

Optimization under uncertainties: an overview with a focus on Gaussian processes

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Content

Optimization under uncertainties: an overview with a focus on Gaussian processes

Problem formulation

- Motivation and the two classes of variables
- Formulations as an optimization of statistical measures
- 2 Methods
 - A pointer to methods without metamodels
 - Approximation methods
 - Approaches based on stochastic gradients
 - Methods with metamodels
 - Overall scheme
 - Choice of x
 - Choice of *u* knowing *x*

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Goals of the class

- Optimization under uncertainty is a huge field: 3480 article have "optimization" and "uncertainty" in their title (google scholar).
- We focus on uncertainties within an optimization problem. There are two aspects:
 - How to formulate the problem.
 - ② How to solve it ← we will mainly cover approaches involving Gaussian processes (as they are the most integrated), and mention connexions.
- We will not cover statistical estimation (in particular simulation methods for reliability), generic adaptive design of experiments for kriging (in particular for constraints) beyond the strict minimum needed.



The deterministic optimization exploits mesh flaws. The robust optimization (mean of ΔP) has two advantages: the final solution accounts for uncertainties in production; the numerical model flaws are avoided.

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Besides this specific example, uncertainties affect simulation models (lack of knowledge, epistemic) and their working conditions (aleatory) and must be accounted for when the simulation is used within an optimization problem.



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The double (x, U) parameterization

- x ∈ X, vector of deterministic, controlled variables over which the optimization is carried out.
- $U : \Omega \to A$, vector of random variables of pdf $p_U(.)$. $\Rightarrow s(x, U), f(x, U), g(x, U)$ 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].

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- x ∈ X, vector of deterministic, controlled variables over which the optimization is carried out. U : Ω → A, vector of random variables of pdf p_U(.).
- Expl with a structure, s(,) is the stress and/or displacement:



- Noise homogeneous to x: r = x + U, both x and U are length, s(x + U, w).
- Noise exogenous to x: U perturbation to the load w, s(r, w + U).
- Noise as an error model for the simulation: s(r, w) + U.

Noise controlled by x: x tolerance class,
 s(r + xU, w) (any parameter of p_U() can be x's).

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Problem formulation: the noisy case

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

$$\min_x f(x, U)$$

such that $g(x, U) \leq 0$



It does not look good : gradients are not defined, what is the result of the optimization ? But sometimes (often!?) one still wants to do it: f() and g() are

inexpensive, large base of u^i 's available \leftarrow application scope of stochastic gradient methods.

Problem formulation: statistical measures

Remove the uncertainty (mathematically) by formulating the problem with statistical risk measures, either as a constrained optimization problem, f(x) = f(x) - f(

$$\min_{x} \mathbb{p}^{t}(x) \quad , \quad \mathbb{p}^{t}(x) = \mathbb{p}^{t} \left(f(x, U) \right)$$

such that $\mathbb{p}^{g}(x) \leq 0 \quad , \quad \mathbb{p}^{g}(x) = \mathbb{p}^{g} \left(g(x, U) \right)$

or through an aggregation of statistical measures (remember f(., U)and g(., U) are dependent), $\min_{v} \rho(x)$, $\rho(x) = \rho(f(x, U), g(x, U))$

or a combination thereof, $\min_{x} p(x)$ s.t. $p^{g}(x) \leq 0$.



Risk measures for the objective function (1/2)

The "robust" formulations, single criteria:

- $p^f \equiv expectation (\mathbb{E})$ as average performance.
 - \equiv variance (\mathbb{V}) as performance dispersion.
 - ≡ quantile (\mathbb{Q}_{α}) as guaranteed performance since α % of the realizations will be better. \mathbb{Q}_{50} , the median, as representative performance. \mathbb{Q}_{100} is the worst-case formulation.
 - \equiv a quantile difference $(\mathbb{Q}_{\alpha} \mathbb{Q}_{1-\alpha})$ as a performance dispersion.
 - \equiv super-quantile as guaranteed performance with an account for extreme values.

