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Bayesian Optimization

— Engineering design under uncertainty using
expensive-to-evaluate numerical models —

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CEA-EDF-INRIA Numerical Analysis Summer School
Université Pierre et Marie Curie (Paris VI)
Paris, 2017, July 3–7

Lecture 1 : From meta-models to UQ

- 1.1 Introduction
- 1.2 Black-box modeling
- 1.3 Bayesian approach
- 1.4 Posterior distribution of a quantity of interest
- 1.5 Complements on Gaussian processes

Lecture 2 : Bayesian optimization (BO)

- 2.1. Decision-theoretic framework
- 2.2. From Bayes-optimal to myopic strategies
- 2.3. Design under uncertainty

References

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1.1 Introduction

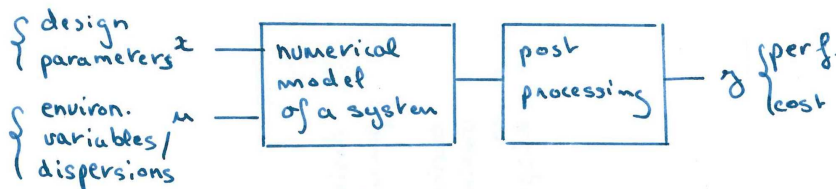
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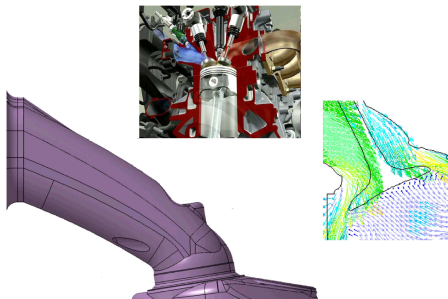
Computer-simulation based design



- ▶ The numerical model might be time- or resource-consuming
- ▶ Design parameters might be subject to dispersions
- ▶ The system might operate under unknown conditions

Computer-simulation based design – Example

- ▶ Computer simulations to design a product or a process, in particular
 - ▶ to find the best feasible values for **design parameters** (optimization problem)
 - ▶ to minimize the probability of failure of a product
- ▶ To comply with European emissions standards, the design parameters of combustion engines have to be carefully optimized
- ▶ The shape of intake ports controls airflow characteristics, which have direct impact on
 - ▶ the performances of the engine
 - ▶ emissions of NO_x and CO
- ▶ $f : \mathbb{X} \subset \mathbb{R}^d \rightarrow \mathbb{R}$ performance as a function of design parameters ($d = 20 \sim 100$)
- ▶ Computing $f(x)$ **takes 5 ~ 20 hours**
- ▶ Objective: estimate $x^* = \operatorname{argmax}_x f(x)$



Simulation of an intake port (Navier-Stokes equ.)
(courtesy of Renault)

Lecture 1 : From meta-models to UQ

1.1 Introduction

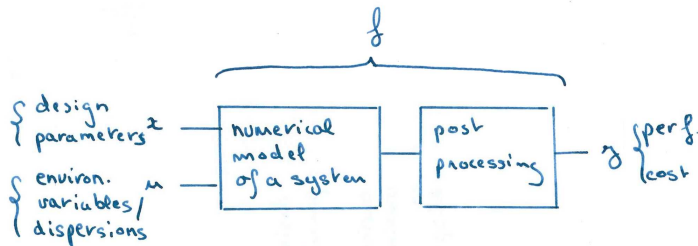
1.2 Black-box modeling

1.3 Bayesian approach

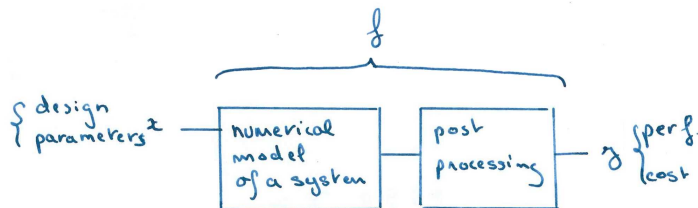
1.4 Posterior distribution of a quantity of interest

1.5 Complements on Gaussian processes

Black-box modeling



Black-box modeling



For simplification \rightarrow drop u

Black-box modeling

- ▶ Let $f : \mathbb{X} \rightarrow \mathbb{R}$ be a real function defined on $\mathbb{X} \subseteq \mathbb{R}^d$, where
 - ▶ \mathbb{X} is the input/parameter domain of the computer simulation under study, or the **factor** (from Latin, “which acts”) space
 - ▶ f is a **performance** or **cost** function (a function of the outputs of the computer simulation)

Black-box modeling

- ▶ Let $x_1, \dots, x_n \in \mathbb{X}$ be n simulations points
- ▶ Denote by

$$z_1 = f(x_1), \dots, z_n = f(x_n)$$

the corresp. simulation results (observations/evaluations of f)

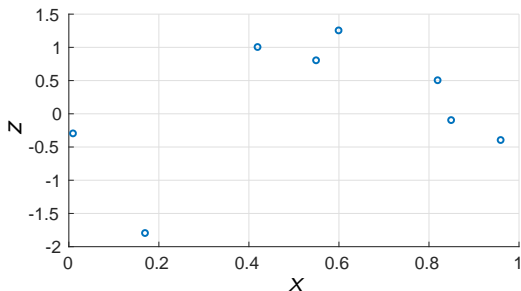
- ▶ Our objective: use the data $\mathcal{D}_n = (x_i, z_i)_{i=1\dots n}$ to **infer properties** about f
- ▶ Example: given a new $x \in \mathbb{R}^d$, predict the value $f(x)$

Black-box modeling

- ▶ f is a black-box, only known through evaluation results: query an evaluation at x , observe the result
 - ▶ Predict the value of f at a given x ?
- the problem is that of constructing an **approximation** / an **estimator** \hat{f}_n of f from \mathcal{D}_n
- ▶ Such a \hat{f}_n also called a **model** or a **meta-model** (because the numerical simulator is a model itself) of f

A simple curve fitting problem

- ▶ Suppose that we are given a data set of n simulation results, i.e., evaluations results of an unknown function $f : [0, 1] \rightarrow \mathbb{R}$, at points x_1, \dots, x_n .
- ▶ A data set of size $n = 8$:



A simple curve fitting problem

- ▶ Any approximation procedure of f consists in building a function $\hat{f}_n = h(\cdot; \theta)$ where $\theta \in \mathbb{R}^l$ is a vector of parameters, to be estimated from \mathcal{D}_n and available prior information
- ▶ Fundamental example: **linear model**

$$\hat{f}_n(x) = h(x, \theta) = \sum_{i=1}^l \theta_i r_i(x)$$

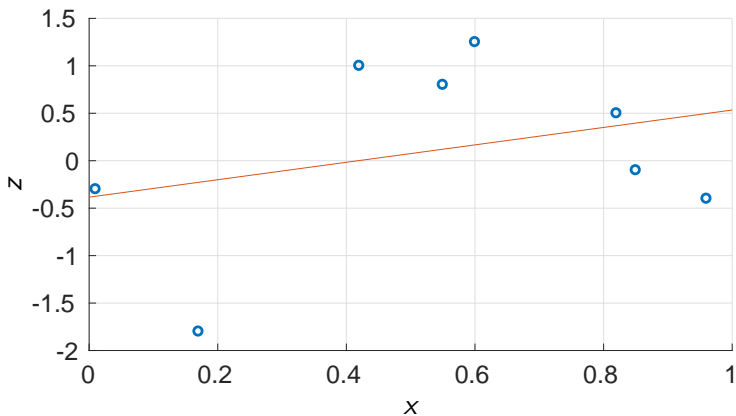
where functions $r_i : \mathbb{X} \rightarrow \mathbb{R}$ are called regressors (e.g., $r_1(x) = 1, r_2(x) = x, r_3(x) = x^2 \dots \rightarrow$ polynomial model)

- ▶ Most classical method to obtain a good value of b :
least squares \rightarrow minimize the sum of squared errors

$$J(\theta) = \sum_{i=1}^n \left(z_i - \hat{f}_n(x_i) \right)^2 = \sum_{i=1}^n \left(z_i - h(x_i; \theta) \right)^2$$

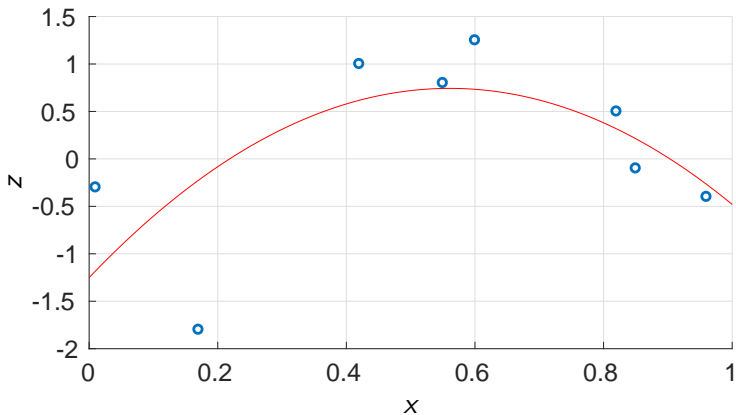
A simple curve fitting problem

► Linear fit



A simple curve fitting problem

► Quadratic fit



A simple curve fitting problem

- ▶ Poor fit!
- ▶ Why? Model capacity is weak
- ▶ Now, as an example, consider the model

$$\hat{f}_n(x) = \theta^t r(x)$$

with

$$r(x) = (1 \cos(2\pi x) \sin(2\pi x) \dots \cos(2m\pi x) \sin(2m\pi x))^t \in \mathbb{R}^{2m+1}$$

(a truncated Fourier series)

- ▶ The increase in the number of parameters yields an **ill-defined** problem ($l \gg n$)

A simple curve fitting problem

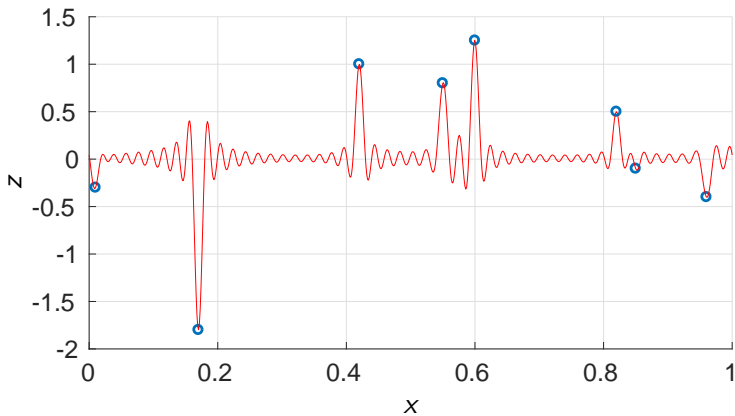
- ▶ When the problem becomes ill-defined (as capacity increases), a classical solution for finding a good value of b is to minimize the sum of an approximation error and a **regularization** term:

$$J(\theta) = \sum_{i=1}^n (z_i - \theta^t r(x_i))^2 + C \|\theta\|_2^2, \quad C > 0$$

- ▶ $\|\theta\|_2^2$ penalizes vectors θ with large elements
- ▶ C strikes a balance between regularization and data fidelity
- ▶ This approach is known as **Tikhonov regularization** (Tikhonov & Arsenin, 1977) → at the basis of numerous approximation methods (ridge regression, splines, RBF, SVM. . .)

A simple curve fitting problem

- ▶ $n = 8, m = 50, l = 101, C = 10^{-8}$



A simple curve fitting problem

- ▶ The regularization principle alone is not enough to obtain a good approximation
- ▶ As modeling capacity increases, **overfitting** may arise

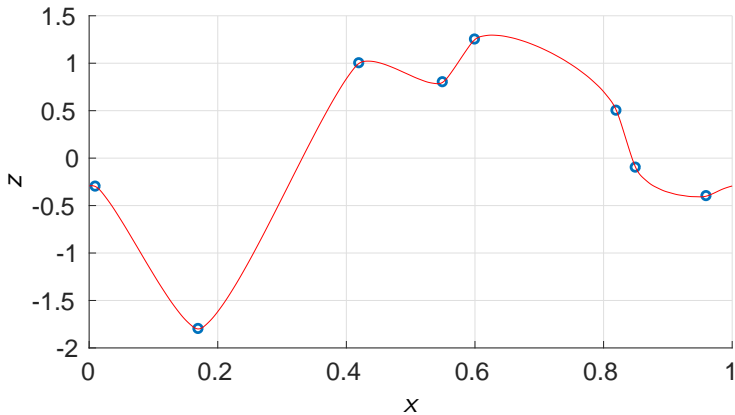
A simple curve fitting problem

- ▶ To avoid overfitting, we should try a regularization that penalizes high frequencies more
- ▶ For instance, take

$$\|\theta\| = \theta_1^2 + \sum_{k=1}^m \frac{\theta_{2k}^2 + \theta_{2k+1}^2}{(1 + (2k\pi)^\alpha)^2}$$

A simple curve fitting problem

- ▶ $n = 8, m = 50, l = 101, C = 10^{-8}, \alpha = 1.3$



A simple curve fitting problem

- ▶ From this example, we can see that the construction of a regularization scheme should result from a procedure that takes into account the data (using cross-validation, for instance) an/or prior knowledge (high frequencies \ll low frequencies, for instance)

Black-box modeling

- ▶ A large number of methods are available in the literature: polynomial regression, splines, NN, RBF...
- ▶ All methods are based on mixing prior information and regularization principles
- ▶ Instances of “regularization” in regression:
 - ▶ t-tests, F-tests, ANOVA, AIC (Akaike info criterion)... in linear regression
 - ▶ Early stopping in NN
 - ▶ Regularized reproducing-kernel regression
 - ▶ 1960 : splines, (Schoenberg 1964, Duchon 1976–1979)
 - ▶ 1970 : ridge regression (Hoerl, Kennard)
 - ▶ 1980 : RBF, (Micchelli 1986, Powel 1987)
 - ▶ 1995 : SVM, (Vapnik 1995)
 - ▶ 1997 : SVR, (Smola 1997) & semi-param SVR (Smola 1999)

Black-box modeling

- ▶ How to choose a regularization scheme?
- ▶ The **Bayesian setting** is a principled approach that makes it possible to construct regularized regressions

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1.5 Complements on Gaussian processes

Why a Bayesian approach?

- ▶ Objective: infer properties about $f : \mathbb{X} \rightarrow \mathbb{R}$ through pointwise evaluations
- ▶ Why a Bayesian approach?
 - ▶ a principled approach to choose a regularization scheme according to prior information
 - ▶ through probability calculus and/or Monte Carlo simulations, the user can infer properties about the unknown function
 - ▶ for instance: given prior knowledge and \mathcal{D}_n , what is the probability that the global maximum of f is greater than a given threshold $u \in \mathbb{R}$?
- ▶ **Main idea:** use a **statistical model of the observations**, together with a **probability model for the parameter** of the statistical model

Some reminders about probabilities

- ▶ Recall that a **random variable** is a function that maps a sample space Ω to an outcome space E (e.g. $E = \mathbb{R}$), and that assigns probabilities (weights) to possible outcomes

Def.

Formally, let (Ω, \mathcal{A}, P) be a probability space, and (E, \mathcal{E}) be a measurable outcome space

→ a random variable X is a measurable function $(\Omega, \mathcal{A}, P) \rightarrow (E, \mathcal{E})$

- ▶ X is used to assign probabilities to events: for instance

$$P(X \in [0, 1]) = P^X([0, 1]) = 1/2$$

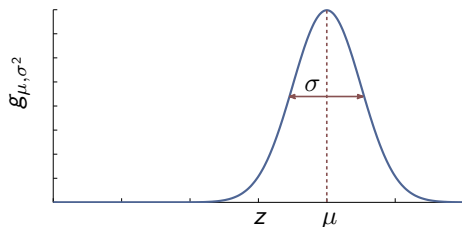
- ▶ Case of a random variable with a density

$$P(X \in [a, b]) = P^X([a, b]) = \int_a^b p^X(x) dx$$

Gaussian random variables

- ▶ A real-valued random variable Z is said to be **Gaussian** $\mathcal{N}(\mu, \sigma^2)$, if it has the continuous **probability density function**

$$g_{\mu, \sigma^2}(z) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2} \frac{(z - \mu)^2}{\sigma^2}\right)$$



Gaussian random variables

- ▶ The **mean** of Z (also called **expectation** or first-order moment) is

$$E(Z) = \int_{\mathbb{R}} z g_{\mu, \sigma^2}(z) dz = \mu$$

and its **second-order** moment is defined as

$$E(Z^2) = \int_{\mathbb{R}} z^2 g_{\mu, \sigma^2}(z) dz = \sigma^2 + \mu^2$$

- ▶ The **variance** of Z is defined as

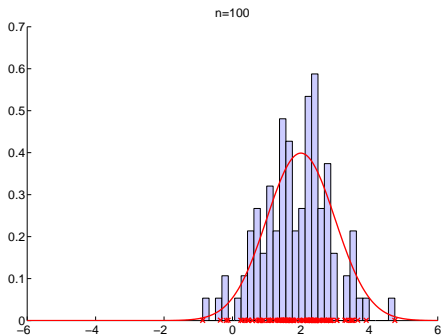
$$\text{var}(Z) = E[(Z - E(Z))^2] = E[Z^2] - E[Z]^2 = \sigma^2$$

Gaussian random variables

- ▶ A Gaussian variable Z can be used as a **stochastic model** of some uncertain real-valued quantity
- ▶ In other words, Z can be thought as a **prior about some uncertain quantity** of interest

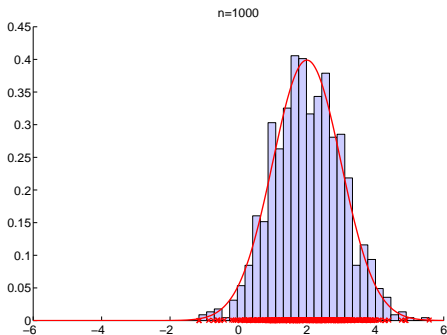
Gaussian random variables

- ▶ Using a random generator, it is possible to “generate” sample values z_1, z_2, \dots of our model $Z \rightarrow$ possible values for our **uncertain quantity of interest**



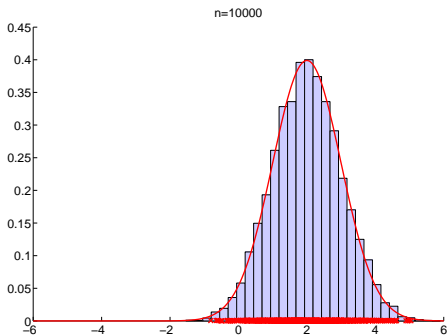
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Gaussian random variables

- ▶ Using a random generator, it is possible to “generate” sample values z_1, z_2, \dots of our model $Z \rightarrow$ possible values for our **uncertain quantity of interest**



(as $n \rightarrow \infty$, the empirical distribution of the realizations tends to the normal distribution)

Bayesian model

Formally, recall that a **statistical model** is a triplet $\mathcal{M} = (\mathcal{Z}, \mathcal{F}, \mathcal{P})$

- ▶ $\mathcal{Z} \rightarrow$ observation space (typically, $\mathcal{Z} = \mathbb{R}^n$)
- ▶ $\mathcal{F} \rightarrow$ σ -algebra on \mathcal{Z}
- ▶ $\mathcal{P} \rightarrow$ parametric family $\{P_\theta; \theta \in \Theta\}$ of probability distributions on $(\mathcal{Z}, \mathcal{F})$

Def.

A **Bayesian model** is defined by the specification of

- ▶ a **parametric statistical model** \mathcal{M} (model of the observations)
- ▶ a **prior probability distribution** Π on $(\Theta, \Xi) \rightarrow$ probability model that describes uncertainty about θ before an observation is made

Example

- ▶ Suppose we repeat measurements of a quantity of interest:
 $z_1, z_2, \dots \in \mathbb{R}$

- ▶ **Model of observations:** $Z_i \stackrel{iid}{\sim} \mathcal{N}(\theta_1, \theta_2), i = 1, \dots, n$

- ▶ The statistical model can formally be written as the triplet

$$\mathcal{M} = \left(\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n), \{ \mathcal{N}(\theta_1, \theta_2)^{\otimes n} \}_{\theta_1, \theta_2} \right)$$

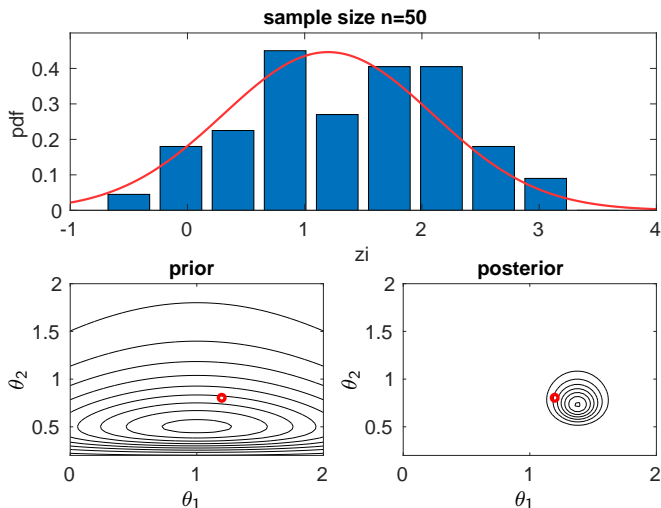
- ▶ Moreover, if we assume a **prior distribution** about θ_1 and θ_2
(e.g. $\theta_1 \sim \mathcal{N}(1, 1), \theta_2 \sim \mathcal{IG}(3, 2)$), we obtain a

Bayesian model

- ▶ From this Bayesian model (model of observations + prior), we can compute the **posterior distribution** of (θ_1, θ_2) given Z_1, \dots, Z_n (will be explained later)

Example

$$n = 50, \theta_1 = 1.2, \theta_2 = 0.8$$



Simple curve fitting problem from a Bayesian approach

- ▶ Recall our simple curve fitting model

$$\hat{f}_n(x) = \theta^t r(x)$$

with

$$r(x) = (1 \cos(2\pi x) \sin(2\pi x) \dots \cos(2m\pi x) \sin(2m\pi x))^t \in \mathbb{R}^{2m+1}$$

- ▶ Bayesian model?

- ▶ Assume the following statistical model for the observations:

$$\begin{cases} Z_i = \xi(x_i) + \varepsilon_i, & i = 1, \dots, n \\ \xi(x) = \theta^t r(x), & x \in \mathbb{X} \\ \varepsilon_i \stackrel{iid}{\sim} \mathcal{N}(0, \sigma_\varepsilon^2) \end{cases}$$

or equivalently,

$$Z_i \stackrel{iid}{\sim} \mathcal{N}(\theta^t r(x_i), \sigma_\varepsilon^2), \quad i = 1, \dots, n$$

- ▶ Moreover, choose a prior distribution for θ :

$$\theta_j \stackrel{\text{indep}}{\sim} \mathcal{N}(0, \sigma_{\theta_j}^2), \quad j = 1, \dots, 2m + 1$$

- ▶ The rvs Z_i constitute a Bayesian model of the observations
- ▶ ξ is a random function / random process \rightarrow prior about f

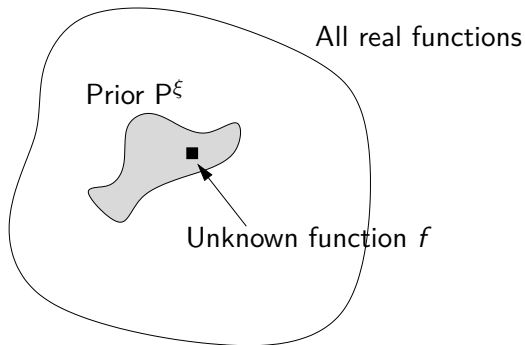
Random process

Def.

