maximization of the expected improvement,

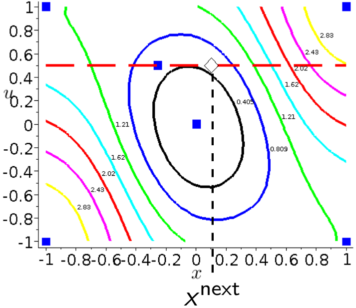
$$x^{\text{next}} \;=\; max_{x\in\mathcal{X}} \text{EI}_Z(x)$$

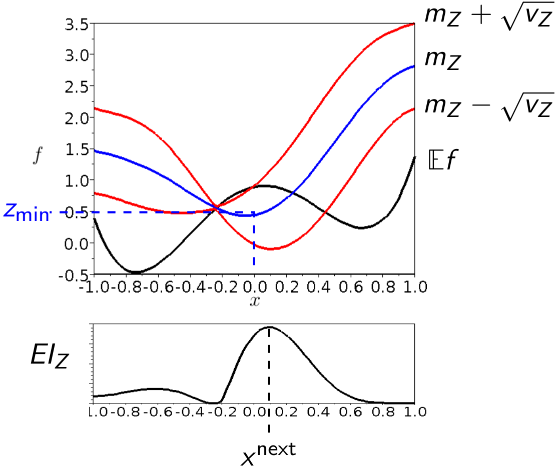
where, remember,

$$\text{EI}_Z(x) = \sqrt{c_Z(x,x)}\,[w(x)\text{cdf}_{\mathcal{N}}(w(x)) + \text{pdf}_{\mathcal{N}}(w(x))] \quad \text{with} \quad w(x) = \frac{z_{\min} - m_Z(x)}{\sqrt{(c_Z(x,x))}}.$$

But $Z(x)$ is not observed so define $z_{\min} := \min(m_Z(X))$.

Start EGO on $Z(x)$ ...




**$x$ ok. What about $u$, which we need to call the simulator?**

# Choose $u$ knowing $x^{\text{next}}$

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

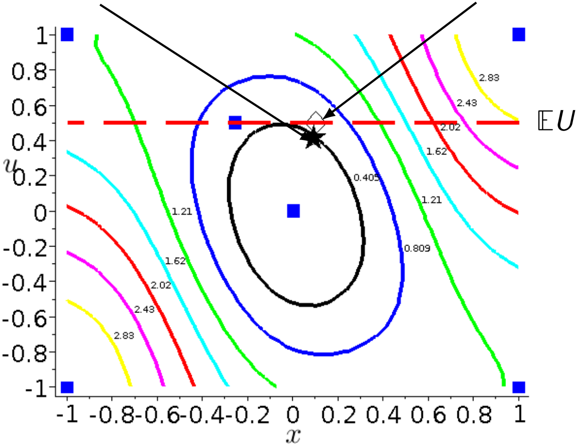
Choose $(x^{t+1}, u^{t+1})$ that provides the most information, i.e., which minimizes the one-step-ahead variance[1] of the integrated process at $x^{\text{next}}$:

$$(x^{t+1}, u^{t+1}) \;=\; \arg \min_{(x,u)\in\mathcal{X}\times\mathcal{A}} \mathbb{V}[Z^{t+1}(x^{\text{next}})]$$

Can be done because the variance can be calculated without calling $f$.

[1] See Stepwise Uncertainty Reduction methods (SUR).

$$x^{t+1} = \arg\min_{(x,u)} \mathbb{V}[Z^{t+1}(x^{\text{next}})] \qquad x^{\text{next}} = \arg\max_x EI_Z^t(x)$$



## $\min_x \mathbb{E}f(x,U)$ with EGO in augmented space

Putting it together:

1 Create an initial Design of Experiments (DoE), $(x^i, u^i, f(x^i,u^i))$

While budget no exhausted or other stopping criterion

Update the conditional GP $Y^t(x,u)$ from last DoE. The updated $Z^t(x)$ stems from it.