Risk measures for the objective function (2/2)

The "robust" formulations, multiple criteria:

- $f \equiv$ a multi-objective formulation accounting for an average performance and a deviation measure [Park et al., 2006], with various subsequent resolution approaches (goal programming, ordering, full Pareto, aggregations) and in particular
 - ≡ a linear combination of average and dispersion measures, typically $\mathbb{E}f(x, U) + \alpha \sqrt{\mathbb{V}f(x, U)}$: minimize average cost penalized by dispersion. For $f(x, U) \sim \mathcal{N}$, it is equivalent to the quantile (e.g. $\alpha = 1.645$ for \mathbb{Q}_{90}).

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Risk measures for the constraints

The "reliable" formulations:

 $p^g \equiv \alpha - \mathbb{P}(g(x, U) \le 0) \le 0$, as at least α % chances of satisfying the constraints.

$$\mathbb{P}(g(x, U) \le 0) = \int_{g(x, u) \le 0} p_U(u) du = \int_{\mathcal{A}} \mathbb{1}_{g(x, u) \le 0} p_U(u) du$$
$$= \mathbb{E}(\mathbb{1}_{g(x, u) \le 0})$$

- \equiv Equivalently, $\mathbb{Q}_{\alpha}(g(x, U)) \leq 0.$
- but other formulations involving $\mathbb{E}g(x, U)$ and $\mathbb{V}g(x, U)$ (common in the litterature) do not match the meaning of what a constraint is. What counts is the risk of not satisfying the constraint, not the average quantity by which it is violated.

Risk measures: illustrations









The choice of the risk measure changes the optimum and the mathematical properties of the problem!

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Risk measures for both objective and constraints

The robust and reliable formulations:

• They are based on the feasible trajectories, $[f(x, U) \mid g(x, U) \leq 0]$, used within the ρ^f measures, e.g., $\mathbb{E}(f(x, U) \mid g(x, U))$,

 \bullet associated to a constraint risk measure $\rho^g.$

An ideal series formulation:

• G(x) the random event "all constraints are satisfied at x", $G(x) \equiv \bigcap_i [g_i(x, U) \le 0] \leftarrow$ now several constraints $g_i(,)$,

$$\min_{x \in \mathcal{X}} \mathbb{Q}_{\alpha}(f(x, U) \mid G(x))$$
such that $\alpha' - \mathbb{P}(G(x)) \leq 0$

(to the best of my knowledge, no contribution to solve this problem: it cumulates the difficulties of quantile estimation and dependent criteria)

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The double loop issue

The cumulation of the search on x with the estimation of the risk measures creates a double loop that takes too long to calculate in the context of expensive functions.

(this, in addition with the importance of taking uncertainties into account, explains the number of articles dealing with both uncertainties and optimization.)



x

Risk estimation loop: at a given x loop on u's to estimate
$$p(x)$$
.

For example, crude Monte Carlo and mean, $\mathbb{E} f(x, t) \approx \frac{1}{2} \sum_{i=1}^{m} f(z(x, t))$

$$-\mathbb{E}f(x,U)\approx \frac{1}{m}\sum_{i=1}^{m}f(s(x,u'))$$

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

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Approximation methods

The original reliability optimization problem (RBDO) is transformed into a problem expressed in terms of *reliability indices*

 $\min_{x \in \mathcal{X}} f(x)$ $\min_{x \in \mathcal{X}} f(x)$ \Rightarrow such that $\mathbb{P}(g(x, U) < 0) > \alpha$ such that $\beta(x) > \beta^{\text{tol}}$ where $\beta^{tol} = \Phi^{-1}(\alpha)$ and the reliability index is solution of $\beta(x) = \arg \min \|v\|$ such that $g(x, T_{vu}(v)) > 0$ and T_{yy} () is a transformation from a vector of random variables V that are standard normal to U, typically the inverse of $v = \Phi^{-1}(CDF(u)) \leftarrow$ trade the cost of an integral for an optimization problem.

See I. Papaioannou's class for transformation, [Hasofer and Lind, 1974] for the reliability indices, [Valdebenito and Schuëller, 2010] for a review of FORM / SORM in optimization R. Le Riche (CNRS) Optimization under uncertainties Sept. 2019 19 / 61



If $g(x, T_{vu}(.))$ is linear in v, there is an equivalence with the probabilities, $\mathbb{P}(g(x, u) \leq 0) = \Phi(\beta(x))$. The equivalence exists also with quadratic $g(x, T_{vu}(.))$, but in general it is an approximation.