A **random process** $\xi : (\Omega, \mathbb{X}) \rightarrow \mathbb{R}$ is a collection of random variables $\xi(\cdot, x) : \Omega \rightarrow \mathbb{R}$ indexed by $x \in \mathbb{X}$

- ▶ Random processes can be viewed as a generalization of random vectors
- ▶ For a fixed $\omega \in \Omega$, the function $\xi(\omega, \cdot) : \mathbb{X} \rightarrow \mathbb{R}$ is called a **sample path**

- ▶ In our Bayesian setting, we can say that
 - ▶ we use a random process ξ as a **stochastic model** of the **unknown** function f
 - ▶ f is viewed as as **sample paths** of ξ
 - ▶ ξ represents **our knowledge about f** before any evaluation has been made
 - ▶ the distribution $\Pi = P^\xi$ is a **prior** about f

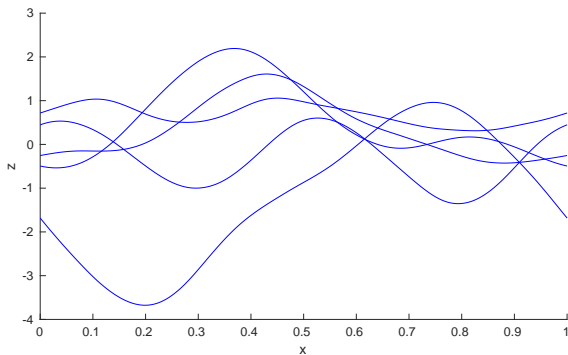


- ▶ Here, $\xi(\omega, \cdot) = \theta(\omega)^t r(\cdot)$
- ▶ Fixing ω (a sample path) amounts to “choosing” a value for the random vector θ

- ▶ Example of sample paths with

$$\begin{cases} \theta_1 \sim \mathcal{N}(0, 1) \\ \theta_{2k}, \theta_{2k+1} \stackrel{\text{indep}}{\sim} \mathcal{N}\left(0, \frac{1}{1+(\omega_0 k)^\alpha}\right), \quad k = 1, \dots, m \end{cases}$$

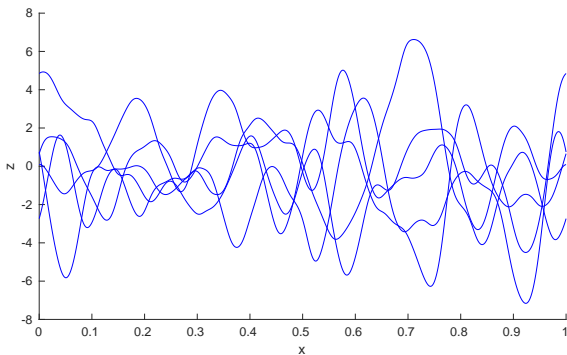
with $\omega_0 = \frac{2\pi}{10}$, $\alpha = 4$



- ▶ Example of sample paths with

$$\begin{cases} \theta_1 \sim \mathcal{N}(0, 1) \\ \theta_{2k}, \theta_{2k+1} \stackrel{\text{indep}}{\sim} \mathcal{N}\left(0, \frac{1}{1+(\omega_0 k)^\alpha}\right), \quad k = 1, \dots, m \end{cases}$$

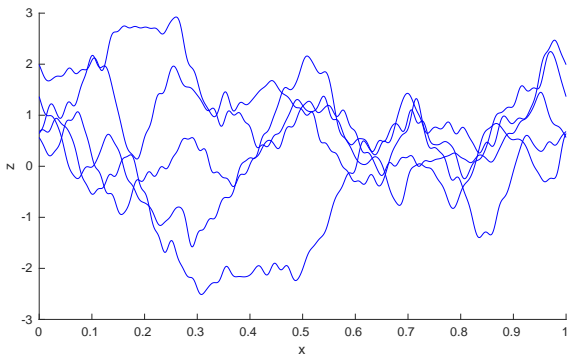
with $\omega_0 = \frac{2\pi}{50}$, $\alpha = 4$



- ▶ Example of sample paths with

$$\begin{cases} \theta_1 \sim \mathcal{N}(0, 1) \\ \theta_{2k}, \theta_{2k+1} \overset{\text{indep}}{\sim} \mathcal{N}\left(0, \frac{1}{1+(\omega_0 k)^\alpha}\right), \quad k = 1, \dots, m \end{cases}$$

with $\omega_0 = \frac{2\pi}{10}$, $\alpha = 1.5$

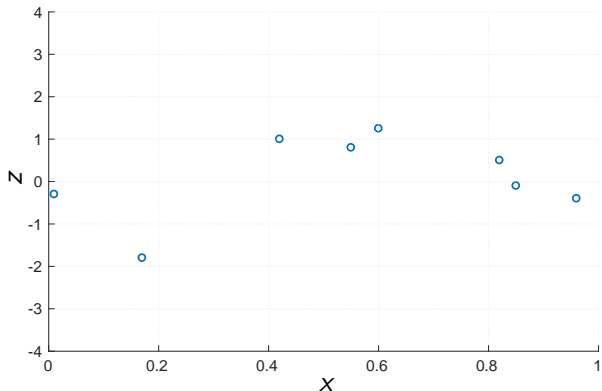


Bayesian approach

- ▶ The **choice of a prior** in a Bayesian approach reflects the **user's knowledge about uncertain parameters**
- ▶ In the case of function approximation \rightarrow **regularity** of the function

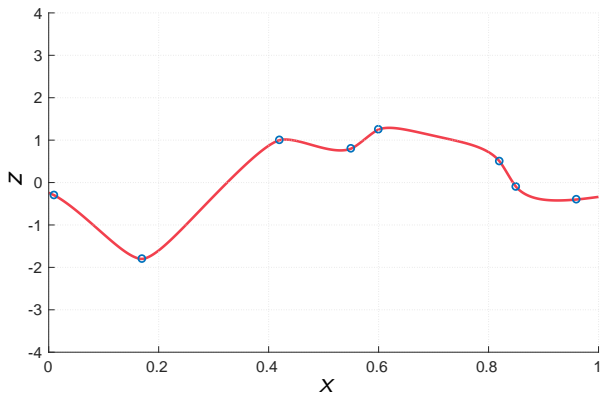
Bayesian approach

- ▶ Where shall we go now?
- ▶ Objective: compute posterior distributions from data



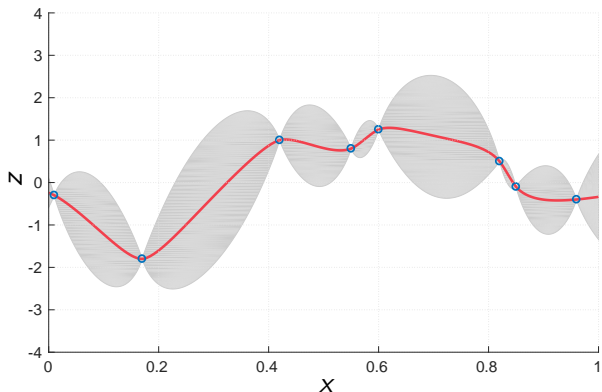
Bayesian approach

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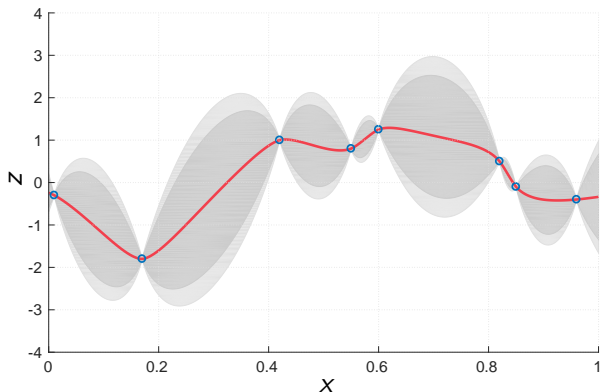
Bayesian approach

- ▶ Where shall we go now?
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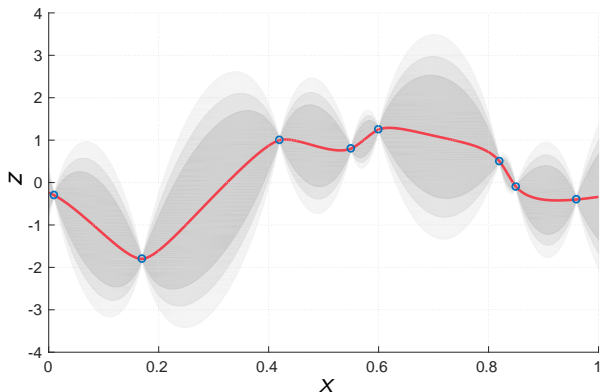
Bayesian approach

- ▶ Where shall we go now?
- ▶ Objective: compute posterior distributions from data



Bayesian approach

- ▶ Where shall we go now?
- ▶ Objective: compute posterior distributions from data



A “simplification” of the Bayesian model for the simple curve fitting problem

- ▶ $\xi = \theta^t r$ (our prior about f) is a **Gaussian process**
- ▶ Why?

Gaussian random vectors

Def.

A real-valued random vector $Z = (Z_1, \dots, Z_d) \in \mathbb{R}^d$ is said to be **Gaussian** iff any linear combination of its components $\sum_{i=1}^d a_i Z_i$, with $a_1, \dots, a_d \in \mathbb{R}$, is a Gaussian variable

- ▶ A Gaussian random vector Z is characterized by its **mean** vector, $\mu = (E[Z_1], \dots, E[Z_d]) \in \mathbb{R}^d$, and the **covariance** of the pairs of components (Z_i, Z_j) , $i, j \in \{1, \dots, d\}$,
 $\text{cov}(Z_i, Z_j) = E[(Z_i - E(Z_i))(Z_j - E(Z_j))]$
- ▶ If $Z \in \mathbb{R}^d$ is a Gaussian vector with mean $\mu \in \mathbb{R}^d$ and covariance matrix $\Sigma \in \mathbb{R}^{d \times d}$, we shall write $Z \sim \mathcal{N}(\mu, \Sigma)$

- ▶ Exercise: Let $Z \sim \mathcal{N}(\mu, \Sigma)$. Determine $E\left(\sum_{i=1}^d a_i Z_i\right)$ and $\text{var}\left(\sum_{i=1}^d a_i Z_i\right)$

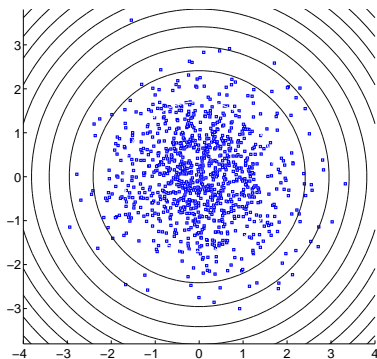
- ▶ The correlation coefficient of two components Z_i and Z_j of Z is defined by

$$\rho(Z_i, Z_j) = \frac{\text{cov}(Z_i, Z_j)}{\sqrt{\text{var}(Z_i)\text{var}(Z_j)}} \in [-1, 1],$$

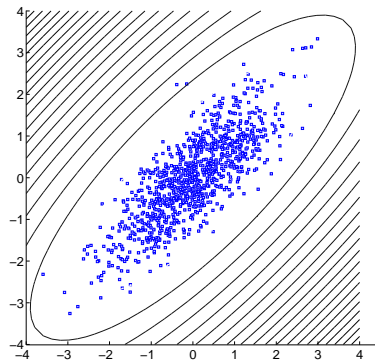
→ measures the similarity between Z_i and Z_j

Gaussian random vectors: correlation

$$\rho = 0$$



$$\rho = 0.8$$



Gaussian random processes

- ▶ Recall that a random process is a set $\xi = \{\xi(x), x \in \mathbb{X}\}$ of random variables indexed by the elements of \mathbb{X}
- ▶ Gaussian random process
 - generalization of a Gaussian random vector

Def.

ξ is a **Gaussian random process** iff, $\forall n \in \mathbb{N}$, $\forall x_1, \dots, x_n \in \mathbb{X}$, and $\forall a_1, \dots, a_n \in \mathbb{R}$, the real-valued random variable

$$\sum_{i=1}^n a_i \xi(x_i)$$

is Gaussian

Application

- ▶ If

$$\begin{cases} \xi(x) = \theta^t r(x), & x \in \mathbb{X} \\ \theta_j \stackrel{\text{indep}}{\sim} \mathcal{N}(0, \sigma_{\theta_j}^2), & j = 1, \dots, 2m + 1 \end{cases}$$

then, $\forall x_1, \dots, x_n \in \mathbb{X}$, and $\forall a_1, \dots, a_n \in \mathbb{R}$,

$$\begin{aligned} \sum_{i=1}^n a_i \xi(x_i) &= \sum_i a_i \left(\sum_j \theta_j r_j(x_i) \right) \\ &= \sum_j \left(\sum_i a_i r_j(x_i) \right) \theta_j \sim \mathcal{N} \left(0, \sum_j \left(\sum_i a_i r_j(x_i) \right)^2 \sigma_{\theta_j}^2 \right) \end{aligned}$$

- ▶ Thus, $\xi = \theta^t r$ is a Gaussian process

Gaussian random processes

- ▶ A Gaussian process is **characterized** by
 - ▶ its **mean function**

$$m : x \in \mathbb{X} \mapsto \mathbb{E}[\xi(x)]$$

- ▶ and its **covariance function**

$$k : (x, y) \in \mathbb{X}^2 \mapsto \text{cov}(\xi(x), \xi(y))$$

- ▶ Notation: $\xi \sim \mathcal{GP}(m, k)$

▶ Exercise: determine $E\left(\sum_{i=1}^d a_i \xi(x_i)\right)$ and $\text{var}\left(\sum_{i=1}^d a_i \xi(x_i)\right)$

▶ What is the distribution of $\sum a_i \xi(x_i)$?

→ The distribution of a linear combination of a Gaussian process $\mathcal{GP}(m, k)$ can be **simply obtained as a function of m and k**

Application

► If

$$\begin{cases} \xi(x) = \theta^t r(x), & x \in \mathbb{X} \\ \theta_j \stackrel{\text{indep}}{\sim} \mathcal{N}(0, \sigma_{\theta_j}^2), & j = 1, \dots, 2m + 1 \end{cases}$$

then,

$$\xi \sim \mathcal{GP}(0, k)$$

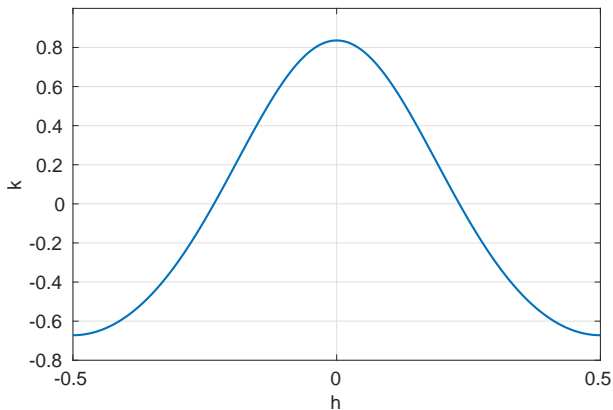
with

$$k : (x, y) \mapsto \sum_j \sigma_{\theta_j}^2 r_j(x) r_j(y)$$

- Covariance function corresponding to

$$\begin{cases} \theta_1 \sim \mathcal{N}(0, 1) \\ \theta_{2k}, \theta_{2k+1} \stackrel{\text{indep}}{\sim} \mathcal{N}\left(0, \frac{1}{1+(\omega_0 k)^\alpha}\right), \quad k = 1, \dots, m \end{cases}$$

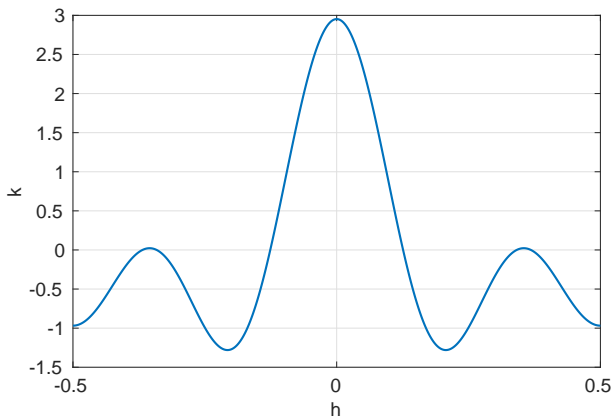
with $\omega_0 = \frac{2\pi}{10}$, $\alpha = 4$



- Covariance function corresponding to

$$\begin{cases} \theta_1 \sim \mathcal{N}(0, 1) \\ \theta_{2k}, \theta_{2k+1} \stackrel{\text{indep}}{\sim} \mathcal{N}\left(0, \frac{1}{1+(\omega_0 k)^\alpha}\right), \quad k = 1, \dots, m \end{cases}$$

with $\omega_0 = \frac{2\pi}{50}$, $\alpha = 4$



The covariance of a Gaussian random process

- ▶ Main properties: a covariance function k is
 - ▶ **symmetric**: $\forall x, y \in \mathbb{X}, k(x, y) = k(y, x)$
 - ▶ **positive**:

$$\forall n \in \mathbb{N}, \forall x_1, \dots, x_n \in \mathbb{X}, \forall a_1, \dots, a_n \in \mathbb{R}, \sum_{i,j=1}^n a_i k(x_i, x_j) a_j \geq 0$$

- ▶ In the following, we shall assume that the covariance of $\xi \sim \mathcal{GP}(m, k)$ is **invariant under translations**, or **stationary**:

$$k(x + h, y + h) = k(x, y), \quad \forall x, y, h \in \mathbb{X}$$

- ▶ When k is stationary, there exists a **stationary covariance** $k_{\text{sta}} : \mathbb{R}^d \rightarrow \mathbb{R}$ such that

$$\text{cov}(\xi(x), \xi(y)) = k(x, y) = k_{\text{sta}}(x - y)$$

Stationary covariances

- ▶ When k is stationary, the variance

$$\text{var}(\xi(x)) = \text{cov}(\xi(x), \xi(x)) = k(0)$$

does not depend on x

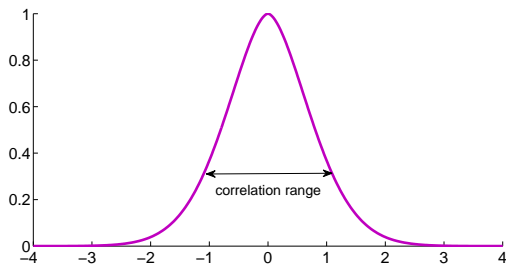
- ▶ The covariance function can be written as

$$k(x - y) = \sigma^2 \rho(x - y),$$

with $\sigma^2 = \text{var}(\xi(x))$, and where ρ is the **correlation function** of ξ .

Stationary covariances

- ▶ The graph of the correlation function is a symmetric “bell curve” shape



- ▶ We have, by C-S,

$$\begin{aligned}\forall h \in \mathbb{X}, |k(h)| &= |\text{cov}(\xi(x), \xi(x+h))| \\ &= |E[(\xi(x) - m(x))(\xi(x+h) - m(x+h))]| \\ &\leq E((\xi(x) - m(x))^2)^{1/2} E((\xi(x+h) - m(x+h))^2)^{1/2} \\ &= k(0)^{1/2} k(0)^{1/2} = k(0)\end{aligned}$$

- ▶ Recall, Bochner's spectral representation theorem

Theorem

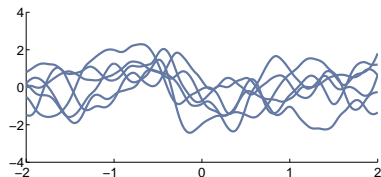
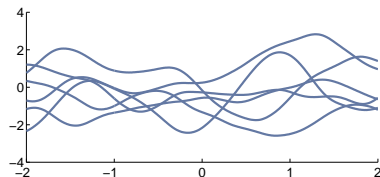
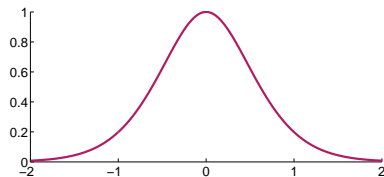
A real function $k(h)$, $h \in \mathbb{R}^d$ is symmetric positive iff it is the Fourier transform of a finite positive measure, i.e.

$$k(h) = \int_{\mathbb{R}^d} e^{i\langle u, h \rangle} d\mu(u),$$

where μ is a finite positive measure on \mathbb{R}^d .

Gaussian process simulation

- ▶ Using a random generator, it is possible to “generate” sample paths f_1, f_2, \dots of a Gaussian process ξ



Gaussian process simulation

How to simulate sample paths of a zero-mean Gaussian random process?

- ▶ Choose a set of points $x_1, \dots, x_n \in \mathbb{X}$
- ▶ Denote by K the $n \times n$ covariance matrix of the random vector $\underline{\xi} = (\xi(x_1), \dots, \xi(x_n))^t$ (NB: $\underline{\xi} \sim \mathcal{N}(0, K)$)
- ▶ Consider the Cholesky factorization of K

$$K = CC^t,$$

with C a lower triangular matrix (such a factorization exists since K is a sdp matrix)

- ▶ Let $\varepsilon = (\varepsilon_1, \dots, \varepsilon_n)^t$ a Gaussian vector with $\varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1)$
- ▶ Then $C\varepsilon \sim \mathcal{N}(0, K)$

“Simplification” of the Bayesian model for the simple curve fitting problem

- ▶ Instead of choosing the model

$$\begin{cases} \xi(x) = \theta^t r(x), & x \in \mathbb{X} \\ \theta_j \stackrel{\text{indep}}{\sim} \mathcal{N}(0, \sigma_{\theta_j}^2), & j = 1, \dots, 2m + 1 \end{cases}$$

simply choose a covariance function k and assume $\xi \sim \mathcal{GP}(0, k)$

- ▶ More details about how to choose k will be given below

Conditional distributions

- ▶ Let X be a random variable modeling an unknown quantity of interest
- ▶ Assume we observe a random variable T , or a random vector $T = (T_1, \dots, T_n)$
- ▶ Provided that T and X are **not independent**, T contains **information about X**
- ▶ Aim: define a **notion of distribution of X “knowing” T**

Conditional probabilities

Recall the following

Def.

Let (Ω, \mathcal{A}, P) be a probability space. Given two events $A, B \in \mathcal{A}$ such that $P(B) \neq 0$, define the **probability of A given B** (or conditional on B) by

$$P(A | B) = \frac{P(A \cap B)}{P(B)}$$

The notion of conditional density

Def.

Assume that the pair $(X, T) \in \mathbb{R}^2$ has a density $p^{(X,T)}$.

Define the **conditional density** of X given the event $T = t$ by

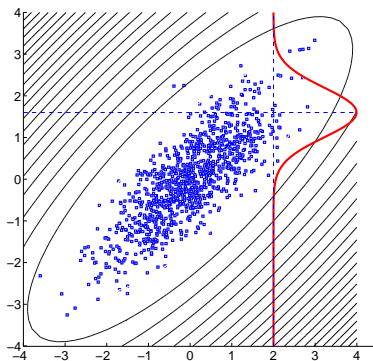
$$p^{X|T}(x | t) = \begin{cases} \frac{p^{(X,T)}(x, t)}{p^T(t)} = \frac{p^{(X,T)}(x, t)}{\int p^{X,T}(x, t) dx} & \text{if } p^T(t) > 0 \\ \text{arbitrary density} & \text{if } p^T(t) = 0. \end{cases}$$

Application

- ▶ Given a Gaussian random vector $Z = (Z_1, Z_2) \sim \mathcal{N}(0, \Sigma)$, what is the distribution of Z_2 “knowing” Z_1 ?
- ▶ Define

$$p^{Z_2|Z_1}(z_2|z_1) = \frac{p^{(Z_2, Z_1)}(z_2, z_1)}{p^{Z_1}(z_1)} = \frac{\sigma_1}{(2\pi)^{1/2}(\det \Sigma)^{1/2}} \exp(-1/2(z^t \Sigma^{-1} z - z_1^2 / \sigma_1^2))$$

→ Gaussian distribution!