2 Maximize EI of $Z^t(x) \;\rightarrow\; x^{\text{next}}$

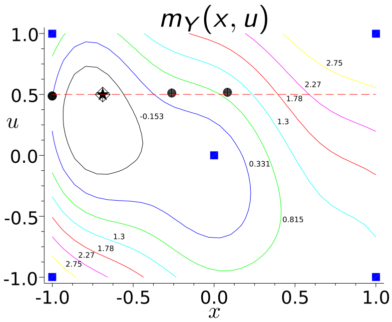
2' & 3 Minimize $\mathbb{V}[Z^{t+1}(x^{\text{next}})] \;\rightarrow\; x^{t+1} \& u^{t+1}$

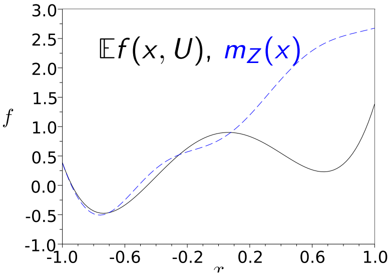
Calculate $f(x^{t+1}, u^{t+1})$, update DoE, $t \leftarrow t+1$

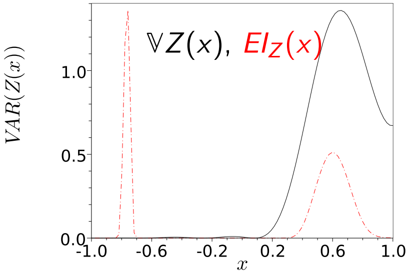
End while

3 (nonlinear, multimodal) sub-optimizations involved but they do not call the expensive $f$. Use a global optimizer (e.g., CMA-ES or restarted BFGS).

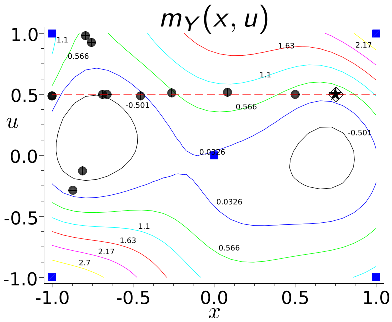
# Example: 2D Camelback function, iteration 6

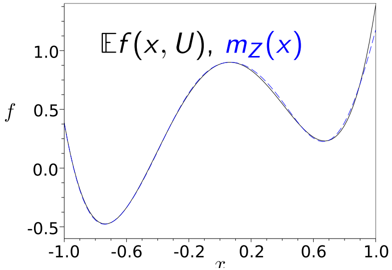


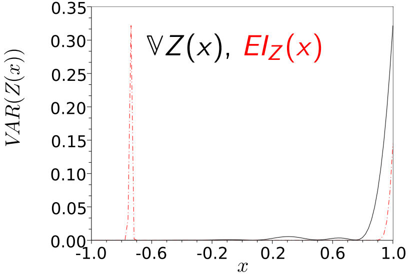



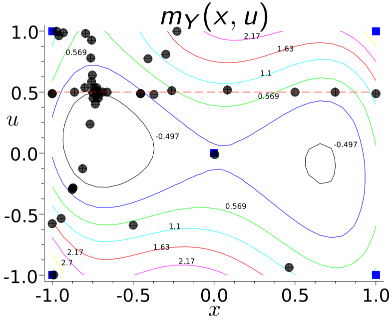
# Example: 2D Camelback function, iteration 14

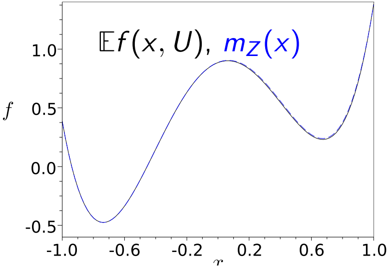


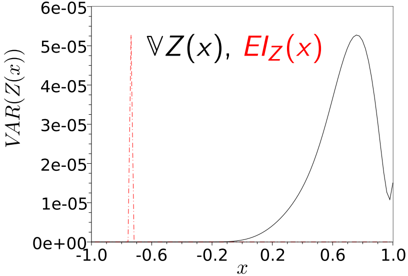



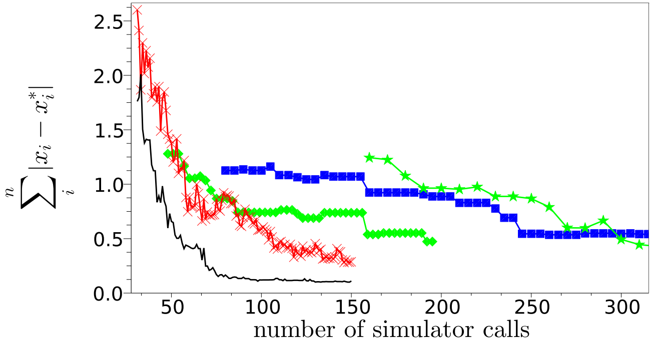
# Example: 2D Camelback function, iteration 50