Approximation methods: 2, 1, 0 loop

2 loops

- Optimization algorithm: proposes x^{t+1}
- Calculate β(x^{t+1}) (reliability analysis, sub-optimization with iteration on u through T_{vu}(v)) and f(x^{t+1})
 Stop or go back to 1

1 loop

• Optimization algorithm: proposes x^{t+1} and approximate reliability analyses, e.g., $\widehat{\beta}(x^{t+1}) = \beta(x^t) + \nabla_x \beta(x^t)(x^{t+1} - x^t)$ Stop or sometimes update approximation $\widehat{\beta}(.)$ and go back to 1

"decoupled"

(find worst uncertainty) $\max_{v} g(x^{t}, T_{vu}(v))$ such that $||v|| = \beta^{\text{tol}}$ (optim with fixed uncertainty) $\min_x f(x)$ such that $g(x, T_{vu}(v^t))$

 v^t

 \rightleftharpoons

x^t

Optimization under uncertainty with stochastic gradients

Many risk measures can be written as sums over u samples:

$$\frac{1}{N} \sum_{i=1}^{N} f(x, u^{i}) \stackrel{N \nearrow}{\to} \mathbb{E}f(x, U)$$
$$\frac{1}{N^{2}} \sum_{i
$$\frac{1}{N} \sum_{i=1}^{N} \mathbb{1}_{g(x, u^{i}) \le 0} \stackrel{N \nearrow}{\to} \mathbb{P}(g(x, U) \le 0)$$$$

which makes them appropriate for stochastic gradients. Parallel with machine learning methods where the u_i 's are data samples.

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Example with the mean minimization, the Arrow-Hurwicz iteration reads

$$\begin{aligned} x^{i+1} &= \mathsf{Proj}_{\mathcal{X}} \left(x^i - \varepsilon_i \nabla_{\!\!x} f(x^i, u^i) \right) \quad , \quad u^i \sim p_U(.) \quad , \\ &\sum_{i \in \mathbb{N}} \varepsilon_i = +\infty \quad , \quad \sum_{i \in \mathbb{N}} \varepsilon_i^2 < +\infty \end{aligned}$$

If $\nabla_x f(x^i, u^i)$ is known and an unbiased noisy sample of $\nabla_x \mathbb{E} f(x, U)$, the algorithm converges to a local minimizer of the mean.

Cf. [Andrieu et al., 2011] for RBDO formulation & theory (like what do you do with the gradient of $\mathbb{1}_{g(x,u_i) \leq 0}$).

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Methods with metamodels (kriging)

- 1 Create an initial Design of Experiments (DoE), (xⁱ, uⁱ, f or g(xⁱ, uⁱ)) and use it to initialize 1/many Gaussian Processes (GPs) (in X or in augmented X, A). Then, there are 2 steps
- 2 Use the GP(s) to choose the next x^{t+1}
- 3 Choose the next u^{t+1} knowing x^{t+1}
- 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.

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Methods with metamodels (kriging)

Ideally, x^{t+1} and u^{t+1} should be such that

- x^{t+1} guides the search towards good regions (low risk estimators): global optimization.
- u^{t+1} helps improve the risk estimators at x^{t+1} : statistical estimation.
- both x^{t+1} and u^{t+1} once evaluated, contributed to an improved GP in important parts of the design space.

It is sometimes possible to build the metamodel in the lower dimensional space of real variables $x^{\text{real}}(x, u)$, for example the earlier radius where $x^{\text{real}} = r = x + u$, Y(x, u) = Z(x + u).

Batch versions: many x^{t+1} 's, many u^{t+1} 's. Ex: brute force Monte Carlo (MC), parallel EGO [Ginsbourger et al., 2010].