- ▶ The random variable denoted by $Z_2 | Z_1$ with density $p^{Z_2|Z_1}(\cdot | Z_1)$ represents the **residual uncertainty** about Z_2 when Z_1 has been observed
- ▶ High correlation → small residual uncertainty

Conditional mean/expectation

- A fundamental notion: conditional expectation

Def.

Assume that the pair (X, T) has a density $p^{(X, T)}$. Define the **conditional mean of X given $T = t$** as

$$E(X | T = t) \triangleq \int_{\mathbb{R}} x p^{X|T}(x|t) dx = h(t)$$

Def.

The random variable $E(X | T) = h(T)$ is called the **conditional expectation of X given T**

Conditional expectation

- ▶ Why conditional expectation is an fundamental notion?
- ▶ We have the following

Theorem

Under the previous assumptions, the solution of the problem

$$\hat{X} = \operatorname{argmin}_Y E[(X - Y)^2]$$

*where the **minimum is taken over all functions of T** is given by*

$$\hat{X} = E(X | T)$$

- ▶ In other words, $E(X | T)$ is the **best approximation** (in the sense of the quadratic mean) **of X by a function of T**

Important properties of conditional expectation

- (1) $E(X | T)$ is a random variable depending on $T \rightarrow$ there exists a function h such that $E(X | T) = h(T)$
- (2) The operator $\pi_H : X \mapsto E(X | T)$ is a (linear) operator of **orthogonal projection** onto the space of all functions of T (for the inner product $X, Y \mapsto (X, Y) = E(XY)$)
- (3) Let $X, Y, T \in L^2$. Then
 - i) $\forall \alpha \in \mathbb{R}, E(\alpha X + Y | T) = \alpha E(X | T) + E(Y | T)$ a.s.
 - ii) $E(E[X | T]) = E(X)$
 - iii) If $X \perp\!\!\!\perp T$, $E(X | T) = E(X)$

Conditional expectation: Gaussian random variables

- ▶ Recall that the space of second-order random variables $L^2(\Omega, \mathcal{A}, P)$ endowed with the inner product $X, Y \mapsto (X, Y) = E(XY)$ is a Hilbert space
- ▶ Gaussian linear space

Def.

A **linear subspace** G of $L^2(\Omega, \mathcal{A}, P)$ is **Gaussian** iff $\forall X_1, \dots, X_n \in G$ and $\forall a_1, \dots, a_n \in \mathbb{R}$ the random variable $\sum_i a_i X_i$ is Gaussian

- ▶ In what follows, assume that G is **centered**, i.e., each element in G is a zero-mean random variable

■ Application

Let $Z = (Z_1, Z_2)$ be a zero-mean Gaussian random vector, with covariance matrix

$$\begin{pmatrix} \sigma_1^2 & \sigma_{1,2} \\ \sigma_{2,1} & \sigma_2^2 \end{pmatrix}$$

Then $E(Z_1 | Z_2)$ is the orthogonal projection of Z_1 onto Z_2 . Thus

$$E(Z_1 | Z_2) = \lambda Z_2$$

with

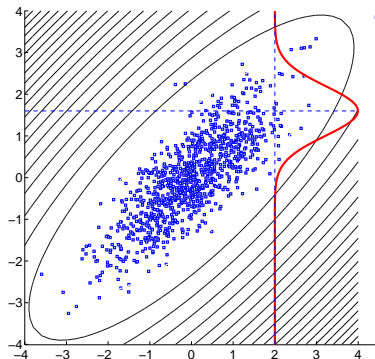
$$(Z_1 - \lambda Z_2, Z_2) = (Z_1, Z_2) - \lambda(Z_2, Z_2) = 0.$$

Hence,

$$\lambda = \frac{\sigma_{1,2}}{\sigma_2^2}$$

Application

- ▶ Let $Z = (Z_1, Z_2) \sim \mathcal{N}(0, \Sigma)$ as above \rightarrow recall that the cond. distrib. of Z_2 given Z_1 is a Gaussian distribution
- ▶ Hence $Z_2 | Z_1 \sim \mathcal{N}(\mu(Z_1), \sigma(Z_1)^2) \rightarrow \mu ? \sigma ?$



- ▶ $\mu = E(Z_2 | Z_1) = \lambda Z_1$ with $\lambda = \frac{\sigma_{1,2}}{\sigma_2^2}$
- ▶ Using the property of the orthogonal projection:

$$\begin{aligned}\sigma^2 &= E((Z_2 - E(Z_2 | Z_1))^2 | Z_1) \\ &\stackrel{\perp}{=} E((Z_2 - E(Z_2 | Z_1))^2) \\ &= E((Z_2 - \lambda Z_1)^2) \\ &\stackrel{\perp}{=} E((Z_2 - \lambda Z_1)Z_2) \\ &= \sigma_2^2 - \lambda\sigma_{1,2}\end{aligned}$$

Generalization

Exercise: Let (Z_0, Z_1, \dots, Z_n) be a centered Gaussian vector.
Determine $E(Z_0 \mid Z_1, \dots, Z_n)$.

Application: computation of the posterior distrib. of a GP

- ▶ Let $\xi \sim \mathcal{GP}(0, k)$
- ▶ Assume we observe ξ at $x_1, \dots, x_n \in \mathbb{X}$
- ▶ Given $x_0 \in \mathbb{X}$, what is the conditional distrib.—or the posterior distrib. in our Bayesian framework—of

$$\xi(x_0) \mid \xi(x_1), \dots, \xi(x_n) ?$$

- ▶ More generally, what is the **posterior distribution** of the random process

$$\xi(\cdot) \mid \xi(x_1), \dots, \xi(x_n) ?$$

Computation of the posterior distribution of a GP

Prop.

Let $\xi \sim \mathcal{GP}(0, k)$. The random process ξ conditioned on $F_n = \{\xi(x_1), \dots, \xi(x_n)\}$, denoted by $\xi | F_n$, is a **Gaussian process** with

- mean $\hat{\xi}_n : x \mapsto \mathbb{E}(\xi(x) | \xi(x_1), \dots, \xi(x_n))$
- covariance $k_n : x, y \mapsto \mathbb{E}((\xi(x) - \hat{\xi}_n(x))(\xi(y) - \hat{\xi}_n(y)))$

Computation of the posterior distrib. of a GP

- ▶ By property of the conditional expectation in Gaussian spaces, for all $x \in \mathbb{X}$, $\hat{\xi}_n(x)$ is a linear combination of $\xi(x_1), \dots, \xi(x_n)$:

$$\hat{\xi}_n(x) := \sum_{i=1}^n \lambda_i(x) \xi(x_i)$$

- ▶ Moreover, the posterior mean $\hat{\xi}_n(x)$ is the orthogonal projection of $\xi(x)$ onto $\text{span}\{\xi(x_i), i = 1, \dots, n\}$, such that
 - ▶ $\hat{\xi}_n(x) = \operatorname{argmin}_Y E[(\xi(x) - Y)^2] \rightarrow$ the variance of the prediction error is minimum
 - ▶ $E(\hat{\xi}_n(x)) = E[E(\xi(x) | F_n)] = E(\xi(x)) = 0 \rightarrow$ unbiased estimation
- ▶ $\hat{\xi}_n(x)$ is the **best linear predictor** (BLP) of $\xi(x)$ from $\xi(x_1), \dots, \xi(x_n)$, also called the **kriging predictor** of $\xi(x)$

Computation of the posterior distrib. of a GP

- ▶ The posterior covariance, also called **kriging covariance**, is given by

$$\begin{aligned}k_n(x, y) &:= \text{cov}(\xi(x) - \hat{\xi}_n(x), \xi(y) - \hat{\xi}_n(y)) \\ &= k(x - y) - \sum_i \lambda_i(x) k(y - x_i).\end{aligned}$$

- ▶ k_n is the covariance function of the **error of prediction**
- ▶ The posterior variance of ξ , also called the **kriging variance**, is defined as

$$\sigma_n^2(x) = \text{var}(\xi(x) - \hat{\xi}_n(x)) = k_n(x, x)$$

- ▶ $\sigma_n^2(x)$ is the variance of the **error of prediction**

Kriging equations

- ▶ How to compute the weights $\lambda_i(x)$ of the posterior mean/kriging predictor?
- ▶ Weights $\lambda_i(x)$ are solutions of a **system of linear equations**

$$K\lambda(x) = k(x)$$

with

- $\lambda(x) = (\lambda_1(x), \dots, \lambda_n(x))^t$
- K : $n \times n$ covariance matrix of the observation vector
- $k(x)$: $n \times 1$ vector with entries $k(x_i, x)$

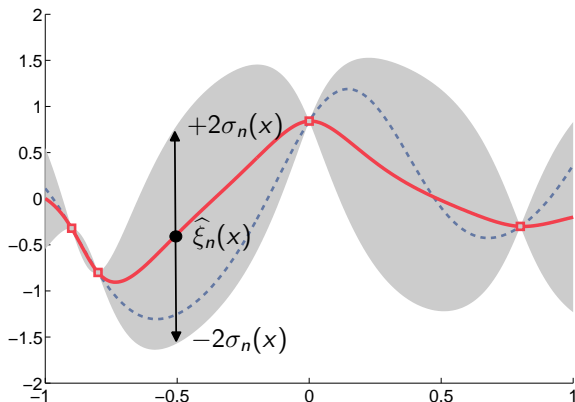
Kriging equations

proof



Posterior distrib. of a GP

- ▶ For all $x \in \mathbb{X}$, the random variable $\xi(x) \mid F_n$ with distrib. $\mathcal{N}(\hat{\xi}_n(x), \sigma_n^2(x))$ represents the **residual uncertainty** about $\xi(x)$ when $\xi(x_1), \dots, \xi(x_n)$ are observed



Software for kriging/GP regression

- ▶ R packages

- ▶ **BACCO** Bayesian analysis of computer code software
- ▶ **fanovaGraph** Building Kriging Models from FANOVA Graphs
- ▶ **DiceKriging** **DiceOptim** **GPareto** Dice and ReDice packages
- ▶ **MuFiCokriging** Multi-Fidelity Cokriging models
- ▶ **RobustInv** Robust inversion based on GP (like KrigInv)
- ▶ **tgp** Treed Gaussian processes
- ▶ ...

Software for kriging/GP regression

▶ Matlab/GNU Octave

- ▶ **DACE** DACE, a matlab kriging toolbox.
- ▶ **FERUM** Finite Element Reliability using Matlab
- ▶ **GPML** Gaussian Processes for Machine Learning
- ▶ **GPstuff** GP Models for Bayesian analysis
- ▶ **scalaGAUSS** Kriging toolbox with a focus on large datasets
- ▶ **Matlab Stat & ML toolbox** GP regression from Mathworks
- ▶ **STK** Small (Matlab/GNU Octave) Toolbox for Kriging
- ▶ **SUMO** **ooDACE** Surrogate Modeling Lab
- ▶ **UQLab** Uncertainty quantification framework in Matlab

▶ Python

- ▶ **scikit-learn** Machine learning in Python
- ▶ **OpenTURNS** Open source lib for UQ
- ▶ **Spearmint** Bayesian optimization
- ▶ **GPy** Gaussian processes framework in Python

Generalization: prediction from noisy observations

- ▶ Let $\xi \sim \text{GP}(0, k)$
- ▶ For $i = 1, \dots, n$, we observe $Z_i = \xi(x_i) + \varepsilon_i$ at points x_i , where the random variables ε_i model an observation noise:
 - ▶ $\varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2)$
 - ▶ independent from ξ
- ▶ As above, the posterior mean $\hat{\xi}_n(x)$ of $\xi(x)$ is obtained as the orthogonal projection of $\xi(x)$ on the linear subspace $\text{span}\{Z_i, i = 1, \dots, n\}$:

$$\hat{\xi}_n(x) = \sum_{i=1}^n \lambda_i(x) Z_i$$

with $\lambda_i(x)$ such that

$$\forall i, \quad \xi(x) - \hat{\xi}_n(x) \perp Z_i$$

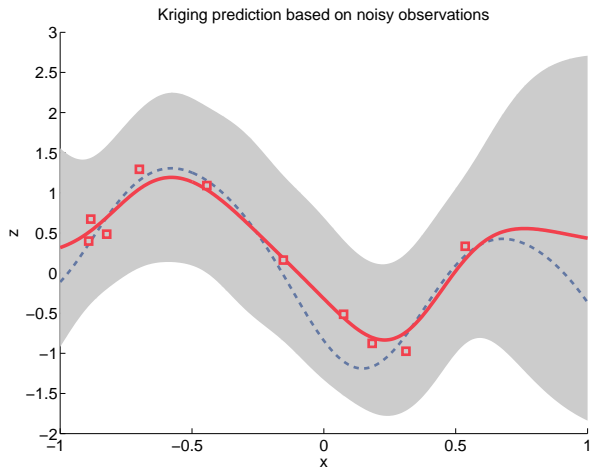
Generalization: prediction from noisy observations

- ▶ Thus, $\forall i$

$$\begin{aligned} & \mathbb{E}[(\xi(x) - \hat{\xi}_n(x))Z_i] \\ &= \mathbb{E}[\xi(x)(\xi(x_i) + \varepsilon_i)] - \sum_{j=1}^n \lambda_j(x) \mathbb{E}[(\xi(x_j) + \varepsilon_j)(\xi(x_i) + \varepsilon_i)] \\ &= k(x, x_i) - \sum_{j=1}^n \lambda_j(x) (k(x_j, x_i) + \sigma^2 \delta_{i,j}) \end{aligned}$$

- ▶ Under matrix form (exercise):

Generalization: prediction from noisy observations



Generalization: prediction from noisy observations

We should use an **approximation instead of an interpolation** in three cases:

- i) The **observations are noisy** (obviously): the computer code is stochastic (for instance, Monte Carlo is used) and running the code twice does not produce the same output
- ii) The **output of the computer code is very irregular** → a smooth approximation is preferred
- iii) The **covariance matrix is ill-conditioned** → adding a small observation noise will regularize the solution of the linear system (why?)

Lecture 1 : From meta-models to UQ

1.1 Introduction

1.2 Black-box modeling

1.3 Bayesian approach

1.4 Posterior distribution of a quantity of interest

1.5 Complements on Gaussian processes

Posterior of a quantity of interest

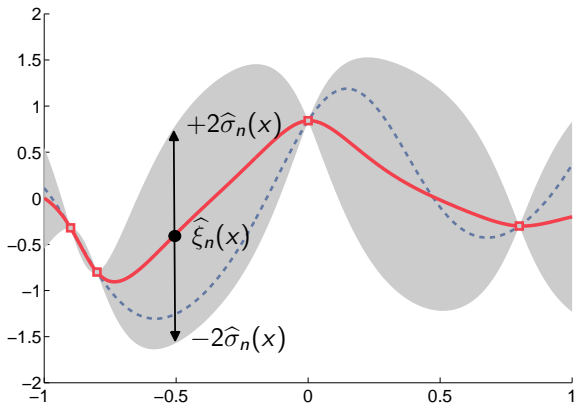
- ▶ Using the posterior distribution of ξ , we can address questions like
 - ▶ What are plausible values for $\xi(x)$ at a given x ? (obviously)
 - ▶ What are plausible values for $\int g(\xi(x)) d\mu(x)$ for given g and μ ?
 - ▶ What are plausible values for the minimum $M = \min_x \xi(x)$?
 - ▶ Where is the minimizer $x^* = \operatorname{argmin}_x \xi(x)$?
 - ▶ What is the probability that $\xi(x)$ exceeds a given threshold?
 - ▶ ...

Example of a quantity of interest: the improvement

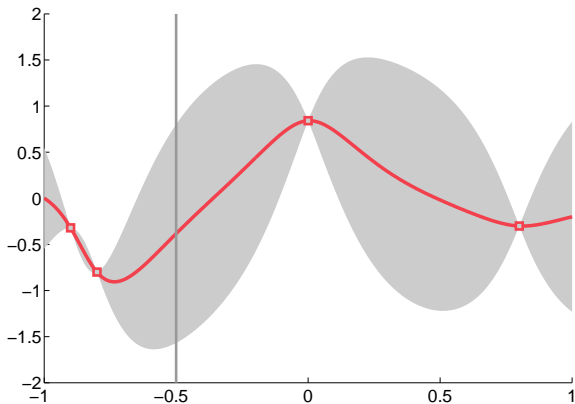
- ▶ Suppose that our objective is to **minimize** an unknown function $f : \mathbb{X} \rightarrow \mathbb{R}$
- ▶ In our Bayesian approach, we choose a GP prior ξ for f (in other words, ξ is a model of f)
- ▶ Objective: construct a sequence $(X_1, X_2, \dots) \in \mathbb{X}$ that converges to $X^* = \operatorname{argmin}_x \xi(x)$
- ▶ Given X_1, \dots, X_{n+1} , how to define and choose a “good” point X_{n+1} in our setting?
- ▶ Let $m_n = \min_{1 \leq i \leq n} \xi(X_i)$
- ▶ A “good” point $x \in \mathbb{X}$ is such that $m_n - \xi(x)$ is large
- ▶ Define the excursion of ξ at x below m_n , a.k.a **the improvement**:

$$I_n = \begin{cases} 0 & \text{if } \xi(x) > m_n \\ m_n - \xi(x) & \text{if } \xi(x) \leq m_n \end{cases}$$

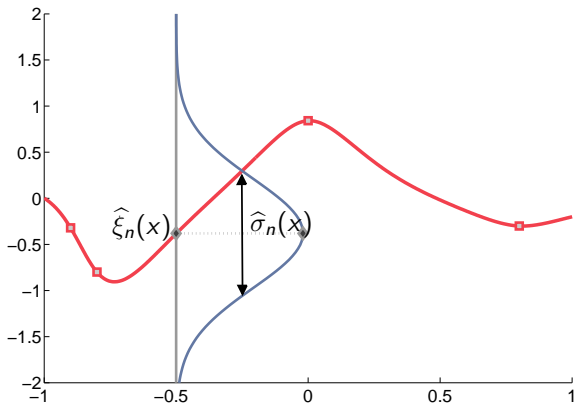
Example of a quantity of interest: the improvement



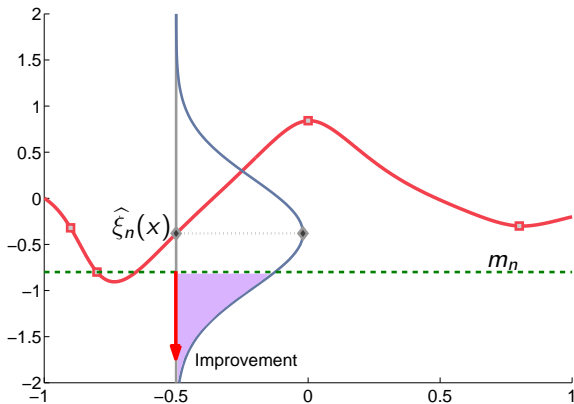
Example of a quantity of interest: the improvement



Example of a quantity of interest: the improvement



Example of a quantity of interest: the improvement



Example of a quantity of interest: the improvement

- ▶ Regions with high values of the **posterior mean** of I_n are promising search regions for the minimum of ξ
- ▶ The posterior mean of I_n may be written as

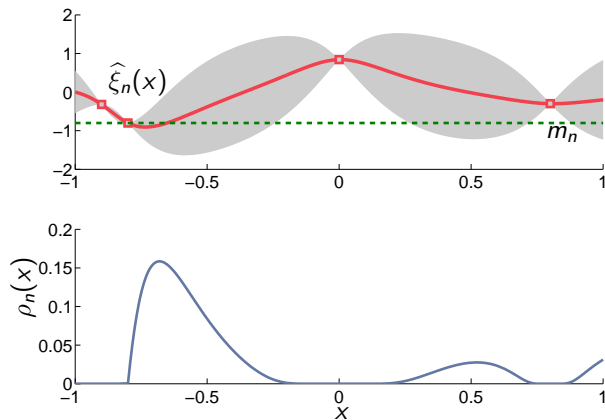
$$\begin{aligned}\rho_n(x) &= E(I_n \mid \xi(X_1), \dots, \xi(X_n)) \\ &= \int_{z=-\inf}^{m_n} (m_n - z) p^{\xi(x) \mid \xi(X_1), \dots, \xi(X_n)}(z) dz \\ &= \gamma(m_n - \hat{\xi}_n(x), \sigma_n^2(x))\end{aligned}$$

with

$$\gamma(z, s) = \begin{cases} \sqrt{s} \Phi' \left(\frac{z}{\sqrt{s}} \right) + z \Phi \left(\frac{z}{\sqrt{s}} \right) & \text{if } s > 0, \\ \max(z, 0) & \text{if } s = 0. \end{cases}$$

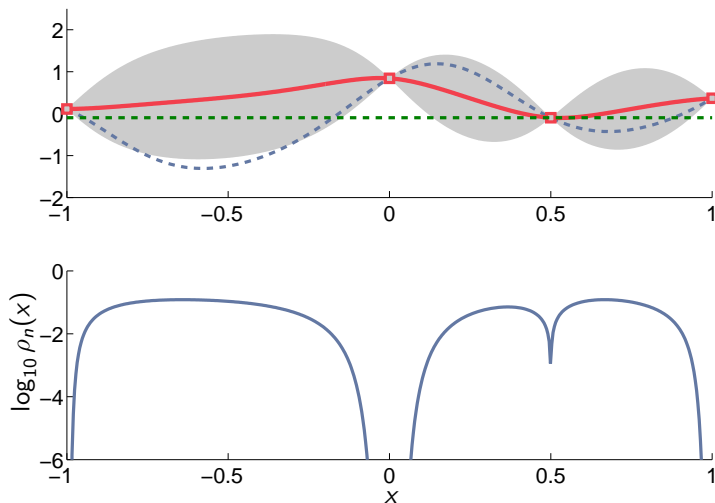
- ▶ ρ_n is called the **expected improvement** [Mockus 78, Schonlau et al. 96, Jones et al. 98]

Example of a quantity of interest: the improvement



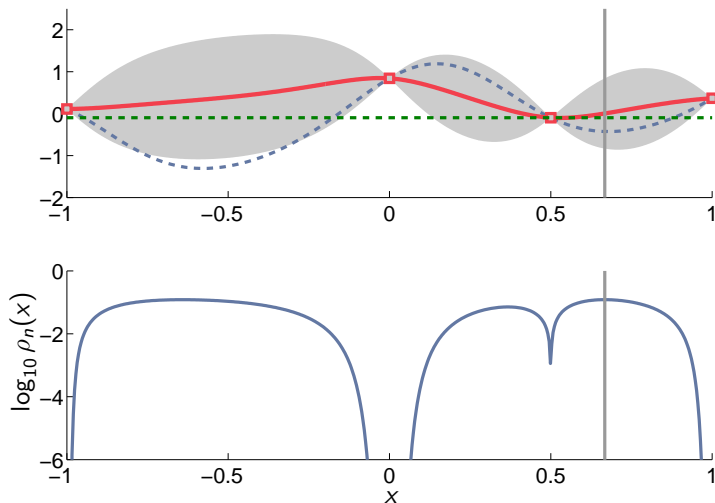
Insertion into an optimization algorithm