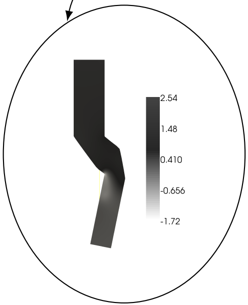



Example: 6D Michalewicz function, convergence averaged over 10 runs




designed with EI-VAR




EI-VAR, MC-kriging, and brute force MC for $N = 3$ (diamonds), 5 (squares), 10 (stars) samples

$\Rightarrow$ working in the augmented space is worth the effort

# Content

**Bayesian optimization under uncertainties**

# Mean minimization with chance constraints

From [El Amri et al., 2019]. The problem is:

$$x^* = \arg\min_{x \in \mathcal{X}} \; \mathbb{E}_U(f(x,U)) \text{ s.t. } \mathbb{P}(g_i(x,U) \leq 0, \; i = 1,\ldots,l) \geq 1 - \alpha \; .$$

- $\mathbb{E}_U[f(x,U)] = z(x)$ ,
- $$\begin{aligned} \mathbb{P}(g_i(x,U) \leq 0, \; i = 1,\ldots,l) \geq 1 - \alpha &\Leftrightarrow \mathbb{E}_U[\mathbb{1}_{\{g_i(x,U)\leq 0, \; i=1,\ldots,l\}}] \geq 1 - \alpha \; , \\ &\Leftrightarrow 1 - \alpha - \mathbb{E}_U[\mathbb{1}_{\{g_i(x,U)\leq 0, \; i=1,\ldots,l\}}] \leq 0 \; , \\ &\Leftrightarrow c(x) \leq 0 \; . \end{aligned}$$

## Problem of interest

$$x^* = \arg\min_{x \in \mathcal{X}} \; z(x) \text{ s.t. } c(x) \leq 0 \; .$$

# BO formulation for chance constraints

Let $F^{(t)}$ and $G_i^{(t)}$ denote the Gaussian processes conditioned on the $t$ observations

$$F^{(t)}(x,u) \sim \mathcal{GP}\left(m_F^{(t)}(x,u), k_F^{(t)}(x,u;x',u')\right),$$
$$\forall i = \{1,\ldots,l\},\; G_i^{(t)}(x,u) \sim \mathcal{GP}\left(m_{G_i}^{(t)}(x,u), k_{G_i}^{(t)}(x,u;x',u')\right).$$

Like in slide 23,

$$Z^{(t)}(x) = \mathbb{E}_U[F^{(t)}(x,U)] \sim \mathcal{GP}(m_Z^{(t)}(x), k_Z^{(t)}(x,x')),$$

and

$$C^{(t)}(x) = 1 - \alpha - \mathbb{E}_U[\mathbb{1}_{\{G_i^{(t)}(x,U)\leq 0,\; i=1,\ldots,l\}}]$$

$C^{(t)}(x)$ is not Gaussian

**The Feasible Improvement**

$$FI^{(t)}(x) = I^{(t)}(x)\mathbb{1}_{(C^{(t)}(x)\leq 0)} = \max(0, z_{\min}^{\text{feas}} - Z^{(t)}(x))\mathbb{1}_{(C^{(t)}(x)\leq 0)},$$

where

$$z_{\min}^{\text{feas}} = \min_{x\in\mathcal{X}_t} m_Z^{(t)}(x) \text{ t.q. } \mathbb{E}[C^{(t)}(x)] \leq 0.$$

$z_{\min}^{\text{feas}}$ is (relatively) easy to calculate because $\mathbb{E}[C^{(t)}(x)]$ is an integral of $\text{CDF}_{\mathcal{N}}$.

This FI is a generalization of that in [Schonlau et al., 1998, Sasena et al., 2002] to non-Gaussian $g$.

## The Expected Feasible Improvement

$$EFI(x) \;=\; \mathbb{E}[(z_{\text{min}}^{\text{feas}} - Z^{(t)}(x))^{+} 1_{\{C^{(t)}(x) \leq 0\}}] \;=\; EI_{Z}^{(t)}(x)\mathbb{P}(C^{(t)}(x) \leq 0)\ .$$

because of the independence between $Z^{(t)}$ and $C^{(t)}$.