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Global optimization methods are a trade-off between

- Intensification in known good regions
- Exploration of new regions



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

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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

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$$\mathsf{EI}(x) = \int_{-\infty}^{+\infty} \max\left(0, (\min(F) - Y(x))\right) \, dy(x) = \cdots = \sqrt{c(x, x)} \left[w(x) \mathsf{cdf}_{\mathcal{N}}(w(x)) + \mathsf{pdf}_{\mathcal{N}}(w(x))\right]$$

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



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



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Let's see how it works... iteration 2



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Let's see how it works... iteration 3



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Let's see how it works... iteration 4



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Let's see how it works... iteration 5



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

- make an initial design of experiments X and calculate the associated F, t = length(F)
- 2 built a GP from (X, F) (max. log-likelihood on σ and θ_i 's)
- X_{t+1} = arg max_x EI(x) (with another optimizer, e.g. CMA-ES [Hansen and Ostermeier, 2001])

• calculate
$$F_{t+1} = f(X_{t+1})$$
, increment t

5 stop
$$(t > t^{max})$$
 or go to 2.

- + EGO provides a good trade-off between intensification and exploration without arbitrary parameters.
- + It requires few function observations to get close to optima.
- $\times\,$ EGO does not converge in the traditional sense: it creates dense samples in the volume of S. The efficiency comes from the order in which points are sampled.

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Consider an optimization problem under uncertainty and its implementation with an estimator

$$\min_{x} p^{f}(x) \xrightarrow{\text{implemented as}} \min_{x} \widehat{p}^{f}(x)$$

Example:
$$\rho^f(x) = \mathbb{E}f(x, U), \ \widehat{\rho}^f(x) = \overline{f(x)} = \frac{1}{N} \sum_{i=1}^N f(x, u^i), u^i \sim p_U().$$

The estimator of the risk, the objective function, is either noisy or biased.

Example of noisy estimator:

Crude MC estimation of mean is noisy and has variance $\mathbb{V}\left(\overline{f(x)}\right) = \frac{1}{N(N-1)} \left(f(x, u^i) - \overline{f(x)}\right)^2$

Example of biased estimator: the common random numbers strategy

Choose a unique set $u_{CRN}^1, \ldots, u_{CRN}^N$, following $p_U()$, for all x's. Use your favorite MC estimator with these u's, e.g., $\overline{f(x)}_{CRN} = \frac{1}{N} \sum_{i=1}^{N} f(x, u_{CRN}^i)$.

In both cases, don't trust the response, consider it noisy.

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GP to guide the optimization of risk estimates

Let's start putting things together.

EGO can be applied to the response $\widehat{p}^{f}(x)$ but 2 changes are needed to account for the noise:







1. Use kriging with noise: $c(X, X) \rightarrow c(X, X) + N(X, X)$ (cf. course [Le Riche and Durrande, 2019])

- Homogeneous nugget, $N(X, X) = \text{diag}(\tau^2)$, and τ is estimated with the other GP parameters in the likelihood maximization.
- Heterogeneous nugget, N(X, X) = diag(τ_i²), the τ_i² are the variances of the risk estimator at the xⁱ's (example with a quantile in [Le Riche et al., 2009]). Cannot be estimated because not enough data points (ill-posed max likelihood).

2 additions to EGO to optimize the estimator $\widehat{p}^{f}(x)$:



2. Don't trust the best observation:

- Let noisy kriging filter out the noise: replace min(F) in the El formula by min(m(X)).
- 2 levels kriging: do a normal EGO on the filtered observations m(F) (i.e., 2 GP models built)

Evolutionary algorithms for uncertain responses

It has been known for some time that population based stochastic optimizers can locate the region of the optimum of noisy functions.

Principle of a CMA-ES algorithm [Hansen and Ostermeier, 2001]:



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The two ingredients are large enough populations and mutations [Beyer and Sendhoff, 2007], [Hansen et al., 2008]. But this goes against cost (number of function calls).

Versions of these algorithms that perform well on noisy functions have cost control mechanisms added:



summary of results on the 2012 noisy testbed of COCO

- A (1,4)-ES with mirrored sampling and sequential selection [Brockhoff et al., 2010].
- The IPOPsaACM = CMA algorithm with increasing population (IPOP) and a surrogate [Loshchilov et al., 2012].

x^{t+1} from kriging in the augmented space

An example of what can be done in optimization under uncertainty with a GP built in the augmented $(\mathcal{X}, \mathcal{A})$ -space of (x, u) variables.