- ▶ The EI algorithm: $X_{n+1} = \operatorname{argmax}_x \rho_n(x)$



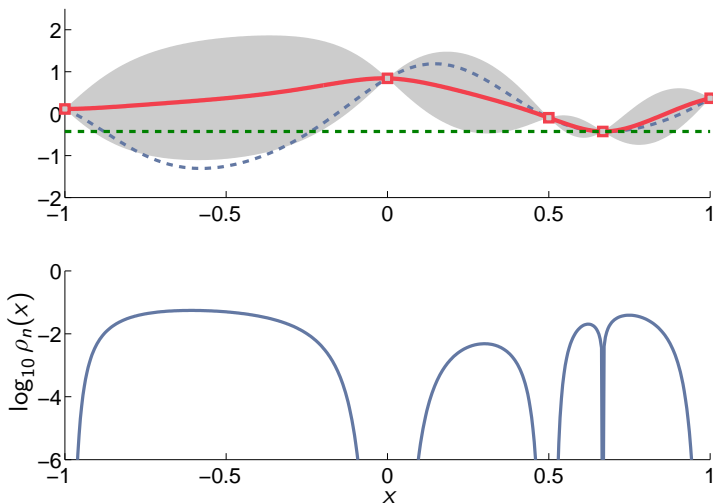
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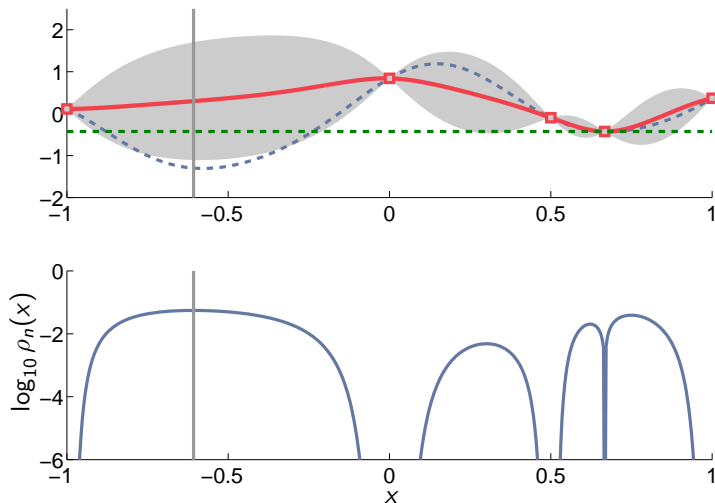
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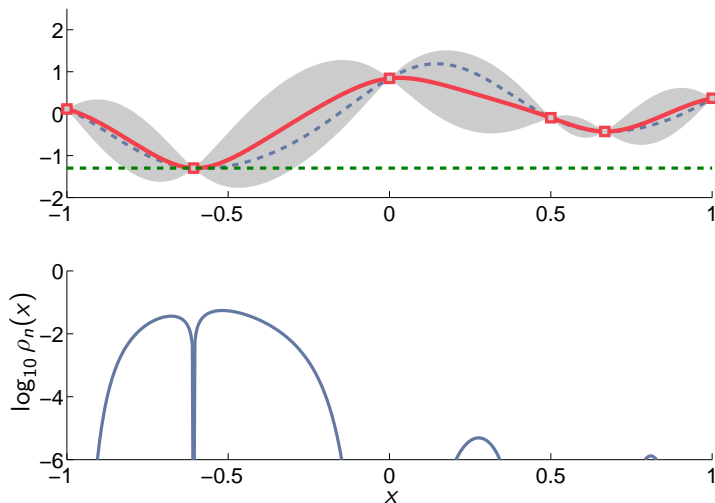
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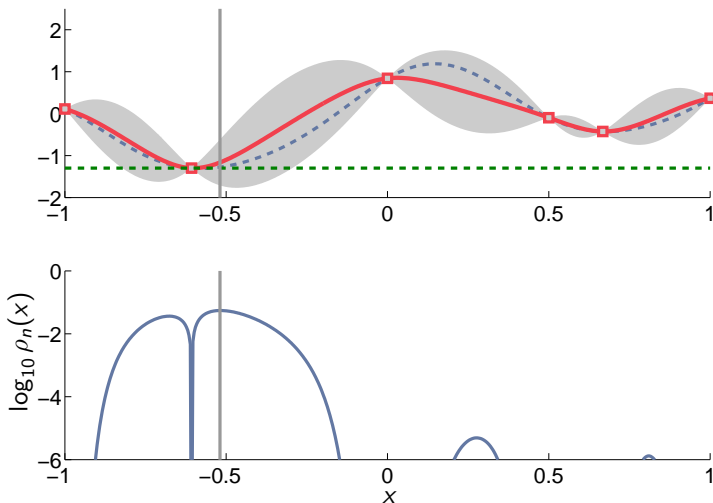
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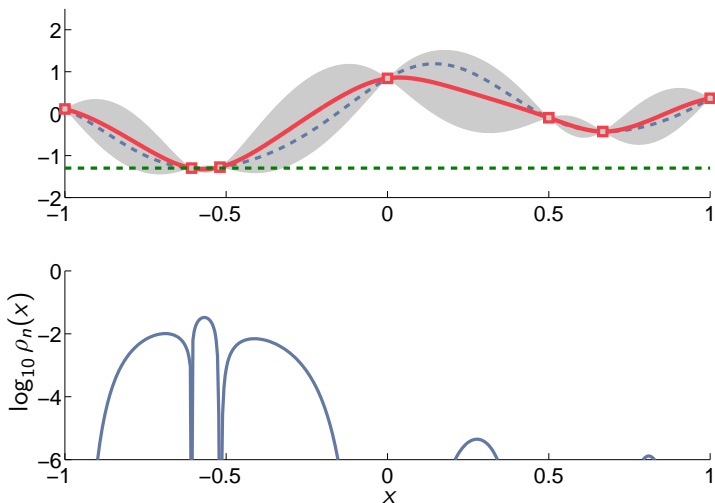
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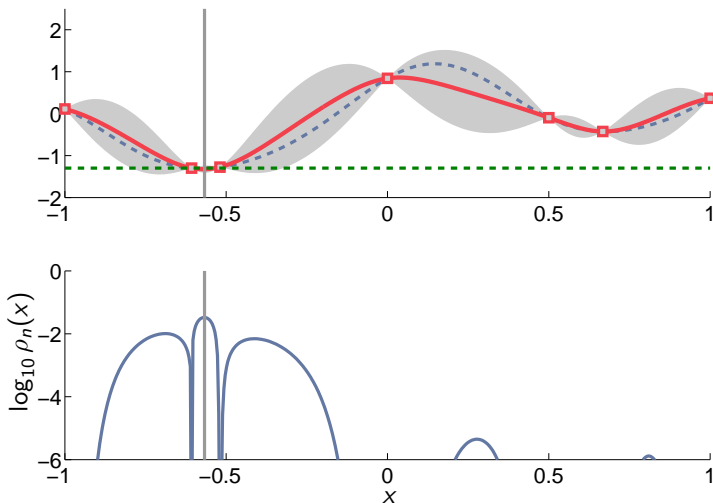
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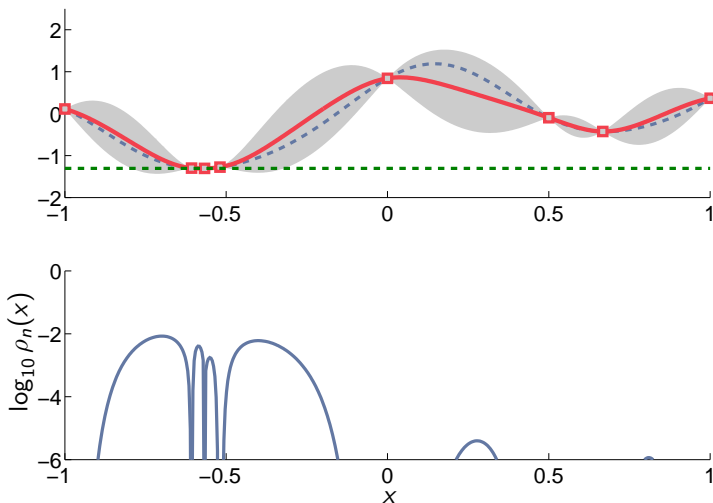
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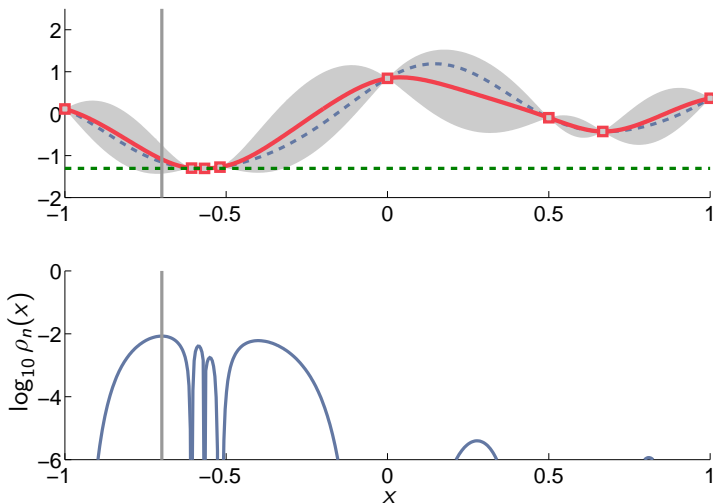
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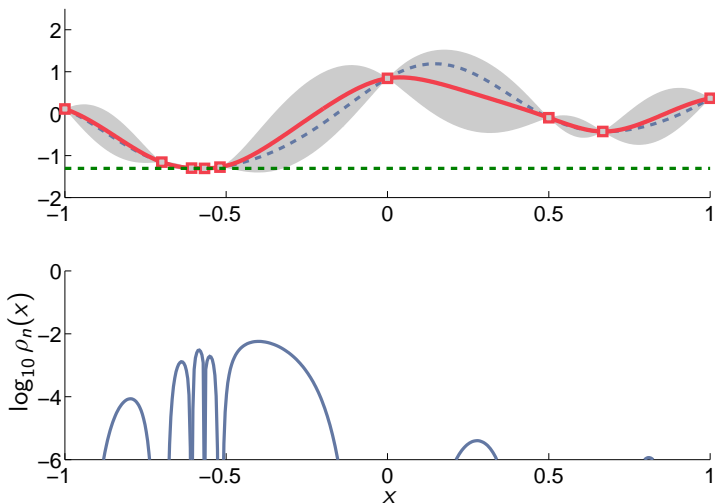
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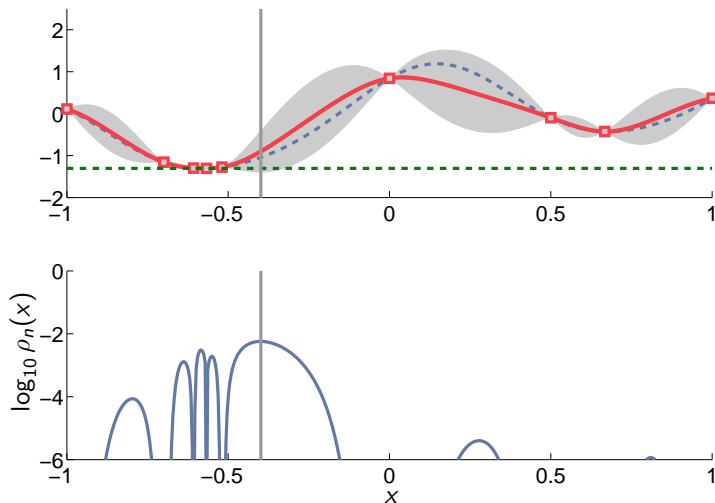
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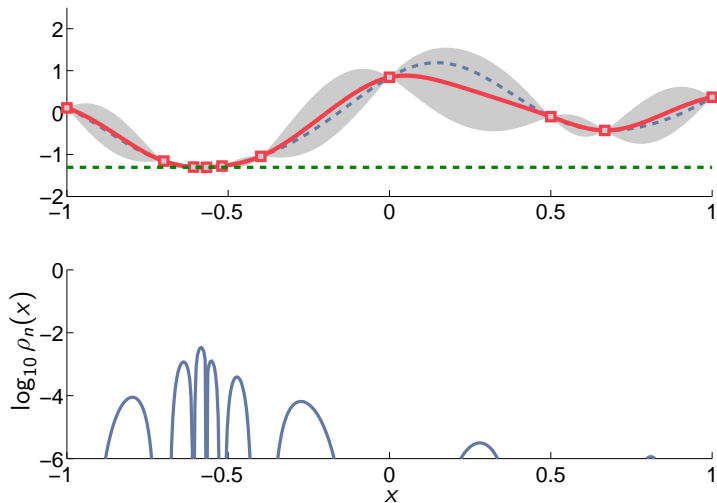
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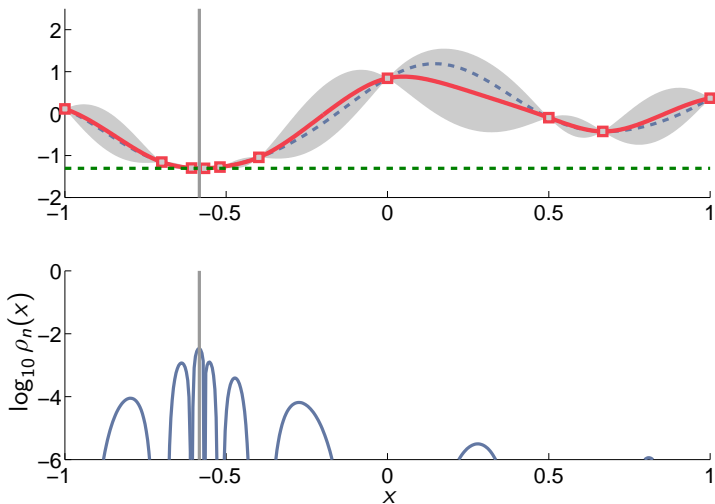
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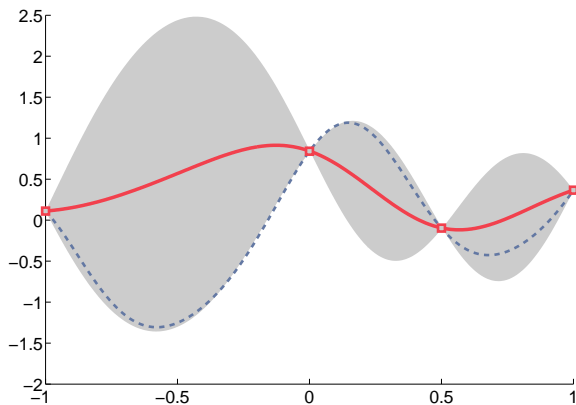
Example of quantity of interest: the minimizer

- ▶ Assume an unknown function $f : \mathbb{X} \rightarrow \mathbb{R}$ and suppose we are interested in seeking its **minimizer**:

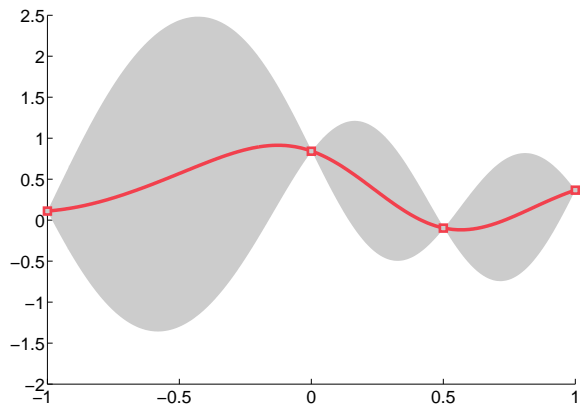
$$x^* = \operatorname{argmin}_x f(x)$$

- ▶ Choose a GP prior ξ for f . Given observations $\xi(x_1), \dots, \xi(x_n)$, what is the posterior distrib. of $X^* = \operatorname{argmin}_x \xi(x)$?
- ▶ Unlike I_n above, the distrib. of X^* does not possess a closed-form expression \rightarrow resort to an **empirical estimation using conditional sample paths**

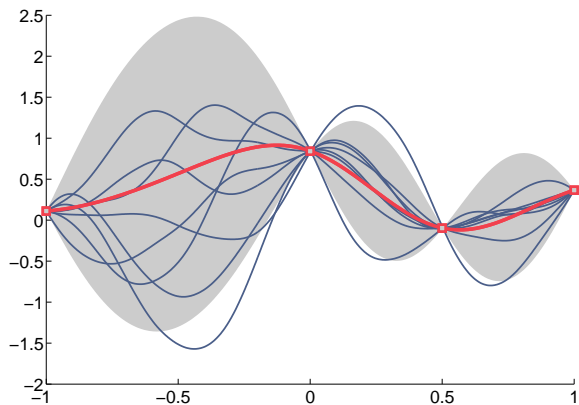
Empirical posterior density of the minimizer



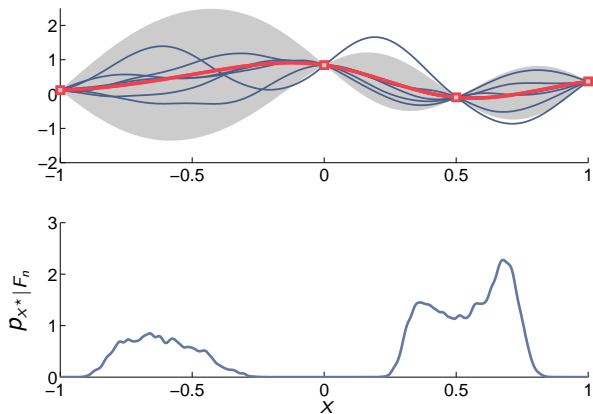
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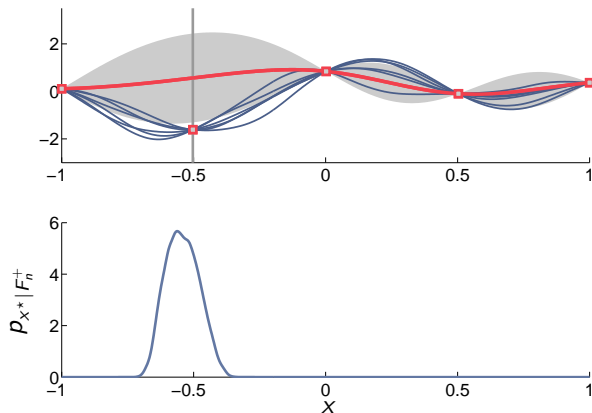
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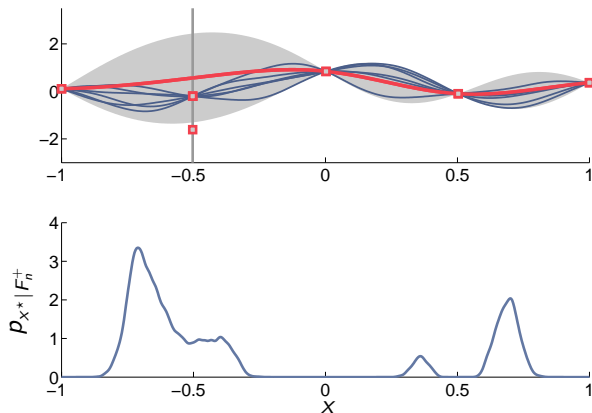
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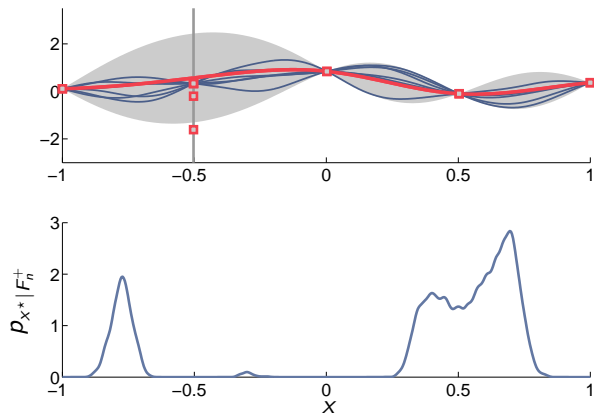
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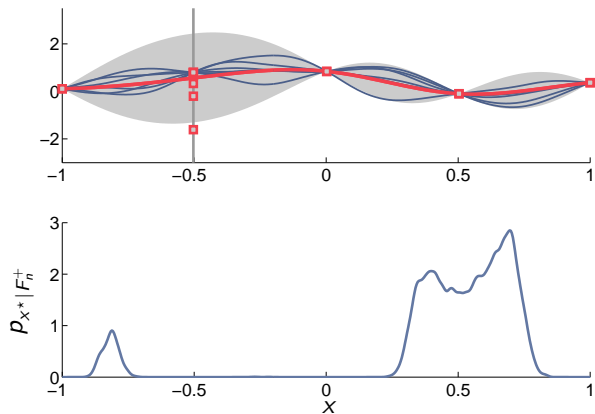
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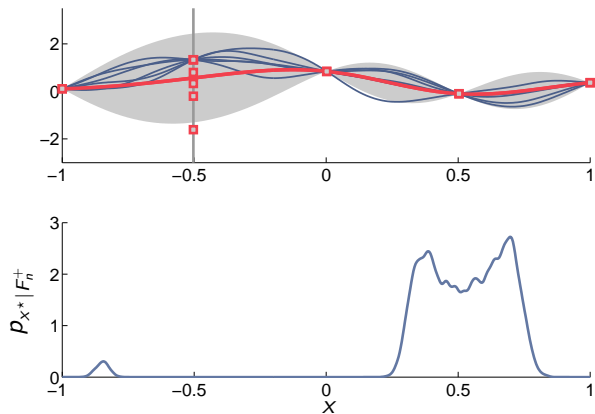
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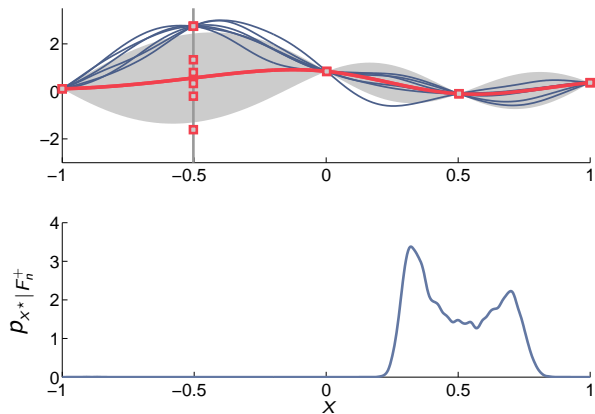
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Lecture 1 : From meta-models to UQ

1.1 Introduction

1.2 Black-box modeling

1.3 Bayesian approach

1.4 Posterior distribution of a quantity of interest

1.5 Complements on Gaussian processes

Choosing a centered Gaussian random process

How to choose the covariance function of a GP $\xi \sim \mathcal{N}(0, k)$?

Regularity properties of a random process

Def.

Given $x_0 \in \mathbb{R}^d$, a random process ξ is said to be **continuous in mean-square** at x_0 iff

$$\lim_{x \rightarrow x_0} E[(\xi(x) - \xi(x_0))^2] = 0$$

Prop.

Let ξ be a second-order random process with continuous mean function and stationary covariance function k . ξ is continuous in mean-square iff k is continuous at zero.

Regularity properties of a random process

Def.

For $x, h \in \mathbb{R}^d$, define the random variable

$$\xi_h(x) = \frac{\xi(x_0 + h) - \xi(x_0)}{\|h\|}$$

ξ is **mean-square differentiable** at x_0 iff there exists a random vector $\nabla\xi(x_0)$ such that

$$\lim_{h \rightarrow 0} \mathbb{E} \left[(\xi_h(x_0) - (\nabla\xi(x_0), h))^2 \right] = 0$$

Prop.

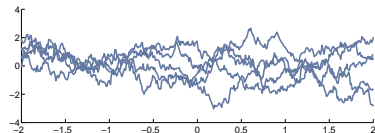
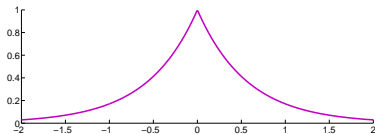
Let ξ be a second-order random process with differentiable mean function and stationary covariance function k . ξ is differentiable in mean-square iff k is two-time differentiable at zero.