The first term, $EI_Z(x)$, is known analytically (sl. 24).
The second, $\mathbb{P}(C^{(t)}(x) \leq 0)$, is estimated by Monte Carlo with Common Random Numbers to have a smooth (although biased) function.
Then,

$$x^{t+1} = \arg\max_{x \in \mathcal{X}} EFI^{(t)}(x).$$

To simplify, here $x^{\text{next}} = x^{t+1}$.

# Sampling criterion

## General principle

Minimize the variance of the measure of progress (I or FI) at the next step $(t+1)$ at the location of interest $(x^{\text{next}})$: $u^{t+1} \;=\; \arg\min_{u\in\mathcal{A}} S(u)$

- In [Janusevskis and Le Riche, 2012], no constraint: $\mathbb{V}(Z^{(t+1)}(x^{t+1}))$
- With chance constraints, ideally: $\mathbb{V}\Big((z_{\min}^{\text{feas}} - Z^{(t+1)}(x^{t+1}))^{+} 1_{\{C^{(t+1)}(x^{t+1})\leq 0\}}\Big)$

## Aggregated variance

A proxy to the variance of the feasible improvement, easier to calculate, is

$$S(\tilde{u}) = \mathbb{V}((z_{\min}^{\text{feas}} - Z^{(t+1)}(x^{t+1}))^{+})\int_{\mathbb{R}^m} \mathbb{V}(1_{\{G_i^{(t+1)}(x^{t+1},u)\leq 0,\ i=1:l\}})p_U(u)du\ .$$

The first term is the variance of the improvement at the next step, the second is the average variance of the feasibility (without confidence).

**Algorithm 1** Bayesian Optimization with chance constraints

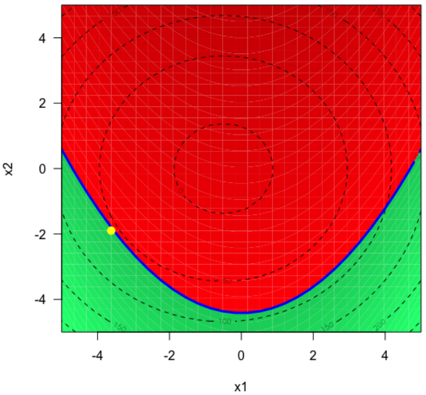
**Require:** Initial DoE in the augmented space $(X^t, U^t)$ and the simulator responses, $\alpha$ confidence level.

**Ensure:** Reliable and robust optimal solution

```
for j = 1 to itermax do
    Create GP models F^(t) and G^(t)_{1...l} for the objective and constraint functions;
    Calculate mean objective GP model Z^(t);
    Maximize EFI to choose x^{t+1};
    Minimize S to choose u^{t+1};
    Call simulator responses f(x^{t+1}, u^{t+1}), g_{1...l}(x^{t+1}, u^{t+1});
    Update DoE with (x^{t+1}, u^{t+1}).
end for
```

# Analytical example

- $f(x,u) = 5(x_1^2 + x_2^2) - (u_1^2 + u_2^2) + x_1(-u_1 + u_2 + 5) + x_2(u_1 - u_2 + 3)$,
- $g(x,u) = -x_1^2 + 5x_2 - u_1 + u_2^2 - 1$.
- where $x \in [-5,5]^2$, $U \sim \mathcal{U}([-5,5]^2)$ and $\alpha = 0.05$.




dashed line: contours of $\mathbb{E}_U f(x,U)$.

green/red: $c(x) \leq 0$ / $c(x) > 0$

yellow bullet: $x^*$

## Analytical example

- Initial Doe $\longrightarrow$ Random LHS (size 8),
- Covariance kernel: Matern 5/2,
- 20 runs,
- $\mathbb{P}(C^{(t)}(x) \leq 0) \approx \frac{1}{M'} \sum_{i=1}^{M'} 1_{\left(1-\alpha-\frac{1}{M}\sum_{j=1}^{M} \mathbb{1}_{\left(g_i^{(t)}(x,u_j)\leq 0\right)} \leq 0\right)}$
  - $M = 300$ (Common Random Numbers), $M' = 1000$ trajectories,
- $\mathbb{V}((z_{\text{min}}^{\text{feas}} - Z^{(t+1)}(x_{t+1}))^+)$
  - 20 realizations of $F^{(t)}(x_{t+1}, \tilde{u})$ (by quantization).