Objective

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



Cf. [Janusevskis and Le Riche, 2012]

- f(x, u) is approximated by $Y^t_{\omega}(x, u)$ $Y^t_{\omega}(x, u)$ the GP conditionned by the DoE at time t, $[(x^1, u^1), f((x^1, u^1)), \dots, (x^t, u^t), f((x^t, u^t))]$
- $\mathbb{E}_U f(x, U)$ 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

$$Z^t_\omega(x) \coloneqq \mathbb{E}_U Y^t_\omega(x, U) = \int_{\mathcal{A}} Y^t_\omega(x, u) p_U(u) du$$

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,

$$x^{next} = max_{x \in \mathcal{X}} El_Z(x)$$

where, remember,

$$\mathsf{El}_Z(x) = \sqrt{c(x,x)} \left[w(x) \mathsf{cdf}_\mathcal{N}(w(x)) + \mathsf{pdf}_\mathcal{N}(w(x))
ight]$$

with $w(x) = rac{z_{\min} - m_Z(x)}{\sqrt{(c_Z(x,x))}}.$

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

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

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Content

Optimization under uncertainties: an overview with a focus on Gaussian processes

- Problem formulation
 - Motivation and the two classes of variables
 - Formulations as an optimization of statistical measures
- Methods

• A pointer to methods without metamodels

- Approximation methods
- Approaches based on stochastic gradients
- Methods with metamodels
 - Overall scheme
 - Choice of x
 - Choice of u knowing x

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Remember optimizers with uncertainty:

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 the GP(s) (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 Choose the next u^{t+1} knowing x^{t+1}
- 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 GP(s), stop or return to 2.

Choosing u knowing x^{next}

- Brute force MC: calculate all [f and g](x^{next}, uⁱ) needed by the risk estimator. Ex: p^f = 1/N ∑_{i=1}^N f(x^{next}, uⁱ), u_i ~ p_U(). Costs N.
- MC-kriging: replace calls to f or g by calls to the metamodel (GP mean). Ex: $\hat{p}^f = 1/N \sum_{i=1}^N m(x^{\text{next}}, u^i)$, $u^i \sim p_U()$. Still need to choose u^{t+1} where to call the true simulator. Simplest: sample it, $u^{t+1} \sim p_U()$. Costs 1. But the augmented GP is not used in the choice.

We now explain two approaches taking advantage of the GP in augmented space:

- Minimize the average function: $\min_x f(x, U)$ continued.
- Reliability problem: $\min_x f(x)$ such that $\mathbb{P}(g(x, U) \le 0) > \alpha$.

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Back to average minimization: u knowing x^{next}

continued, from [Janusevskis and Le Riche, 2012]

 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 \rightarrow one choice of (x, u).

Choose (x^{t+1}, u^{t+1}) that provides the most information, i.e., which minimizes the one-step-ahead variance¹ of the integrated process at x^{next}.

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

¹See Stepwise Uncertainty Reduction methods (SUR). R. Le Riche (CNRS) Optimization under uncertainties

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

Putting it together:

- 1 Create an initial Design of Experiments (DoE), (xⁱ, uⁱ, f(xⁱ, uⁱ))
 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 El 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).

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Example: 2D Camelback function, iteration 6



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Example: 2D Camelback function, iteration 14



Example: 2D Camelback function, iteration 50



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



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

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RBDO in the augmented space

From [Moustapha et al., 2016]

Problem to solve:

 $\min_{x\in\mathcal{X}}f(x) \text{ such that } \mathbb{Q}_{\alpha}(g(x,U))\leq 0 \quad (\Leftrightarrow \mathbb{P}(g(x,U)\leq 0)\geq \alpha)$

Method:

- x^{t+1} given by a 1+1-CMA-ES optimization algorithm
- *u*^{t+1} comes from a deviation number that is small when the GP is near but inaccurate at the quantile level,

$$u^{t+1} = \arg \min_{u \in \mathcal{A}} \frac{\widehat{q}_{\alpha}(x^{t+1}) - m(x^{t+1}, u)}{v(x^{t+1}, u)}$$

where $\widehat{q}_{\alpha}(x) = m(x, u^{\lfloor N\alpha:N \rfloor})$ • Calculate $f(x^{t+1})$, $g(x^{t+1}, u^{t+1})$, update and loop as usual.

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