Regularity properties of a random process

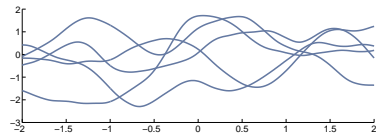
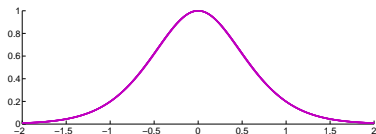
- ▶ Differentiability of the covariance function **at the origin** \rightarrow **mean-square differentiability** of ξ

Influence of the regularity

mean-square continuity



three-time mean-square
differentiability



Choice of a covariance

- ▶ A Gaussian process prior carries a high amount of information about f
 - it is often difficult to elicit such a prior before any evaluation is made
- ▶ Covariance function of ξ is usually assumed to belong to some **parametric class of positive definite functions**
- ▶ Parameter values assumed to be unknown
- ▶ Two approaches:
 1. The parameters can be estimated from the evaluation results by **maximum likelihood**, and then used as if they were known (plug-in approach)
 2. We can assume a prior distrib. for the parameters of the covariance and use a **fully Bayesian approach**

Choice of a parametrized covariance function: the Matérn covariance

- ▶ The **Matérn covariance** function is a conventional covariance function in the literature of computer experiments
→ offers the possibility to adjust the regularity of ξ with a single parameter

- ▶ The Matérn function:

$$\kappa_\nu(h) = \frac{1}{2^{\nu-1}\Gamma(\nu)} \left(2\nu^{1/2}h\right)^\nu \mathcal{K}_\nu \left(2\nu^{1/2}h\right), \quad h \in \mathbb{R} \quad (1)$$

with

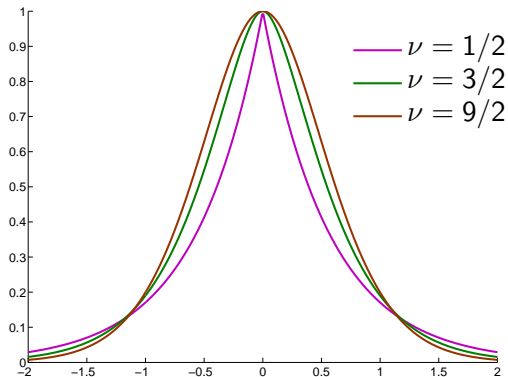
- Γ the Gamma function
- \mathcal{K}_ν the modified Bessel function of the second kind

- ▶ To model a real-valued function defined over $\mathbb{X} \subset \mathbb{R}$, we use the Matérn covariance:

$$k_\theta(h) = \sigma^2 \kappa_\nu(|h|/\rho), \quad h \in \mathbb{R} \quad (2)$$

Choice of a parametrized covariance function: the Matérn covariance

Matérn covariance in one dimension $\sigma^2 = 1$, $\rho = 0.8$



ξ is p -time mean-square differentiable iff $\nu > p$

Choice of a parametrized covariance function: the Matérn covariance

- ▶ To model a function f defined over $\mathbb{X} \subset \mathbb{R}^d$, with $d > 1$, we use the anisotropic form of the Matérn covariance:

$$k_{\theta}(x, y) = \sigma^2 \kappa_{\nu} \left(\sqrt{\sum_{i=1}^d \frac{(x_{[i]} - y_{[i]})^2}{\rho_i^2}} \right), \quad x, y \in \mathbb{R}^d \quad (3)$$

where $x_{[i]}, y_{[i]}$ denote the i^{th} coordinate of x and y , and the positive scalars ρ_i represent scale parameters

- ▶ Since $\sigma^2 > 0, \nu > 0, \rho_i > 0, i = 1, \dots, d$, in practice, we consider the vector of parameters

$$\theta = \{\log \sigma^2, \log \nu, -\log \rho_1, \dots, -\log \rho_d\} \in \mathbb{R}^{d+2}$$

→ makes parameter estimation easier

Parameter estimation by maximum likelihood

- ▶ Assume ξ is a zero-mean Gaussian process
- ▶ The log-likelihood of the data $\underline{\xi}_n = (\xi(x_1), \dots, \xi(x_n))^t$ can be written as

$$\ell(\underline{\xi}_n; \theta) = -\frac{n}{2} \log(2\pi) - \frac{1}{2} \log \det K(\theta) - \frac{1}{2} \underline{\xi}_n^t K(\theta)^{-1} \underline{\xi}_n, \quad (4)$$

where $K(\theta)$ is the covariance matrix of $\underline{\xi}_n$, which depends on the parameter vector θ

- ▶ The log-likelihood can be maximized using a gradient-based search method

Prediction of a Gaussian process with unknown mean function

- ▶ In the domain of computer experiments, the mean of a Gaussian process is generally written as a linear parametric function

$$m(\cdot) = \beta^t \varphi(\cdot), \quad (5)$$

with

- β a vector of unknown parameters
 - $\varphi = (\varphi_1, \dots, \varphi_l)^t$ an l -dimensional vector of functions (in practice, polynomials)
- ▶ Simplest case: the mean function is an unknown constant m , in which case $\beta = m$ and $\varphi : x \in \mathbb{X} \mapsto 1$

Prediction of a Gaussian process with unknown mean function

- ▶ Define the linear space of functions

$$\mathcal{P} = \left\{ x \mapsto \sum_{i=1}^l \beta_i \varphi_i(x); \beta_i \in \mathbb{R} \right\},$$

- ▶ Define Λ the linear space of finite-support measures on \mathbb{X} , i.e.

$$\lambda \in \Lambda \implies \lambda = \sum_{i=1}^n \lambda_i \delta_{x_i} \text{ for some } n \in \mathbb{N}$$

- ▶ For $f : \mathbb{X} \rightarrow \mathbb{R}$, and $\lambda = \sum_{i=1}^n \lambda_i \delta_{x_i} \in \Lambda$,

$$\langle \lambda, f \rangle = \int_{\mathbb{X}} f \, d\lambda = \sum_{i=1}^n \lambda_i f(x_i)$$

- ▶ Define the linear subspace $\Lambda_{\mathcal{P}^\perp} \subset \Lambda$ of finite-support measures vanishing on \mathcal{P} , i.e.

$$\lambda \in \Lambda_{\mathcal{P}^\perp} \implies \langle \lambda, f \rangle = \int_{\mathbb{X}} f \, d\lambda = \sum_{i=1}^n \lambda_i f(x_i) = 0, \quad \forall f \in \mathcal{P}$$

Prediction of a Gaussian process with unknown mean function

- ▶ Let ξ be a Gaussian random process with an unknown mean in \mathcal{P} , and a covariance function k
- ▶ For $x \in \mathbb{X}$, the (intrinsic) kriging predictor $\widehat{\xi}_n(x)$ of $\xi(x)$ from $\xi(x_1), \dots, \xi(x_n)$ is the linear projection

$$\widehat{\xi}_n(x) = \sum_i \lambda_i(x) \xi(x_i)$$

of $\xi(x)$ onto $\text{span}\{\xi(x_i), i = 1, \dots, n\}$ such that the variance of the error $\xi(x) - \widehat{\xi}_n(x)$ is minimized, under the constraint

$$\delta_x - \sum \lambda_i(x) \delta_{x_i} \in \Lambda_{\mathcal{P}^\perp}$$

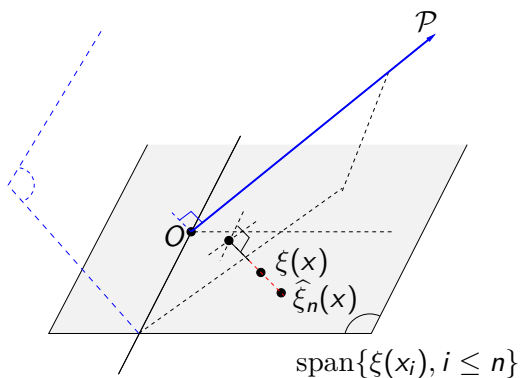
i.e.,

$$\langle \delta_x - \sum \lambda_i(x) \delta_{x_i}, \varphi_j \rangle = \varphi_j(x) - \sum \lambda_i(x) \varphi_j(x_i) = 0, \quad j = 1, \dots, l$$

- ▶ The requirement $\delta_x - \sum \lambda_i(x) \delta_{x_i} \in \Lambda_{\mathcal{P}^\perp}$ makes the kriging predictor **unbiased, even if the mean of ξ is unknown**

Prediction of a Gaussian process with unknown mean function

$\hat{\xi}_n(x)$ is the linear projection of $\xi(x)$ onto $\text{span}\{\xi(x_1), \dots, \xi(x_n)\}$ orthogonally to \mathcal{P}



Prediction of a Gaussian process with unknown mean function

- ▶ The weights $\lambda_i(x; x_n)$ are again solutions of a **system of linear equations**, which can be written under a matrix form as

$$\begin{pmatrix} K & \underline{\varphi}^t \\ \underline{\varphi} & 0 \end{pmatrix} \begin{pmatrix} \lambda(x) \\ \mu(x) \end{pmatrix} = \begin{pmatrix} k(x) \\ \varphi(x) \end{pmatrix}, \quad (6)$$

with

- $\underline{\varphi}$ an $l \times n$ matrix with entries $\varphi_i(x_j)$, $i = 1, \dots, l$, $j = 1, \dots, n$
- μ a vector of Lagrange coefficients
- K , $\lambda(x)$, $k(x)$ as above

Prediction of a Gaussian process with unknown mean function

- ▶ When the mean is unknown, the **kriging covariance function** (the covariance of the error of prediction) is given by

$$\begin{aligned}k_n(x, y) &:= \text{cov} \left(\xi(x) - \widehat{\xi}_n(x), \xi(y) - \widehat{\xi}_n(y) \right) \\ &= k(x - y) - \lambda(x)^t k(y) - \mu(x)^t \varphi(y).\end{aligned}$$

Prop.

Let k be a covariance function and assume $m \in \mathcal{P}$.

$$\text{If } \begin{cases} \xi \mid m \sim \mathcal{GP}(m, k) \\ m : x \mapsto \beta^t \varphi(x), \beta \sim U(\mathbb{R}^l) \end{cases} \quad \text{then } \xi \mid F_n \sim \mathcal{GP} \left(\widehat{\xi}_n(\cdot), k_n(\cdot, \cdot) \right)$$

with $U(\mathbb{R}^l)$ the (improper) uniform distribution over \mathbb{R}^l

→ justifies the use of kriging in a **Bayesian framework** provided that the covariance function of ξ is known

Parameter estimation with unknown mean function

- ▶ Objective: estimate the covariance parameters of a Gaussian process with unknown mean
- ▶ **Restricted Maximum Likelihood (REML)** approach → maximize the **likelihood of the increments** (or generalized increments) of the data
- ▶ Let ξ be a Gaussian process with an **unknown mean** function in \mathcal{P} and $\underline{\xi}_n$ the random vector of observations at points x_i , $i = 1, \dots, n$
- ▶ Let $\underline{\varphi} = (\varphi_i(x_j))_{i,j=1}^{l,n}$ be the $l \times n$ matrix of basis functions of \mathcal{P} evaluated on $\{x_1, \dots, x_n\}$.

Parameter estimation with unknown mean function

- ▶ Since the dimension of \mathcal{P} is l , the dimension of the space of the measures with support $\{x_1, \dots, x_n\}$ that cancel out the functions of \mathcal{P} is $n - l$.
- ▶ Assume an $n \times (n - l)$ matrix W with rank $n - l$ has been found, such that

$$\underline{\varphi}W = 0.$$

(The columns of W are in the kernel of $\underline{\varphi}$.)

- ▶ Then $Z = W^T \underline{\xi}_n$ is a Gaussian random vector taking its values in \mathbb{R}^{n-l} , with **zero mean** and covariance matrix

$$W^T K(\theta) W$$

where $K(\theta)$ is the covariance matrix of $\underline{\xi}_n$ with entries $k_\theta(x_i - x_j)$

REML

- ▶ The random vector Z is a **contrast vector**
- ▶ The log-likelihood of the contrasts is given by

$$L(z | \theta) = -\frac{n-l}{2} \log 2\pi - \frac{1}{2} \log \det(W^t K(\theta) W) - \frac{1}{2} z^t (W^t K(\theta) W)^{-1} z.$$

REML

- ▶ Various methods may be employed to compute the matrix W
- ▶ We favor the QR decomposition of $\underline{\varphi}^T$

$$\underline{\varphi}^T = (Q_1 \mid Q_2) \begin{pmatrix} R \\ 0 \end{pmatrix},$$

where $(Q_1 \mid Q_2)$ is an $n \times n$ orthogonal matrix and R is a $l \times l$ upper triangular matrix

- ▶ It is trivial to check that the columns of Q_2 form a basis of the kernel of $\underline{\varphi}$
- ▶ So we may chose $W = Q_2$
- ▶ Note that $W^T W = I_{n-l}$.

Books

- ▶ **M. Stein**, Interpolation of Spatial Data: Some Theory for kriging, Springer, 1999
- ▶ **T. Santner, B. Williams and W. Notz**, The Design and Analysis of Computer Experiments, Springer, 2003
- ▶ **C. Rasmussen and C. Williams**, Gaussian processes for Machine Learning, MIT Press, 2006
- ▶ **A. Forrester, A. Sóbester and A. Keane**, Engineering design via surrogate modelling: a practical guide, John Wiley & Sons, 2008

Lecture 1 : From meta-models to UQ

- 1.1 Introduction
- 1.2 Black-box modeling
- 1.3 Bayesian approach
- 1.4 Posterior distribution of a quantity of interest
- 1.5 Complements on Gaussian processes

Lecture 2 : Bayesian optimization (BO)

- 2.1. Decision-theoretic framework
- 2.2. From Bayes-optimal to myopic strategies
- 2.3. Design under uncertainty

References

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 - ▶ optimization using tools from Bayesian UQ

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- ▶ In this lecture we adopt this second (more constructive !) definition

Lecture 2 : Bayesian optimization (BO)

2.1. Decision-theoretic framework

2.2. From Bayes-optimal to myopic strategies

2.3. Design under uncertainty

Decision-theoretic framework

Decision-theoretic framework (cont'd)

- ▶ How does this relate to optimization ?

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- ▶ The agent is the optimization algorithm (or you, if you will)

Ingredients of a BDT problem

- ▶ a set of all possible “states of nature”
- ▶ a prior distribution over the states of nature
- ▶ a description of the decisions we have to make
- ▶ and the corresponding “transitions”
- ▶ a loss function (or utility function)

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 1. the **content of the black box** (expensive numerical model)
 2. for stochastic simulators: **future responses** of the simulator
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 4. ...

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Notation

$$\Omega = \{\text{all possible states } \omega \text{ of nature}\}$$

States of nature: example

- ▶ Consider the following setting
 - ▶ a **deterministic** numerical model
 - ▶ input space $\mathbb{X} \subset \mathbb{R}^d$, output space \mathbb{R}^p
 - ▶ **no environmental** variables in the problem

- ▶ States of nature for this setting
 - ▶ $\Omega = \{f : \mathbb{X} \rightarrow \mathbb{R}^p \mid f \text{ such that } \dots\}$

States of nature: example

- ▶ Consider the following setting
 - ▶ a deterministic numerical model
 - ▶ input space $\mathbb{X} \subset \mathbb{R}^d$, output space \mathbb{R}^p
 - ▶ no environmental variables in the problem
- ▶ States of nature for this setting
 - ▶ $\Omega = \{f : \mathbb{X} \rightarrow \mathbb{R}^p \mid f \text{ such that } \dots\}$
 - ▶ e.g., $d = 1$, $p = 1$, $\mathbb{X} = [0; 1]$ and $\Omega = C(\mathbb{X}; \mathbb{R})$
- ▶ Until further notice, we will use this simple (but important) setting to illustrate the basics of Bayesian optimization

Uncertainty quantification (reminder from Lecture #1)

- ▶ The true state of nature $\omega^* \in \Omega$ is **unknown**
- ▶ Example (cont'd)
 - ▶ a function $f^* \in \Omega = C(\mathbb{X}; \mathbb{R})$ is inside the black box ($\omega^* \equiv f^*$)
 - ▶ we don't “know” $f^*(x)$ until we run the code with input x

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- ▶ Bayesian approach to UQ
 - ▶ our knowledge of ω^* is encoded by a **probability distribution** on the set Ω of all possible ω 's
 - ▶ technically: proba on (Ω, \mathcal{F}) for some σ -algebra $\mathcal{F} \dots$

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 - ▶ technically: proba on (Ω, \mathcal{F}) for some σ -algebra $\mathcal{F} \dots$
- ▶ Sequence of decisions \Rightarrow **sequence of distributions** P_0, P_1, \dots
 - ▶ P_n corresponds to the agent's beliefs after the n^{th} decision
 - ▶ A **prior distribution** P_0 needs to be specified

Uncertainty quantification: consequences

- ▶ For clarity, consider again the case of a **deterministic model**:
 - ▶ an **unknown function** $f \in \Omega$ is in the black box

Uncertainty quantification: consequences

- ▶ For clarity, consider again the case of a deterministic model:
 - ▶ an unknown function $f \in \Omega$ is in the black box
 - ▶ Given a proba P on Ω , we can
 - ▶ compute the **probability** of any (measurable) statement about f
 - ▶ compute the **expectation** of any (measurable) function of f
- i.e., the unknown f can be **treated as random**

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Convenient notation

ξ = random function that represents the unknown f

- ▶ we will write, e.g., $E_n(\xi(x))$ instead of $\int_{\Omega} f(x) P_n(df)$ ☺

Decision-theoretic framework (cont'd)

- ▶ How does this relate to optimization ?
- ▶ The agent is the optimization algorithm (or you, if you will)

Ingredients of a BDT problem

- ▶ a set of all possible “states of nature”
- ▶ a prior distribution over the states of nature
- ▶ a description of the decisions we have to make
- ▶ and the corresponding “transitions”
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Decisions

- ▶ Several types of decisions in an optimization procedure:
 - ▶ intermediate decisions
 - ▶ stopping decision
 - ▶ final decision

Decisions: intermediate decisions

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- ▶ Intermediate decisions (simple setting)
 - ▶ **running the numerical model** with a given input $x \in \mathbb{X}$
 - ▶ getting the corresponding output (deterministic or random)

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 - ▶ final decision
- ▶ Intermediate decisions (simple setting)
 - ▶ running the numerical model with a given input $x \in \mathbb{X}$
 - ▶ getting the corresponding output (deterministic or random)
- ▶ Intermediate decisions (various extensions)
 - ▶ parallel computing: **batches** of input values
 - ▶ multi-fidelity: choosing the right **fidelity level**
 - ▶ variable run-time: choosing when to **stop a computation**
 - ▶ ...

Decisions: stopping decision

- ▶ Several types of decisions in an optimization procedure:
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 - ▶ **stopping decision**
 - ▶ final decision

- ▶ Stopping decision (standard setting)
 - ▶ a **budget of evaluations**, or computation time, is given
 - ▶ the stopping decision is trivial in this case

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- ▶ Stopping decision (standard setting)
 - ▶ a budget of evaluations, or computation time, is given
 - ▶ the stopping decision is trivial in this case
- ▶ Digression: taking the cost of observations into account?
 - ▶ *in principle*, BO can deal with the stopping decision too
 - ▶ in practice, difficult to translate into a loss (see later)
 - ▶ some “BO papers” propose heuristic stopping rule

Decisions: final decision

- ▶ Several types of decisions in an optimization procedure:
 - ▶ intermediate decisions
 - ▶ stopping decision
 - ▶ **final decision**

- ▶ Final decision (ex: single-objective minimization pb.)
 - ▶ an **estimate of the minimizer** $x^* = \operatorname{argmin}_{x \in \mathbb{X}} f(x)$
 - ▶ and/or an **estimate of the minimum** $M^* = \min_{x \in \mathbb{X}} f(x)$

with \mathbb{X} a “known” input space

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- ▶ Other settings

- ▶ **multi-objective**: Pareto set / Pareto front (see later),
- ▶ **inequality constraints** (see later), equality constraints (harder !)
- ▶ quasi-optimal region (sublevel set)...

Decisions: standard setting and notations

- ▶ From now on we focus on the “standard” setting
 - ▶ **intermediate decisions \equiv evaluations** (known comput. cost)
 - ▶ stopping: a **budget of N evaluations** is given

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Notations

$X_n(\omega)$ = the n^{th} evaluation point

$D_{N+1}(\omega)$ = the “final decision” (estimate of the QoI)

$\underline{D}(\omega) = (X_1(\omega), \dots, X_N(\omega), D_{N+1}(\omega))$

Transitions: conditioning probability measures

- ▶ Recall that
 - ▶ the agent's knowledge at time n is described by P_n
 - ▶ the $(n + 1)^{\text{th}}$ decision induces a transition $P_n \rightarrow P_{n+1}$

Decisions: standard setting and notations

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$\underline{D}(\omega) = (X_1(\omega), \dots, X_N(\omega), D_{N+1}(\omega))$

- ▶ We cannot use information that is not yet available
 - ▶ $X_n(\omega)$ depends on ω through F_{n-1} only
 - ▶ $D_{N+1}(\omega)$ depends on ω through F_N only
 - ▶ \underline{D} is a decision strategy (sequence of decision rules)

Transitions: examples

- ▶ Example (cont'd)
 - ▶ single-output, deterministic code
 - ▶ $I_n = (X_n, \xi(X_n))$ and $F_n = (X_1, \xi(X_1), \dots, X_n, \xi(X_n))$
 - ▶ $\xi(X_i) = f^*(X_i)$ is the true, scalar, value of the model at X_i

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- ▶ Many other (interesting) settings are possible !
 - ▶ **stochastic simulators**
 - ▶ the output is a random draw $Z_n \sim$ some distrib. $P^{Z_n|X_n}$
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 - ▶ variable run-times, “simulation failures”...

Decision-theoretic framework (cont'd)

- ▶ How does this relate to optimization ?
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Loss function

- ▶ To guide the decisions of the Bayesian agent, we need to specify a **loss function** L

Notation

$$L : \Omega \times \mathbb{D} \rightarrow \mathbb{R}$$

$$(\omega, \underline{d}) \mapsto L(\omega, \underline{d})$$

where \mathbb{D} is the set of all possible sequences of decisions

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where \mathbb{D} is the set of all possible sequences of decisions

- ▶ The **Bayes-optimal strategy** is, by definition:

$$\begin{aligned} \underline{D} &= \operatorname{argmin} E_0(L(\underline{D})) \\ &= \operatorname{argmin} \int_{\Omega} L(\omega, \underline{D}(\omega)) P_0(d\omega) \end{aligned}$$

where \underline{D} ranges over all strategies

Loss function: example

- ▶ Example (cont'd)
 - ▶ Assume that we want to find the minimizer of f
 - ▶ $\underline{d} = (x_1, \dots, x_n, \hat{x})$
 - ▶ with \hat{x} our estimate of $\operatorname{argmin} f$

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- ▶ $\underline{d} = (x_1, \dots, x_n, \hat{x})$

- ▶ with \hat{x} our estimate of $\operatorname{argmin} f$

- ▶ A standard loss function for this situation is the **linear loss**:

$$L(f, \underline{d}) = L(f, \hat{x}) = f(\hat{x}) - \min f$$

(a.k.a. **opportunity cost**, a.k.a. **instantaneous regret**)

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- ▶ Remarks

- ▶ L coincides with the L^1 loss of the estimator $f(\hat{x})$

$$f(\hat{x}) \geq \min f \quad \Rightarrow \quad L(f, \hat{x}) = |f(\hat{x}) - \min f|$$

- ▶ L is a **terminal loss** (does not depend on $X_1, \xi(X_1), \dots$)

Decision-theoretic framework (cont'd)

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- ▶ Our BDT framework is complete, let's use it 😊

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Lecture 2 : Bayesian optimization (BO)

2.1. Decision-theoretic framework

2.2. From Bayes-optimal to myopic strategies

2.3. Design under uncertainty

Problem statement

- ▶ Assume a standard BO setting
 - ▶ fixed budget N , terminal cost only
 - ▶ $L(\omega, \underline{d}) = L(\omega, d_{N+1})$
 - ▶ intermediate decisions \equiv evaluations
 - ▶ one at a time, possibly noisy (stochastic simulator)
 - ▶ $F_n = (X_1, Z_1, \dots, X_n, Z_n)$

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 - ▶ $F_n = (X_1, Z_1, \dots, X_n, Z_n)$
- ▶ Recall the **Bayes-optimal strategy** (algorithm):

$$\begin{aligned}\underline{D}^{\text{Bayes}} &= \operatorname{argmin}_{\underline{D}} E_0(L(D_{N+1})) \\ &= \operatorname{argmin}_{\underline{D}} \int_{\Omega} L(\omega, D_{N+1}(\omega)) P_0(d\omega)\end{aligned}$$

where \underline{D} ranges over all strategies $\underline{D} = (X_1, \dots, X_N, D_{N+1})$

Problem statement

What does this $\underline{D}^{\text{Bayes}}$ look like ?