## Analytical example: alternative BO algorithms

- Algorithm 2:

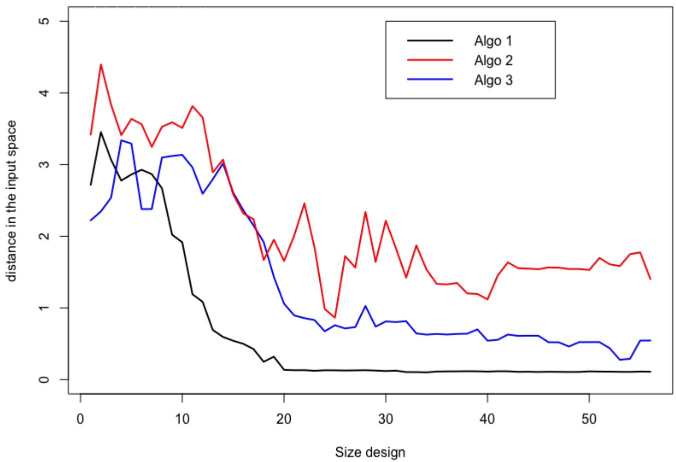
$$
\begin{aligned}
x^{t+1} &= \arg\max_x EI_Z^{(t)}(x) \quad \text{s.t.} \quad m_G^{(t)}(x,u)^{\lfloor(1-\alpha)M\rfloor:M} \leq 0 \\
u^{t+1} &\sim p_U()
\end{aligned}
$$

- Algorithm 3 ([Moustapha et al., 2016]):

$$
\begin{aligned}
x^{t+1} &= \arg\max_x EI_Z^{(t)}(x) \quad \text{s.t.} \quad m_G^{(t)}(x,u)^{\lfloor(1-\alpha)M\rfloor:M} \leq 0 \\
u^{t+1} &= \arg\min_u \frac{|m_G^{(t)}(x^{t+1},u)|}{\sigma_G^{(t)}(x^{t+1},u)}
\end{aligned}
$$

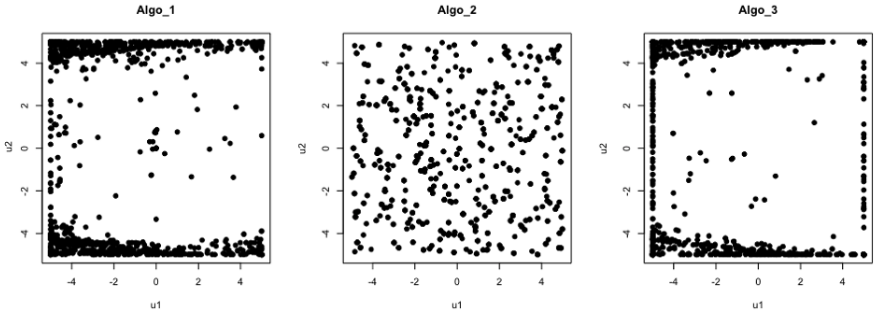
## **Analytical example**: convergence

$$\hat{x} \longmapsto ||\hat{x} - x^*|| \text{ where } \hat{x} = \arg\min_{x \in X^t} m_Z^{(t)}(x) \text{ t.q. } \mathbb{E}[C^{(t)}(x)] \leq 0.$$




EFI & aggregated variance are efficient at converging to $x^*$ through the feasible space

## **Analytical example**: $U$ samples




Algo 1 breaks the symmetry in $u_1$ because it accounts for both the objective and the constraint (Algo 2 and 3 account only for the constraint): $|x_2^*| > |x_1^*|$ makes $u_1 \approx -5$ contribute more to the improvement.

# Conclusions

- What is the solution in the end? Solve the problem one last time on GP means.
- For optimization under uncertainties, building statistical models in the joint space is complicated, not cheap, but it is worth it.
- Many improvements are needed:
  - Other risk measures
  - Simpler risk measure to optimize (they are all multimodal)
  - Parallel (batch versions): generate many $x^{t+1}$ and $u^{t+1}$ in an optimal way (e.g., [Ginsbourger et al., 2010])
  - ...

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