Can we actually **build an optimal Bayesian algorithm** ?

Problem statement (more precisely)

- ▶ Recall that
 - ▶ $X_{n+1}(\omega)$ must depend on ω through F_n only
 - ▶ $D_{N+1}(\omega)$ must depend on ω through F_N only

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Notations

$$X_{n+1} = \varphi_n(X_1, Z_1, \dots, X_n, Z_n) = \varphi_n(F_n)$$

$$D_{N+1} = \varphi_N(X_1, Z_1, \dots, X_N, Z_N) = \varphi_N(F_N)$$

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- ▶ Goal: find the functions $\varphi_0, \dots, \varphi_N$

Lecture 2 : Bayesian optimization (BO)

2.2. From Bayes-optimal to myopic strategies

The optimal terminal decision

Optimal choice of the last evaluation

Bayes-optimal versus “practical Bayes” optimization

Sampling criteria for multi-objective and/or constrained optimization

Optimal terminal decision

Notation

$E_n = E(\cdot | F_n)$ = conditional expectation with respect to F_n
= expectation with respect to the probability P_n

Optimal terminal decision

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= expectation with respect to the probability P_n

- ▶ Consider any incomplete strategy X_1, \dots, X_N
- ▶ Claim: the **optimal terminal decision** is

$$D_{N+1} = \varphi_N^{\text{Bayes}}(X_1, Z_1, \dots, X_N, Z_N) = \text{argmin}_d E_N(L(d))$$

where d runs over all possible values for the terminal decision

Optimal terminal decision: proof

- ▶ Take **any strategy** $\underline{D} = (X_1, \dots, X_N, D_{N+1})$
- ▶ Consider the **modified strategy** $\underline{D}' = (X_1, \dots, X_N, D'_{N+1})$
where $D'_{N+1} = \varphi_N^{\text{Bayes}}(X_1, Z_1, \dots, X_N, Z_N)$

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where $D'_{N+1} = \varphi_N^{\text{Bayes}}(X_1, Z_1, \dots, X_N, Z_N)$
- ▶ Then, by definition of φ_N^{Bayes} ,

$$\begin{aligned} E_N(L(D_{N+1})) &= E_N(L(d))|_{d=D_{N+1}} \\ &\geq \min_d E_N(L(d)) = E_N(L(D'_{N+1})) \end{aligned}$$

Optimal terminal decision: proof

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- ▶ and thus

$$\begin{aligned} E_0(L(D_{N+1})) &= E_0(E_N(L(D_{N+1}))) \\ &\geq E_0(E_N(L(D'_{N+1}))) = E_0(L(D'_{N+1})) \quad \blacksquare \end{aligned}$$

Vocabulary: posterior (Bayes) risk at time N

- ▶ Define the **posterior risk** at time N for the decision d :

$$R_N(d) = E_N(L(d))$$

(“risk” is a synonym for “expected loss”)

Vocabulary: posterior (Bayes) risk at time N

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(“risk” is a synonym for “expected loss”)

- ▶ Define the **posterior Bayes risk** at time N :

$$R_N^{\text{Bayes}} = \min_d R_N(d)$$

- ▶ Remember: the min attained for $d = \varphi_N^{\text{Bayes}}(F_N)$

Example (cont'd): linear loss

- ▶ Recall the setting
 - ▶ goal: minimize f
 - ▶ $d_{N+1} = \hat{x}$ is an estimate of $X^*(f) = \operatorname{argmin} f$
 - ▶ $L(f, \hat{x}) = f(\hat{x}) - \min f$

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 - ▶ $L(f, \hat{x}) = f(\hat{x}) - \min f$
- ▶ Compute the **posterior risk** at time N for a given $\hat{x} \in \mathbb{X}$:

$$\begin{aligned}R_N(\hat{x}) &= \mathbb{E}_N(L(\xi, \hat{x})) = \mathbb{E}_N(\xi(\hat{x}) - \min \xi) \\ &= \hat{\xi}_N(\hat{x}) - \mathbb{E}_N(\min \xi)\end{aligned}$$

Example (cont'd): linear loss

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- ▶ Compute the posterior risk at time N for a given $\hat{x} \in \mathbb{X}$:

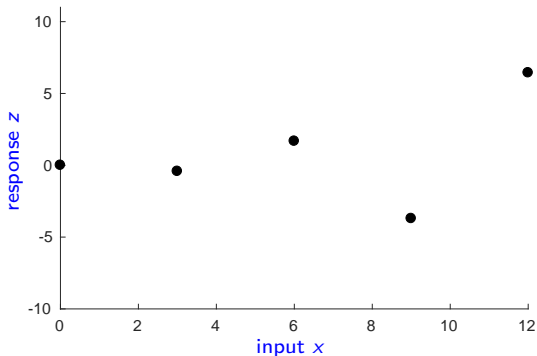
$$\begin{aligned}R_N(\hat{x}) &= E_N(L(\xi, \hat{x})) = E_N(\xi(\hat{x}) - \min \xi) \\ &= \hat{\xi}_N(\hat{x}) - E_N(\min \xi)\end{aligned}$$

- ▶ Thus the optimal terminal decision is

$$D_{N+1}^{\text{Bayes}} = \hat{X}^{\text{Bayes}} = \operatorname{argmin}_{x \in \mathbb{X}} \hat{\xi}_N(x)$$

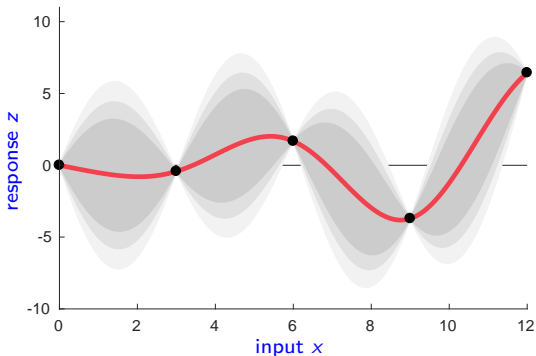
Example (cont'd): linear loss

Assume that $n = N = 5$ (a small budget indeed).



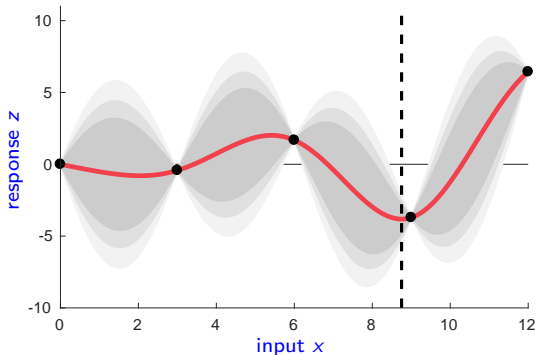
Example (cont'd): linear loss

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Example (cont'd): linear loss

Assume that $n = N = 5$ (a small budget indeed).



Example (cont'd): the L^1 loss, variant

- ▶ To summarize, we have for this example

$$\hat{X}^{\text{Bayes}} = \operatorname{argmin} \hat{\xi}_N$$

$$R_N^{\text{Bayes}} = \min \hat{\xi}_N - E_N(\min \xi)$$

- ▶ Remark: in general, $\hat{X}^{\text{Bayes}} \notin \{X_1, \dots, X_N\}$
 - ▶ the value of the function at \hat{X}^{Bayes} is not known

Example (cont'd): the L^1 loss, variant

- ▶ To summarize, we have for this example

$$\hat{X}^{\text{Bayes}} = \operatorname{argmin} \hat{\xi}_N$$

$$R_N^{\text{Bayes}} = \min \hat{\xi}_N - E_N(\min \xi)$$

- ▶ Remark: in general, $\hat{X}^{\text{Bayes}} \notin \{X_1, \dots, X_N\}$
 - ▶ the value of the function at \hat{X}^{Bayes} is not known

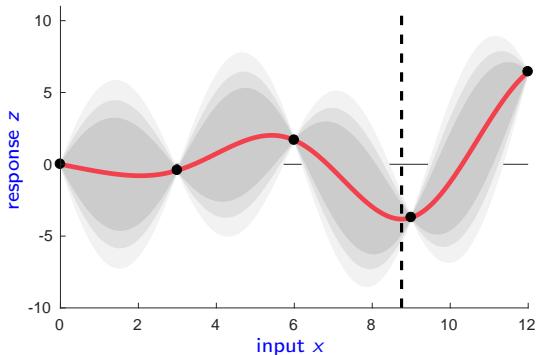
- ▶ Variant: restrict the terminal decision to $\{X_1, \dots, X_N\}$

$$\hat{X}^{\text{Bayes},1} = \operatorname{argmin}_{x \in \{X_1, \dots, X_N\}} \xi(x)$$

$$R_N^{\text{Bayes},1} = \min_{i \leq N} \xi(X_i) - E_N(\min \xi)$$

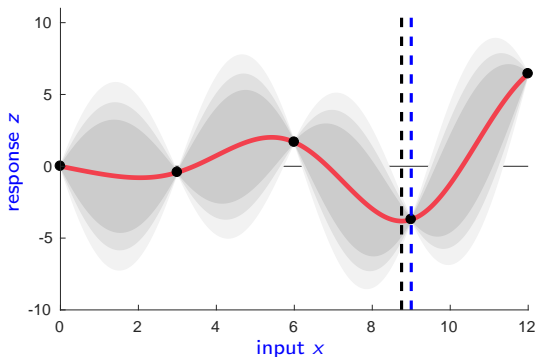
Example (cont'd): linear loss

Assume that $n = N = 5$ (a small budget indeed).



Example (cont'd): linear loss

Assume that $n = N = 5$ (a small budget indeed).



Remark: the two estimates are equal when $\hat{\xi}$ does not “overshoot”
(e.g., for a Brownian motion prior)

Lecture 2 : Bayesian optimization (BO)

2.2. From Bayes-optimal to myopic strategies

The optimal terminal decision

Optimal choice of the last evaluation

Bayes-optimal versus “practical Bayes” optimization

Sampling criteria for multi-objective and/or constrained optimization

Finding X_N^{Bayes} (last evaluation point)

- ▶ Let us focus now on the **last evaluation point**
 - ▶ recall that $\underline{D} = (X_1, \dots, X_{N-1}, X_N, D_{N+1})$

Finding X_N^{Bayes} (last evaluation point)

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Notation

$E_{n,x}(Y)$ will mean: “compute $E_n(Y)$, assuming that $X_{n+1} = x$ ”

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Notation

$E_{n,x}(Y)$ will mean: “compute $E_n(Y)$, assuming that $X_{n+1} = x$ ”

- ▶ For example, if $Y = g(X_1, Z_1, \dots, X_n, Z_n, X_{n+1}, Z_{n+1})$,

$$E_{n,x}(Y) = E_n(g(X_1, Z_1, \dots, X_n, Z_n, x, Z_x))$$

where Z_x denotes the result of a new evaluation at x

Finding X_N^{Bayes} (last evaluation point)

- ▶ Given $x_N \in \mathbb{X}$, consider the following strategy at time $N - 1$:
 - 1) first, **evaluate at $X_N = x_N$** ,
 - 2) then, act optimally, i.e., **use $D_{N+1}^{\text{Bayes}} = \varphi_N^{\text{Bayes}}(F_N)$**

Finding X_N^{Bayes} (last evaluation point)

- ▶ Given $x_N \in \mathbb{X}$, consider the following strategy at time $N - 1$:
 - 1) first, evaluate at $X_N = x_N$,
 - 2) then, act optimally, i.e., use $D_{N+1}^{\text{Bayes}} = \varphi_N^{\text{Bayes}}(F_N)$
- ▶ The corresponding **posterior risk at time $N - 1$** is

$$R_{N-1}(x_N) = \mathbb{E}_{N-1, x_N} \left(L(D_{N+1}^{\text{Bayes}}) \right) = \mathbb{E}_{N-1, x_N} \left(R_N^{\text{Bayes}} \right)$$

Finding X_N^{Bayes} (last evaluation point)

- ▶ Given $x_N \in \mathbb{X}$, consider the following strategy at time $N - 1$:
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- ▶ Claim: the **optimal decision rule** for the last evaluation is

$$X_N^{\text{Bayes}} = \varphi_{N-1}(F_{N-1}) = \operatorname{argmin}_{x_N \in \mathbb{X}} R_{N-1}(x_N)$$

Finding X_N^{Bayes} (last evaluation point)

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$$X_N^{\text{Bayes}} = \varphi_{N-1}(F_{N-1}) = \operatorname{argmin}_{x_N \in \mathbb{X}} R_{N-1}(x_N)$$

- ▶ Remark: R_{N-1} is used as a “**sampling criterion**”
(a.k.a. “infill criterion”, a.k.a. “merit function”...)

Finding X_N^{Bayes} : proof

- ▶ For **any strategy** $\underline{D} = (X_1, \dots, X_{N-1}, X_N, D_{N+1})$,

$$\begin{aligned} E_{N-1}(L(D_{N+1})) &= E_{N-1}(R_N(F_N, D_{N+1})) \\ &\geq E_{N-1}(R_N^{\text{Bayes}}(F_N)) = R_{N-1}(F_{N-1}, X_{N-1}) \end{aligned}$$

Finding X_N^{Bayes} : proof

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- ▶ Let $\underline{D}' = (X_1, \dots, X_{N-1}, X'_N, D'_{N+1})$,
where $X'_N = \varphi_{N-1}^{\text{Bayes}}(F_{N-1})$ and $D'_{N+1} = \varphi_N^{\text{Bayes}}(F_{N-1}, X'_N, Z'_N)$

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- ▶ Then $E_{N-1}(L(D'_{N+1})) = R_{N-1}^{\text{Bayes}}(F_{N-1}) \leq R_{N-1}(F_{N-1}, X_{N-1})$

Finding X_N^{Bayes} : proof

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- ▶ Then $E_{N-1}(L(D'_{N+1})) = R_{N-1}^{\text{Bayes}}(F_{N-1}) \leq R_{N-1}(F_{N-1}, X_{N-1})$
- ▶ Thus $E_0(L(D_{N+1})) \geq E_0(L(D'_{N+1}))$ ■

Finding X_N^{Bayes} : example (cont'd)

- ▶ Recall our **linear loss** example

$$\hat{X}^{\text{Bayes}} = \operatorname{argmin} \hat{\xi}_N$$

$$R_N^{\text{Bayes}} = \min \hat{\xi}_N - E_N(\min \xi)$$

Finding X_N^{Bayes} : example (cont'd)

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$$\hat{X}^{\text{Bayes}} = \operatorname{argmin} \hat{\xi}_N$$

$$R_N^{\text{Bayes}} = \min \hat{\xi}_N - E_N(\min \xi)$$

- ▶ Compute the **posterior risk** at time $N - 1$

$$\begin{aligned} R_{N-1}(F_{N-1}, x_N) &= E_{N-1, x_N} \left(R_N^{\text{Bayes}}(F_N) \right) \\ &= E_{N-1, x_N} \left(\min \hat{\xi}_N \right) - E_{N-1}(\min \xi) \end{aligned}$$

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- ▶ The **optimal decision** at time $N - 1$ is

$$X_N = \operatorname{argmin}_{x_N} E_{N-1, x_N} \left(\min \hat{\xi}_N \right)$$

(first appears (in english) in Mockus, Tiesis & Žilinskas, 1978)

Finding X_N^{Bayes} : example (cont'd)

- ▶ Equivalently,

$$X_N = \operatorname{argmax}_{x_N} \underbrace{\min \hat{\xi}_{N-1} - E_{N-1, x_N}(\min \hat{\xi}_N)}_{\rho_{N-1}^{\text{KG}}(x_N) \geq 0}$$

Finding X_N^{Bayes} : example (cont'd)

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- ▶ Nowadays called the **Knowledge Gradient (KG)** criterion
(Frazier, Powell & co-authors, 2008, 2009, 2011)

Finding X_N^{Bayes} : example (cont'd)

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- ▶ Remarks
 - ▶ applicable to “noisy” observations as well
 - ▶ a.k.a. simulation-based optimization

Finding X_N^{Bayes} : example (cont'd)

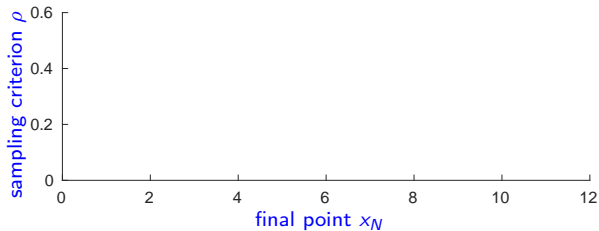
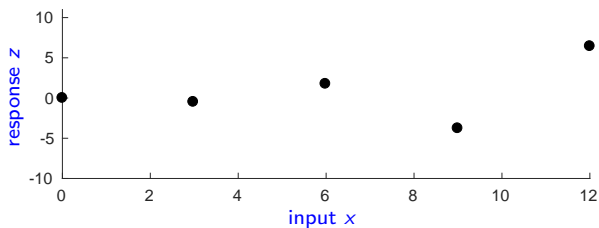
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(Frazier, Powell & co-authors, 2008, 2009, 2011)
- ▶ Remarks
 - ▶ applicable to “noisy” observations as well
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 - ▶ even with a GP prior, ρ^{KG} is **not exactly computable** in general
 - ▶ idea: approx. max over a finite grid (more about that later)

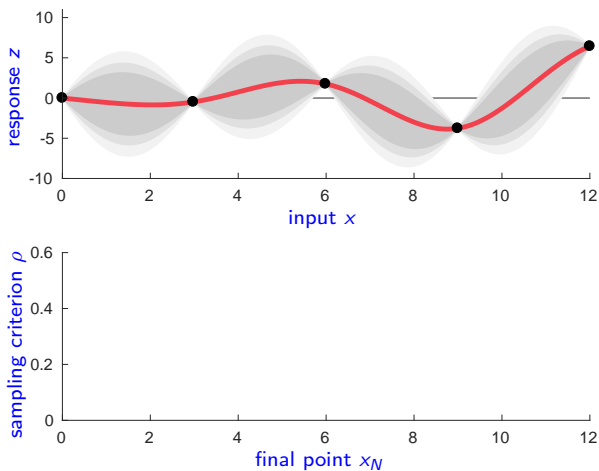
Finding X_N^{Bayes} : example (cont'd)

Same example as before, $n = 5$, but assume now that $N = 6$.



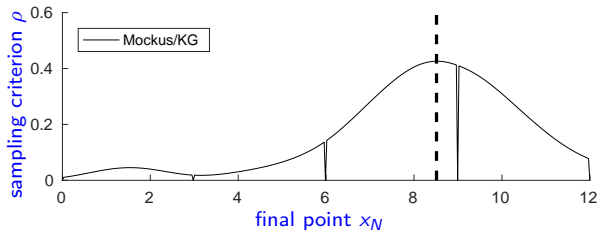
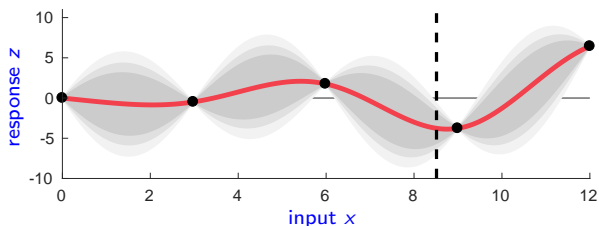
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Finding X_N^{Bayes} : example (cont'd)

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Warning: $X_N \neq \operatorname{argmax} \hat{\xi}_{N-1}$ (uncertainty is taken into account)

Finding X_N^{Bayes} : example, variant (cont'd)

- ▶ Recall the following variant

$$\hat{X}^{\text{Bayes},1} = \operatorname{argmin}_{x \in \{X_1, \dots, X_N\}} \xi(x)$$

$$R_N^{\text{Bayes},1} = \min_{i \leq N} \xi(X_i) - E_N(\min \xi)$$

Finding X_N^{Bayes} : example, variant (cont'd)

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- ▶ Set $M_n = \min_{i \leq n} \xi(X_i)$. The optimal decision at time $N - 1$ is

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- ▶ This is the **Expected Improvement (EI)** criterion
(Mockus et al 1978; Jones, Schonlau & Welch, 1998)

Finding X_N^{Bayes} : example, variant (cont'd)

- ▶ Recall the following variant

$$\hat{X}^{\text{Bayes},1} = \operatorname{argmin}_{x \in \{X_1, \dots, X_N\}} \xi(x)$$

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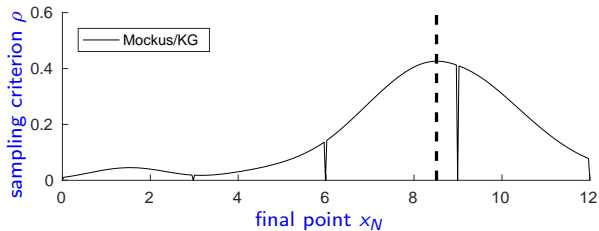
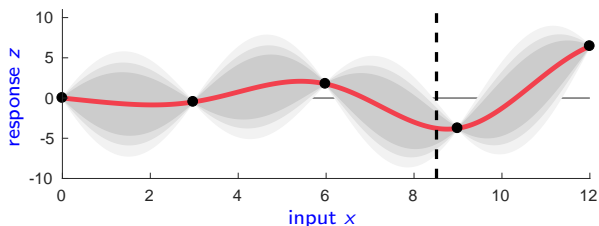
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- ▶ This is the Expected Improvement (EI) criterion
(Mockus et al 1978; Jones, Schonlau & Welch, 1998)
- ▶ **Computable analytically** for GP priors \Rightarrow most commonly used
(for *deterministic* numerical models)

Finding X_N^{Bayes} : example (cont'd)

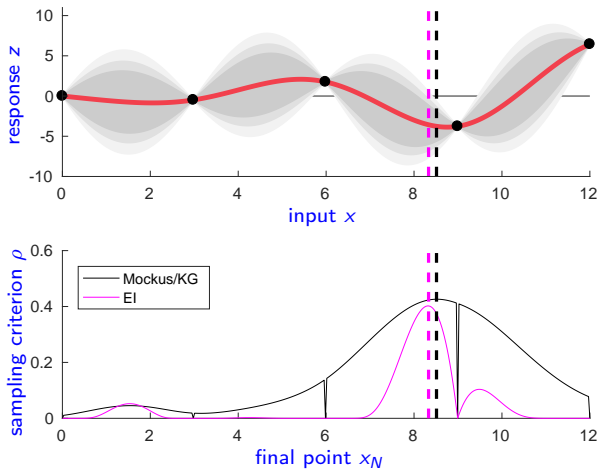
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Finding X_N^{Bayes} : example (cont'd)

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Lecture 2 : Bayesian optimization (BO)

2.2. From Bayes-optimal to myopic strategies

The optimal terminal decision

Optimal choice of the last evaluation

Bayes-optimal versus “practical Bayes” optimization

Sampling criteria for multi-objective and/or constrained optimization

The Bayes-optimal strategy

- ▶ Recall the **optimal terminal decision rule**

$$\varphi_N^{\text{Bayes}}(F_N) = \operatorname{argmin}_d E_N(L(d))$$

$$R_N^{\text{Bayes}}(F_N) = \min_d E_N(L(d))$$

The Bayes-optimal strategy

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- ▶ Recall the **optimal rule for the last evaluation**

$$\varphi_{N-1}^{\text{Bayes}}(F_{N-1}) = \operatorname{argmin}_{x_N} E_{N-1, x_N} \left(R_N^{\text{Bayes}}(F_N) \right)$$

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The Bayes-optimal strategy

- ▶ The entire **Bayes-optimal strategy** can be written similarly: $\forall n$,

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- ▶ This is called backward induction (or dynamic programming)
- ▶ So what ? Can we use this ?

The Bayes-optimal strategy

- ▶ More explicitly, the optimal decision for the first evaluation is

$$X_1 = \operatorname{argmin}_{x_1} E_{0,x_1} \left(\min_{x_2} E_{1,x_2} \left(\dots \right. \right. \\ \left. \left. \min_{x_N} E_{N-1,x_N} \left(\min_d E_N (L(d)) \right) \right) \right)$$

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- ▶ **Very difficult to use in practice** beyond $N = 1$ or 2
 - ▶ each “min” is an optim. problem that needs to be solved...
 - ▶ each “ $E_{n,x}$ ” is an integral that needs to be computed...
 - ▶ none of them are tractable, even for the nicest (GP) priors ☹

Practical Bayesian optimization: myopic strategies

- ▶ Practical BO algorithms use, in general, **myopic strategies**
 - ▶ a.k.a. one-step look-ahead strategies
 - ▶ principle: **make each decision as if it were the last one**
 - ▶ Bayes-optimal if $N = 1$, sub-optimal otherwise

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Generic myopic BO algorithm

- ▶ For n from 0 to $N - 1$
 - ▶ Compute $X_{n+1} = \operatorname{argmin}_x E_{n, x_{n+1}}(\bar{L}_{n+1})$
 - ▶ Make an evaluation at X_{n+1}
- ▶ Output $D_{N+1} = \operatorname{argmin} E_N(L(d))$

Practical Bayesian optimization: hyper-parameters

- ▶ GP models have **hyper-parameters** θ (variance, range, etc.)
 - ▶ **fully Bayes** approach (see Benassi 2013, chap. III, and refs)
 1. set up prior distributions on the hyper-parameters
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 - ▶ **plug-in** approach
 - ▶ use $P_n^\theta \approx \delta_{\hat{\theta}_n}$, with $\hat{\theta}_n$ an estimator of θ (MML, LOO-CV...)
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Generic myopic BO algorithm with hyper-parameter estimation

- ▶ Init: (space-filling) DoE of size n_0 (rule of thumb: $n_0 = 10d$)
- ▶ For n from n_0 to $N - 1$
 - ▶ once in a while, Estimate hyper-parameters (plug-in/fully Bayes)
 - ▶ Compute $X_{n+1} = \operatorname{argmin}_x E_{n, x_{n+1}}(\bar{L}_{n+1})$
 - ▶ Make an evaluation at X_{n+1}
- ▶ Output $D_{N+1} = \operatorname{argmin} E_N(L(d))$

Practical Bayesian optimization: EGO

STK demo

... single-objective box-constrained optimization
with the EI criterion and a plug-in approach
(a.k.a. the “EGO” algorithm) ...

Practical Bayesian optimization: optimization

- ▶ Each iteration involves an **auxiliary optimization problem**

Practical Bayesian optimization: optimization

- ▶ Each iteration involves an auxiliary optimization problem
- ▶ Various approaches to solve it
 - ▶ **Fix grid** or **IID random search**
 - ▶ OK for low-dimensional, simple problems
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 - ▶ **External solvers**
 - ▶ ex: DiceOptim → Rgenoud (genetic + gradient)
 - ▶ ex: Janusvekis & Le Riche (2013) → CMA-ES

Practical Bayesian optimization: optimization

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 - ▶ ex: DiceOptim → Rgenoud (genetic + gradient)
 - ▶ ex: Janusvekis & Le Riche (2013) → CMA-ES
 - ▶ **Sequential Monte Carlo** (Benassi, 2013; Feliot et al, 2017)
 - ▶ sample according to a well-chosen sequence of densities

Practical Bayesian optimization: optimization

- ▶ Each iteration involves an auxiliary optimization problem
- ▶ Various approaches to solve it
 - ▶ **Fix grid** or **IID random search**
 - ▶ OK for low-dimensional, simple problems
 - ▶ if accurate convergence is not needed
 - ▶ **External solvers**
 - ▶ ex: DiceOptim \rightarrow Rgenoud (genetic + gradient)
 - ▶ ex: Janusvekis & Le Riche (2013) \rightarrow CMA-ES
 - ▶ **Sequential Monte Carlo** (Benassi, 2013; Feliot et al, 2017)
 - ▶ sample according to a well-chosen sequence of densities
- ▶ Bayesian optimization \Rightarrow run-time **overhead**
 - ▶ depends on the model, sampling criterion, optimizer, etc.
 - ▶ BO is appropriate for **expensive-to-evaluate** numerical models

Lecture 2 : Bayesian optimization (BO)

2.2. From Bayes-optimal to myopic strategies

The optimal terminal decision

Optimal choice of the last evaluation

Bayes-optimal versus “practical Bayes” optimization

Sampling criteria for multi-objective and/or constrained optimization

Multi-objective problems

- ▶ **Several objective functions** to be minimized: $f = (f_1, \dots, f_p)$
 - ▶ $f_j : \mathbb{X} \rightarrow \mathbb{R}, 1 \leq j \leq p$

Multi-objective problems

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Pareto domination relation

$$z \prec z' \quad \text{if (def)} \quad \begin{cases} z_j \leq z'_j & \text{for all } j \leq p, \\ z_j < z'_j & \text{for at least one } j \leq p. \end{cases}$$

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- ▶ The goal is to find (estimate)
 - ▶ the **Pareto set** $\mathbb{P} = \{x \in \mathbb{X} : \nexists x' \in \mathbb{X}, f(x') \prec f(x)\}$
(a.k.a. set of Pareto-efficient solutions)

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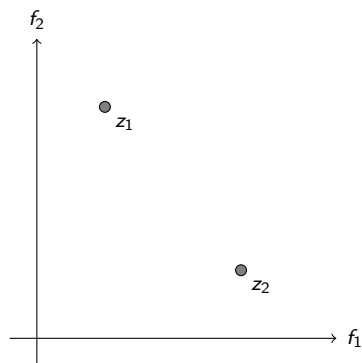
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(a.k.a. set of Pareto-efficient solutions)
 - ▶ and/or the **Pareto front** $\{z \in \mathbb{R}^p : \exists x \in \mathbb{P}, z = f(x)\}$
(a.k.a. Pareto frontier, Pareto boundary...)

Multi-objective problems

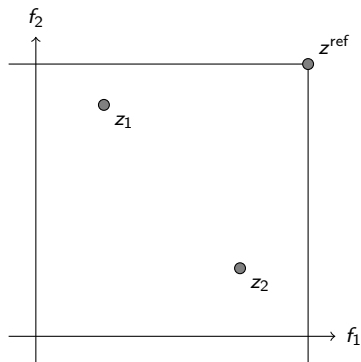
- ▶ EHVI: a natural extension of EI (Emmerich et al, 2006)



Noiseless evaluations

Multi-objective problems

- ▶ EHVI: a natural extension of EI (Emmerich et al, 2006)

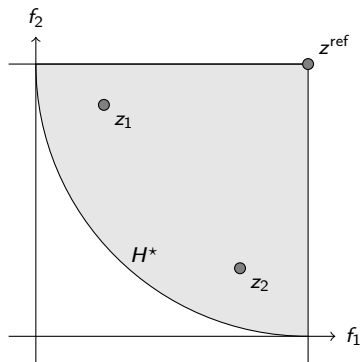


Noiseless evaluations

$$\mathbb{B} = \prod_{j=1}^p]-\infty; z_j^{\text{ref}}]: \text{ bounding box}$$

Multi-objective problems

- ▶ EHVI: a natural extension of EI (Emmerich et al, 2006)



Noiseless evaluations

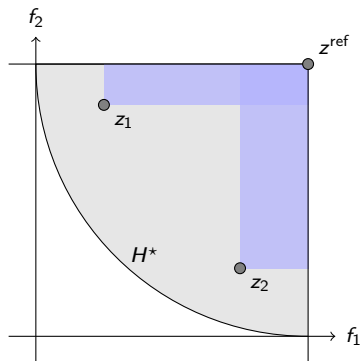
$\mathbb{B} = \prod_{j=1}^p]-\infty; z_j^{\text{ref}}]$: bounding box

True **dominated region**:

$$H^*(f) = \{z \in \mathbb{B}, \exists x \in \mathbb{X}, f(x) \preceq z\}$$

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Loss function:

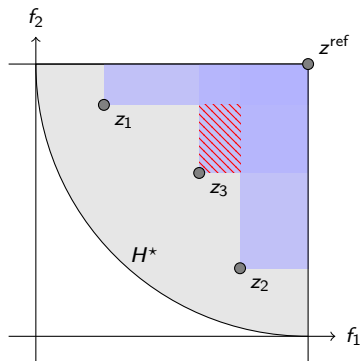
$$L(f, \hat{H}) = |H^*(f) \Delta \hat{H}|$$

Best "safe" estimator:

$$H_n = \{z \in \mathbb{B}, \exists i \leq n, f(X_i) \preceq z\}$$

Multi-objective problems

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$$\rho_n^{\text{EHVI}}(x_{n+1}) = E_{n, x_{n+1}} (|H_{n+1} \setminus H_n|)$$

Multi-objective problems

- ▶ Implementation

- ▶ Exactly computable for independent GP priors, $2 \leq p \lesssim 5$
- ▶ **Implemented** in STK (Matlab/Octave), GPareto (R)...
- ▶ Dependent priors, larger p : Monte Carlo approx.

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STK demo

... bi-objective optimization with the EHVI criterion ...

*code by Etienne Leloup, Guillaume Maistre-Bazin, Lucain Pouget
CentraleSupelec final year project for CEA DIF*

Inequality-constrained problems

- ▶ **Single-objective, inequality-constrained** problem:
 - ▶ $f = (f_o, f_{c,1}, \dots, f_{c,q})$, with
 - ▶ $f_o : \mathbb{X} \rightarrow \mathbb{R}$, to be minimized,
 - ▶ $f_{c,j} : \mathbb{X} \rightarrow \mathbb{R}$, $1 \leq j \leq q$, must be ≤ 0 .

Inequality-constrained problems

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 - ▶ $f_{c,j} : \mathbb{X} \rightarrow \mathbb{R}$, $1 \leq j \leq q$, must be ≤ 0 .
- ▶ Consider the following **loss function**

$$L(f, \hat{x}) = \begin{cases} f_o(\hat{x}) - f_o^* & \text{if } f_c(\hat{x}) \leq 0, \\ +\infty & \text{otherwise.} \end{cases}$$

where $f_o^* = \min_{x: f_c(x) \leq 0} f_o(x)$

Inequality-constrained problems

- ▶ Assuming
 - ▶ noiseless evaluations,
 - ▶ independent priors on objective and constraint functions,
 - ▶ $\exists i \leq n, \xi_c(X_i) = f_c(X_i) \leq 0$,

the following myopic criterion follows (Schonlau et al, 1998)

$$\rho_n^{\text{EIC}}(x_{n+1}) = \rho_{o,n}^{\text{EI}}(x_{n+1}) \cdot \underbrace{\prod_{j=1}^q P_n(\xi_{c,j}(x_{n+1}) \leq 0)}_{\text{Proba of Feasibility (PF)}}.$$

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- ▶ **Easy for independent GP priors** (most commonly used)
- ▶ Dependent priors: harder... (but see Williams et al, 2010)

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- ▶ Implementation
 - ▶ Easy for independent GP priors (most commonly used)
 - ▶ Dependent priors: harder... (but see Williams et al, 2010)
- ▶ Again, **many other approaches** have been proposed
 - ▶ See Feliot et al (2017, section 2.3) and references therein

Et maintenant une page de pub !

- ▶ BMOO algorithm (Feliot et al 2017)
 - ▶ **Unified EI/EHVI/EIC criterion**
 - ▶ well-defined even when no feasible point is known
 - ▶ **Efficient SMC technique** for criterion optimization
 - ▶ SMC = Sequential Monte Carlo
 - ▶ extends the work of Benassi (2013)

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Announcement

Paul Feliot's PhD defense will take place

on **Wednesday, July 12, 2017**, 2 PM,

at CentraleSupélec (Gif). Venez nombreux !

Miscellaneous references for further reading

- ▶ **Information-based** BO: a different approach
 - ▶ Risk = **entropy** of the minimizer
 - ▶ See Villemonteix et al (2009), Hennig & Schueller (2012), Hernandez-Lobáto and co-authors (2014, 2015...)

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 - ▶ **Constrained**: Augmented Lagrangian methods (Gramacy et al, 2016; Picheny et al, 2016)

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 - ▶ Ginsbourger et al (2010), Chevalier & Ginsbourger (2013), Chevalier et al (2014), Marmin et al (2015)
- ▶ **Noisy evaluations** / stochastic simulators
 - ▶ will be discussed in the next part 😊

Lecture 2 : Bayesian optimization (BO)

2.1. Decision-theoretic framework

2.2. From Bayes-optimal to myopic strategies

2.3. Design under uncertainty

Lecture 2 : Bayesian optimization (BO)

2.3. Design under uncertainty

Overview of possible approaches

Optimization of a mean response

RBDO (and other formulations)

Design under uncertainty

- ▶ Standard **design optimization** problem:
 - ▶ Minimize one **objective** (“cost”) **function** $f_o(x)$
 - ▶ or several objective functions $f_{o,1}(x), \dots, f_{o,p}(x)$
 - ▶ under the **constraints** $f_{c,j}(x) \leq 0, 1 \leq j \leq q$
- ▶ Some objective/constraint functions are **expensive to evaluate**

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“Design under uncertainty” framework

- ▶ objective functions: $f_{o,j}(x, u), 1 \leq j \leq p$
- ▶ constraint functions: $f_{c,j}(x, u), 1 \leq j \leq q$
- ▶ where u denotes **factors that the designer cannot control**

(a few words on the) Worst-case approach

- ▶ Principle of the **worst-case** (minimax) approach
 - ▶ Define an **uncertainty set** \mathbb{U}
 - ▶ Optimize by considering the **worst** $u \in \mathbb{U}$

(a few words on the) Worst-case approach

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 - ▶ Define an uncertainty set \mathbb{U}
 - ▶ Optimize by considering the worst $u \in \mathbb{U}$
- ▶ For instance, assuming a single-objective problem:

$$\text{minimize } \max_{u \in \mathbb{U}} f_o(x, u)$$

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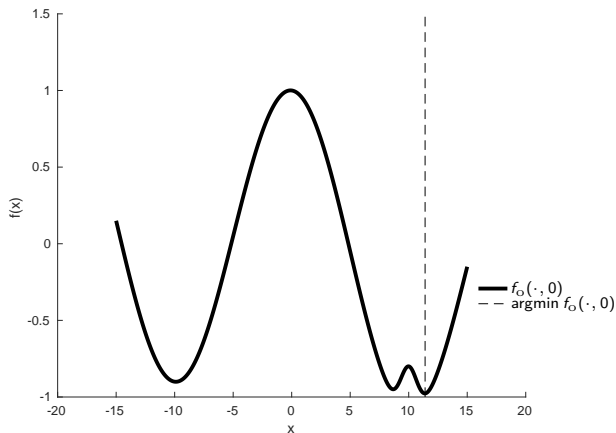
$$\text{minimize } \max_{u \in \mathbb{U}} f_o(x, u)$$

- ▶ If the problem has constraints, they become:

$$\forall j \leq q, \forall u \in \mathbb{U}, f_{c,j}(x, u) \leq 0$$

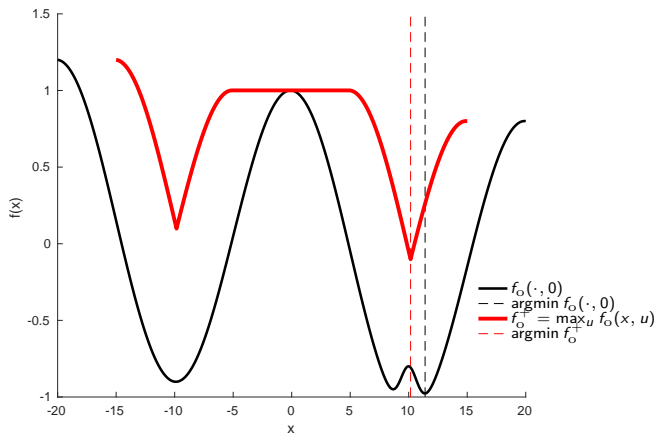
Example 1: Illustration of the worst-case approach

Example: $f_o(x, u) = \tilde{f}(x + u)$, with $u \in \mathbb{U} = [-\delta; \delta]$, $\delta = 5$



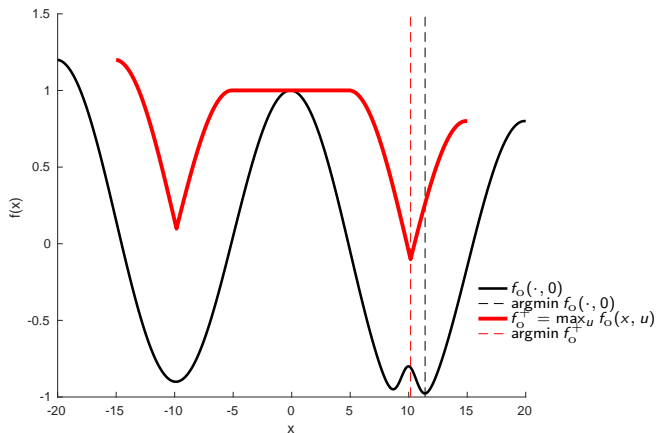
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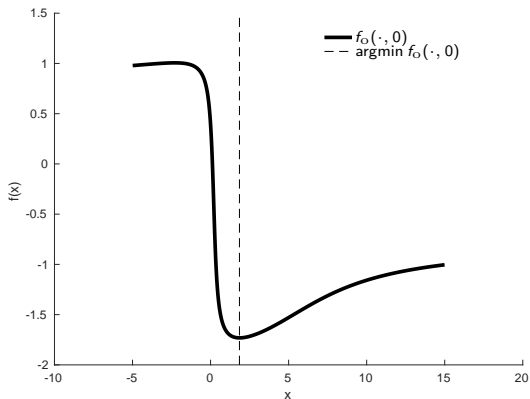
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Remark: very conservative, the **nominal performance** is ignored

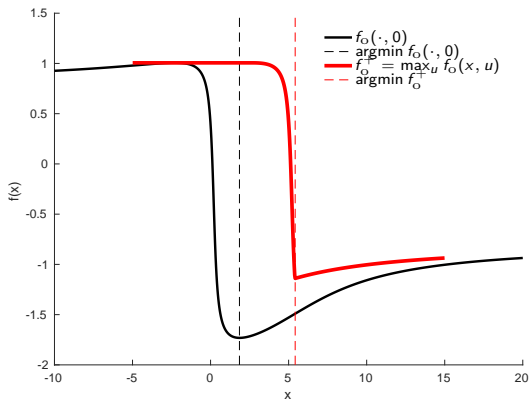
Example 2: Illustration of the worst-case approach

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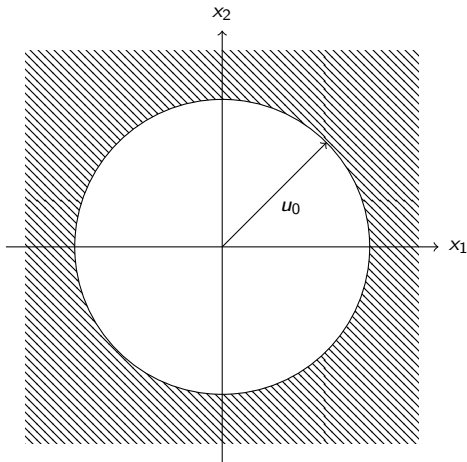
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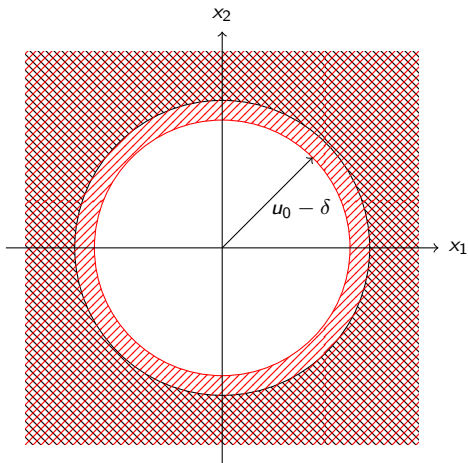
Another example: worst-case approach for a constraint

Example: $f_c(x, u) = \|x\|^2 - u^2$



Another example: worst-case approach for a constraint

Example: $f_c(x, u) = \|x\|^2 - u^2$, with $u \in \mathcal{U} = [u_0 - \delta; u_0 + \delta]$



(a few more words on the) Worst-case approach

- ▶ In **this lecture**, we will **focus on the probabilistic** approach

(a few more words on the) Worst-case approach

- ▶ In this lecture, we will focus on the probabilistic approach
- ▶ See Marzat, Walter & Piet-Lahanier (2013, 2016) for a “BO treatment” of the worst-case approach (using relaxation)

(a few more words on the) Worst-case approach

- ▶ In this lecture, we will focus on the probabilistic approach
- ▶ See Marzat, Walter & Piet-Lahanier (2013, 2016) for a “BO treatment” of the worst-case approach (using relaxation)
- ▶ An issue of terminology: in the math literature,
 - ▶ “robust optimization” refers mainly to the worst-case setting (see Ben Tal et al (2009), Bertsimas et al (2011) and refs)
 - ▶ the probabilistic approach is called stochastic programming
- ▶ while engineers use the word “robust” for both 😊

The probabilistic approach

- ▶ From now, we focus on the **probabilistic approach**
 - ▶ u is considered as **random** $\rightarrow U \sim P^U$
 - ▶ can be a random vector ($\in \mathbb{R}^m$), or a more complicated object

Problem formulations

- ▶ Various “robust” formulations can be considered for the design problem, depending mainly on
 - ▶ the number of objective functions,
 - ▶ the presence of (expensive-to-evaluate) constraints,
 - ▶ and, of course, how we want to deal with U_{real} .

Problem formulations

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 - ▶ the number of objective functions,
 - ▶ the presence of (expensive-to-evaluate) constraints,
 - ▶ and, of course, how we want to deal with U_{real} .
- ▶ In the following, we focus on
 - ▶ **single objective** problems
 - ▶ in the “**environmental variables**” setting
- ▶ and discuss two important cases:
 - ▶ optimization of the **averaged objective** function
 - ▶ **reliability-based design optimization** (RBDO), a.k.a. “chance constrained” optimization, and other formulations

Lecture 2 : Bayesian optimization (BO)

2.3. Design under uncertainty

Overview of possible approaches

Optimization of a mean response

RBDO (and other formulations)

Optimization of a mean response

- ▶ Assume

- ▶ **single objective** $f = f_o$, expensive to evaluate
- ▶ **no** (expensive-to-evaluate) **constraints**
- ▶ remark: cheap constraints allowed in the definition of $\mathbb{X} \subset \mathbb{R}^d$
- ▶ **“environmental variables”** setting

Optimization of a mean response

- ▶ Assume
 - ▶ single objective $f = f_o$, expensive to evaluate
 - ▶ no (expensive-to-evaluate) constraints
 - ▶ remark: cheap constraints allowed in the definition of $\mathbb{X} \subset \mathbb{R}^d$
 - ▶ “environmental variables” setting

- ▶ Consider once again the L^1 loss function

$$\begin{aligned} L((f, u_{\text{real}}), \hat{x}) &= \left| f(\hat{x}, u_{\text{real}}) - \min_x f(x, u_{\text{real}}) \right| \\ &= f(\hat{x}, u_{\text{real}}) - \min_x f(x, u_{\text{real}}) \end{aligned}$$

Optimization of a mean response

- ▶ Compute the **posterior risk** at time N for an estimate $\hat{x} \in \mathbb{X}$

$$E_N(L((\xi, U_{\text{real}}), \hat{x})) = E_N(\xi(\hat{x}, U_{\text{real}})) - E_N(\min \xi(\cdot, U_{\text{real}}))$$

Optimization of a mean response

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where $\bar{\xi}(x) = \int \xi(x, u) P^U(du)$

Optimization of a mean response

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where $\bar{\xi}(x) = \int \xi(x, u) P^U(du)$

- ▶ Same L^1 risk (ignoring last term) as if we were dealing with the

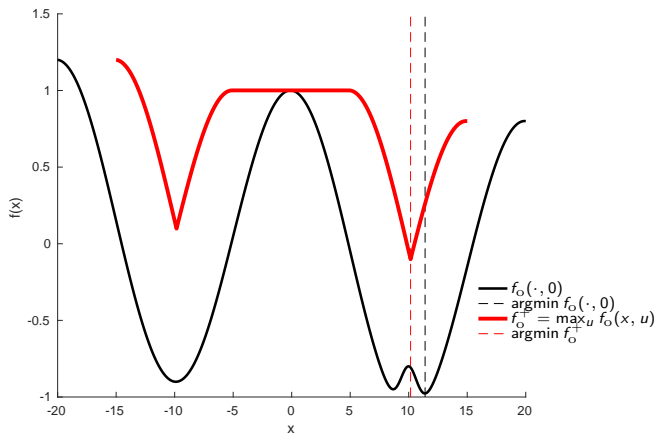
Equivalent “deterministic” problem

$$\min_x \bar{f}(x), \quad \text{with } \bar{f}(x) = \int f(x, u) P^U(du)$$

(Remark: this formulation occurs very naturally in a BO framework 😊)

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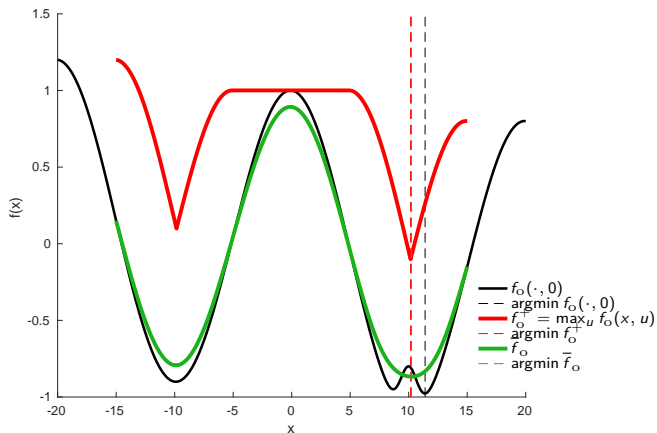
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Example 1: Worst-case versus probabilistic approach

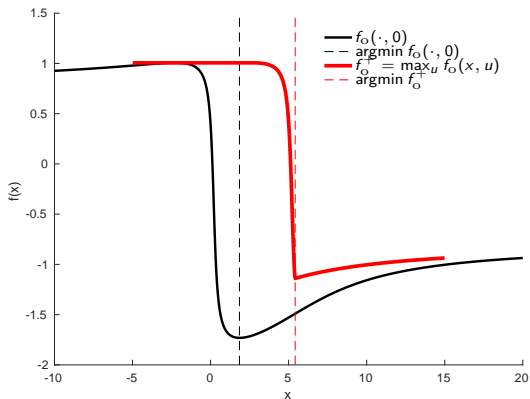
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$\bar{f}_o = E(f_o(\cdot, U))$, with $U \sim \mathcal{N}(0, s^2)$, s.t. $P(|U| \leq \delta) = 99.9\%$

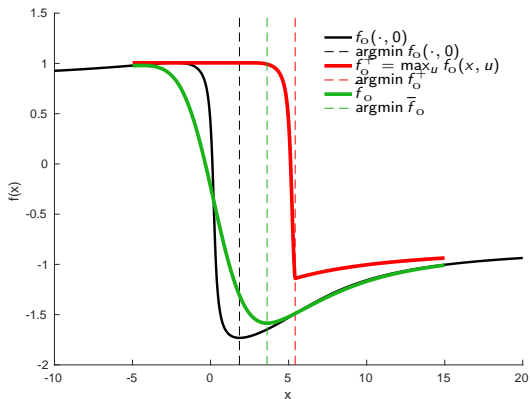
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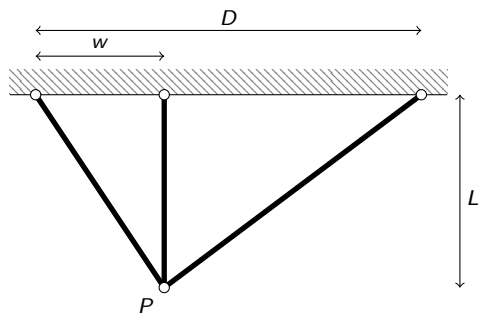
Example 2: Worst-case versus probabilistic approach

Example: $f_o(x, u) = \tilde{f}(x + u)$, with $u \in \mathbb{U} = [-\delta; \delta]$, $\delta = 5$



$\bar{f}_o = E(f_o(\cdot, U))$, with $U \sim \mathcal{N}(0, s^2)$, s.t. $P(|U| \leq \delta) = 99.9\%$

Example 3: Three-bar truss (Koski, 1985; Das, 1997)



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 - ▶ minimize $E_U(\|y\|)$
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 - ▶ under the constraints: $x_{\min} \leq x \leq x_{\max}$, $V \leq V_{\max}$
- ▶ Remark about constraints
 - ▶ The constraint $V \leq V_{\max}$ is **cheap to evaluate**

$$V = a_1 \sqrt{L^2 + w^2} + a_2 L + a_3 \sqrt{L^2 + (D - w)^2}$$

- ▶ Additional constraints: $|\sigma_j| \leq \sigma_{\max}$ can be checked a posteriori

Breaking the “double loop”

- ▶ Natural “double loop” approach
 - ▶ outer loop: ordinary **optimization** algorithm applied to \bar{f}
 - ▶ inner loop: **integration** (MC, quadrature. . .) to compute \bar{f}

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- ▶ Natural “double loop” approach
 - ▶ outer loop: ordinary optimization algorithm applied to \bar{f}
 - ▶ inner loop: integration (MC, quadrature...) to compute \bar{f}
- ▶ Drawback: typically require large number of evaluations
- ▶ Bayesian optimization **breaks the double loop** 😊
 - ▶ Construct a Bayesian model for f , not \bar{f}
 - ▶ Remark: can be achieved using other surrogate-model based approaches (see Janusevskis & LeRiche, 2013, and refs therein)

Prior model

- ▶ There are **two functions of interest** in this setting
 - ▶ the one that can be observed, i.e., $f : (x, u) \mapsto f(x, u)$,
 - ▶ and the one that want to optimize: $\bar{f} = \int f(\cdot, u) P^U(du)$
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Gaussian process priors are, again, very convenient

If $\underbrace{\xi \sim \mathcal{GP}(m, k)}_{\text{defined on } \mathbb{X} \times \mathbb{U}}$, then $\underbrace{\bar{\xi} \sim \mathcal{GP}(m_{\bar{\xi}}, k_{\bar{\xi}})}_{\text{defined on } \mathbb{X}}$,

with

$$m_{\bar{\xi}}(x) = \int m(x, u) P^U(du)$$
$$k_{\bar{\xi}}(x, y) = \iint k((x, u), (y, v)) P^U(du) P^U(dv)$$

Proof

- ▶ $\bar{\xi}$ is Gaussian by linearity of the integral
- ▶ Computation of the mean function: exchange \int and E

$$\begin{aligned}m_{\bar{\xi}}(x) &= E\left(\bar{\xi}(x)\right) = E\left(\int \xi(x, u) P^U(du)\right) \\ &= \int m(x, u) P^U(du)\end{aligned}$$

- ▶ Computation of the covariance function: idem with bilinearity

$$\begin{aligned}k_{\bar{\xi}}(x, y) &= \text{cov}\left(\bar{\xi}(x), \bar{\xi}(y)\right) \\ &= \text{cov}\left(\int \xi(x, u) P^U(du), \int \xi(x, v) P^U(dv)\right) \\ &= \iint k((x, u), (y, v)) P^U(du) P^U(dv)\end{aligned}\quad \blacksquare$$

Prior model (cont'd)

- ▶ Actually, we can say much better:

Jointly Gaussian processes

If $\xi \sim \mathcal{GP}(m, k)$, then ξ and $\bar{\xi}$ are jointly Gaussian, and

$$k_{\xi, \bar{\xi}}((x, u), y) = \text{cov}(\xi(x, u), \bar{\xi}(y)) = \int k((x, u), (y, v)) P^U(dv)$$

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- ▶ Remark: $m_{\bar{\xi}}$, $k_{\bar{\xi}}$ and $k_{\xi, \bar{\xi}}$ can be **computed exactly**
 - ▶ if P^U is **discrete** ($P^U = \sum_{j=1}^{n_U} w_j \delta_{u_j}$)
 - ▶ if P^U is (a mixture of) **Gaussian**(s), for some particular k
 - ▶ see Girard (2004) for exact formulas & approximations

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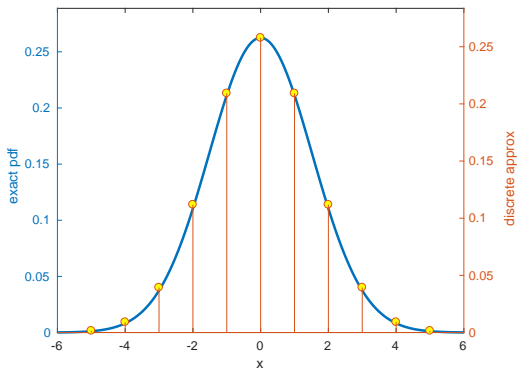
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 - ▶ if P^U is (a mixture of) Gaussian(s), for some particular k
 - ▶ see Girard (2004) for exact formulas & approximations
- ▶ Important **special case**: $\xi(x, u) = \tilde{\xi}(x + u)$
 - ▶ If ξ is a GP iff $\tilde{\xi}$ is a GP
 - ▶ $m_{\xi}(x, u) = m_{\tilde{\xi}}(x + u)$ and $k_{\xi}((x, u), (u, v)) = k_{\tilde{\xi}}(x + u, y + v)$

Examples 1 and 2: discretization of P^U

- ▶ In the two examples, $Prob^U = \mathcal{N}(0, s^2)$, with $s = 1.52$
 - ▶ $P(|U| \leq 5) \approx 99.9\%$

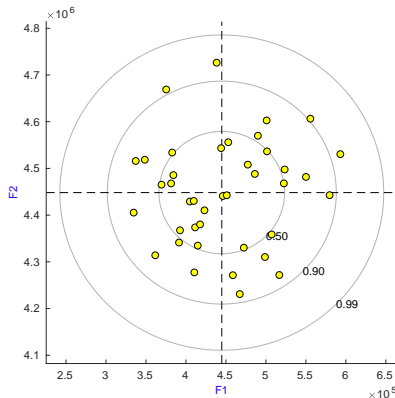
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- ▶ In the two examples, $Prob^U = \mathcal{N}(0, s^2)$, with $s = 1.52$
 - ▶ $P(|U| \leq 5) \approx 99.9\%$
- ▶ We choose to use a **regular discretization with $n_U = 11$ points**
 - ▶ points regularly spaced on $[-5; 5]$
 - ▶ weights computed using the normal cdf (using mid-points)



Example 3: discretization of P^U

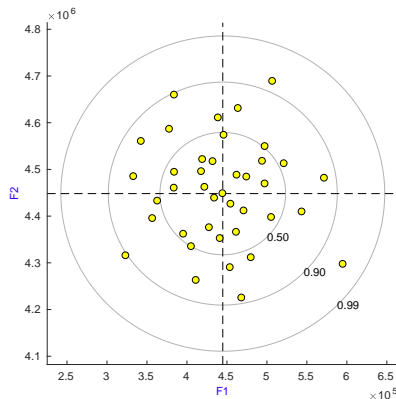
► Here, $U = \begin{pmatrix} F_1 \\ F_2 \end{pmatrix}$ and $P^U = \mathcal{N} \left(\begin{pmatrix} \mu_{F_1} \\ \mu_{F_2} \end{pmatrix}, \begin{pmatrix} \sigma_{F_1}^2 & 0 \\ 0 & \sigma_{F_2}^2 \end{pmatrix} \right)$



Monte Carlo sample of size $n_U = 50$

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Quasi Monte Carlo (QMC) sample of size $n_U = 50$

Sampling strategy: what ?

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 - ▶ i.e, what do we need to provide to run the numerical model ?

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 - ▶ numerical model $f : (x, u) \mapsto f(x, u)$, defined on $\mathbb{X} \times \mathbb{U}$
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 - ▶ at each step, we must select a pair $(X_{n+1}, U_{n+1}) \in \mathbb{X} \times \mathbb{U}$
- ▶ Important special case
 - ▶ $f(x, u) = \tilde{f}(x + u)$
 - ▶ in this case, we must simply **select a point** $X_{n+1} \in \mathbb{X}$
- ▶ In the following slides we assume the general case
(adaptation to the special case poses no difficulty)

Sampling strategy: how ?

- ▶ How do we build a sampling strategy for this problem ?
 - ▶ in this lecture, we will **apply the standard BO machinery**
 - ▶ L^1 loss \rightarrow risk \rightarrow “EI like” myopic strategy

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 - ▶ **other strategies** are proposed in the literature
 - ▶ Williams et al 2000; Janusevkis et Le Riche 2013
 - ▶ Entropy-based methods could be used as well (Villemonais et al 2009, Hennig & Schueller 2012...)

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 - ▶ Williams et al 2000; Janusevkiš et Le Riche 2013
 - ▶ Entropy-based methods could be used as well (Villemonteix et al 2009, Hennig & Schueller 2012...)
- ▶ Assume now the L^1 loss
- ▶ Recall the **posterior risk** at time N for an estimate $\hat{x} \in \mathbb{X}$:

$$E_N(L((\xi, U_{\text{real}}), \hat{x})) = E_N(\bar{\xi}(\hat{x})) - E_N(\min_{\mathbb{X}} \xi(\cdot, U_{\text{real}}))$$

Sampling strategy: one step look-ahead

- ▶ Let \bar{L}_n denote the **expected loss** that we would get **if we stopped at time n** :

$$\begin{aligned}\bar{L}_n &= \min_{\mathbb{X}} E_n(\bar{\xi}(x)) - E_n(\min_{\mathbb{X}} \xi(\cdot, U_{\text{real}})) \\ &= \min_{\mathbb{X}} m_{\bar{\xi}, n} - E_n(\min_{\mathbb{X}} \xi(\cdot, U_{\text{real}}))\end{aligned}$$

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- ▶ The **one-step look-ahead** (myopic) strategy is

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- ▶ Formally, looks like the KG criterion of Frazier & co, but...

Sampling strategy: one step look-ahead

- ▶ Comparison with KG as presented in the literature

	evaluations	optimization
KG	$\xi(x) + \mathcal{N}\text{noise}$	$\min \xi$
here	$\xi(x, u)$	$\min \bar{\xi}$

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 1. the function to be optimized is not observable directly,
 2. the evaluation results and the function to be optimized are jointly Gaussian.
- ▶ Good news: we can then derive an implementable **Approximate KG** criterion as in Scott et al (2011)

Approximate KG criterion (AKG)

- ▶ Let $\mathbb{X}_n^{\text{ref}} \subset \mathbb{X}$ denote some finite “reference set”
- ▶ Let $\tilde{x}_{n+1} = (x_{n+1}, u_{n+1})$. The **AKG criterion** is:

$$\rho_n^{\text{AKG}}(\tilde{x}_{n+1}) = \min m_{\bar{\xi}, n} - E_{n, \tilde{x}_{n+1}} \left(\min m_{\bar{\xi}, n+1} \right) \geq 0$$

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 - ▶ with $\mathbb{X}_n^{\text{ref}} = \{X_1, \dots, X_n\}$
- ▶ Implementation ?
 - ▶ It is **exactly computable** (but not easy to compute...)
 - ▶ Available in STK (Matlab/Octave), DiceOptim (R)...

Optimization of a mean response: demos

STK demo

... One dimensional illustration: examples 1 and 2 ...

STK demo

... Minimization of the mean displacement
in the 3-bar truss example ...

(a few words about) The case of stochastic simulators

- ▶ Good news
 - ▶ the **same sampling criteria can be used** in both cases (environmental variables / stochastic simulators)...
 - ▶ ...provided that the observations and the objective function are **jointly Gaussian**.

(a few words about) The case of stochastic simulators

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- ▶ **Review/benchmark** of existing criteria: Picheny et al (2013)
 - ▶ AKG emerges has one of the most efficient criteria
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 - ▶ (Entropy-based criteria not benchmarked)
- ▶ What about simulators with truly **non-Gaussian output** ?
 - ▶ “batch trick” (CLT)
 - ▶ see also Browne et al (2016)...

Lecture 2 : Bayesian optimization (BO)

2.3. Design under uncertainty

Overview of possible approaches

Optimization of a mean response

RBDO (and other formulations)

Reliability-based (design) optimization (RBO, RBDO)

- ▶ Assume

- ▶ a **single objective** $f = f_o$, often cheap to evaluate
- ▶ one or several **expensive-to-evaluate constraints** $f_{c,1}, \dots, f_{c,q}$
- ▶ “**environmental variables**” setting

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 - ▶ “environmental variables” setting
- ▶ The so-called RB(D)O formulation reads:

Reliability-based (a.k.a. chance-constrained) optimization

Minimize

$$\bar{f}_o(x), \quad \text{where } f_o(x) = E_U(f_o(x, U))$$

under the constraints: $x \in \mathbb{X}$ and

$$\forall j \leq q, \quad P_U(f_{c,j}(x, U) > 0) \leq p_j^{\text{tol}}$$

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 - ▶ outer loop: ordinary optimization algorithm with constraints
 - ▶ inner loop: reliability analysis method to compute the constraints
- ▶ Again, surrogate-based methods should be able to “break the double loop” by building a model on $\mathbb{X} \times \mathbb{U}$

Why RBDO is harder than mean-response optimization

- ▶ because the **thresholds p_j^{tol}** are usually **small**
 - ▶ MC-type approx. $P^U \approx \frac{1}{m} \sum_j \delta_{u_j}$ becomes very expensive or infeasible
 - ▶ Dedicated techniques (e.g., FORM/SORM, IS, subset simulation) needed for an **efficient evaluation of the constraints**

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- ▶ BO: the distribution of $P_U(\xi_{c,j}(x, U) > 0)$ is intractable
 - ▶ **Posterior mean/variance** can be written as integrals (see, e.g., Villemonteix 2008 chap III), but...
 - ▶ ... the posterior distribution is **not Gaussian** even if ξ_c is !
 - ▶ Very difficult to derive Bayesian **sampling criteria** that can be implemented efficiently...

Bayesian RBDO algorithms ?

- ▶ A few GP-based algorithms have been proposed, notably:
 - ▶ Bichon et al (2009): **EGO+EGRA** algorithm
 - ▶ Dubourg and co-authors (2011a, 2011b): **RBDO-N2LA**

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- ▶ Complex, “weakly Bayesian” algorithms... e.g., RBDO-N2LA:

Algorithm 2 Adaptive surrogate-based nested RBDO strategy

```

1:  $\theta^{(0)}, \theta^L, \theta^U, j := 0$ 
2: for  $i = 1$  to  $n$  do
3:    $\theta_0^i := \min_{\theta \in \mathcal{D}_\theta} F_N^{-1}(v_i, \theta)$ 
4:    $\theta_0^i := \max_{\theta \in \mathcal{D}_\theta} F_N^{-1}(v_i, \theta)$ 
5: end for
6:  $\mu := x + 1 \cdot \mathbb{1}_{\mathcal{D}_x}, \mathcal{K} := \emptyset$ 
7:  $k := \Phi^{-1}(97.5\%), \epsilon_1 := 10^{-1}$ 
8: Refine := true, Optimize := true
9: while Refine and Optimize do
10:  while Refine do
11:     $G := \text{RefineKrigingModel}(n, k, \epsilon_1) \mapsto \text{Use Algorithm 1}$ 
12:  end while
13:   $\hat{F}^i := \{x : \mu_G(x) \leq 0\}$ 
14:   $\hat{\beta}^i, \nabla_{\mathbf{x}} \hat{\beta}^i := \text{ReliabilityAnalysis}(\hat{F}^i, \theta^{(i)})$ 
15:   $\epsilon^{(i)} := \epsilon(\theta^{(i)}), \nabla_{\mathbf{x}} \epsilon^{(i)} := \nabla_{\mathbf{x}} \epsilon(\theta^{(i)})$ 
16:   $f^{(i)} := f(\theta^{(i)}), \nabla_{\mathbf{x}} f^{(i)} := \nabla_{\mathbf{x}} f(\theta^{(i)})$ 
17:   $d^{(i)} := \text{SolveQuasiSQP}(\epsilon^{(i)}, f^{(i)}, \hat{\beta}^i, \nabla_{\mathbf{x}} \epsilon^{(i)}, \nabla_{\mathbf{x}} f^{(i)}, \nabla_{\mathbf{x}} \hat{\beta}^i)$ 
18:   $s^{(i)} := \text{GoldsteinAmpeStepSizeRule}(\epsilon, f, \hat{\beta}, d^{(i)})$ 
19:   $\theta^{(i+1)} := \theta^{(i)} + s^{(i)} d^{(i)}$ 
20:  for  $l = -1, 0, +1$  do
21:     $\hat{F}^{i+l} := \{x : \mu_G(x) + l k \sigma_G(x) \leq 0\}$ 
22:     $\hat{\beta}^{i+l} := \text{ReliabilityAnalysis}(\hat{F}^{i+l}, \theta^{(i+1)})$ 
23:  end for
24:  Refine :=  $\max(\hat{\beta}^{i+1} - \hat{\beta}^i, \hat{\beta}^i - \hat{\beta}^{i-1}) > \epsilon_1$ 
25:  Optimize :=  $|\theta^{(i+1)} - \theta^{(i)}| > \epsilon_0$  or  $|\epsilon^{(i+1)} - \epsilon^{(i)}| > \epsilon_2$ 
      or  $3 \mid f_i > 0$  or  $\hat{\beta} < \beta_0$ 
26: end while
    
```

Algorithm 1 Population-based adaptive refinement strategy

```

1:  $\mathcal{X} = \emptyset, \mathcal{Y} = \emptyset$ 
2:  $n := x \mapsto w(x)$ 
3:  $k := \Phi^{-1}(97.5\%), \epsilon_1 := 10^{-1}$ 
4: Refine := true
5:  $\mathcal{M} := \emptyset$ 
6: while Refine do
7:    $\mathcal{P} := \text{MCMCAlgorithm}(\mathcal{X})$ 
8:    $\mathcal{X}_{\text{new}} := \text{KMMeansAlgorithm}(\mathcal{P}, K)$ 
9:    $\mathcal{Y}_{\text{new}} := \mathcal{Y}(\mathcal{X}_{\text{new}})$ 
10:   $\mathcal{X} := \{\mathcal{X}, \mathcal{X}_{\text{new}}\}, \mathcal{Y} := \{\mathcal{Y}, \mathcal{Y}_{\text{new}}\}$ 
11:   $G := \text{MaximumLikelihoodKrigingModel}(\mathcal{X}, \mathcal{Y}, f, \nabla_{\mathbf{x}} f, R(\bullet, \ell), \ell_x, \ell_y)$ 
12:   $\mathbb{P}\{x \in \mathcal{M}\} := x \mapsto \Phi\left(\frac{k \sigma_G(x) - \mu_G(x)}{\sigma_G(x)}\right) - \Phi\left(\frac{-k \sigma_G(x) - \mu_G(x)}{\sigma_G(x)}\right)$ 
13:   $\mathcal{W} := x \mapsto \mathbb{P}\{x \in \mathcal{M}\} w(x)$ 
14:  for  $l = -1, 0, +1$  do
15:     $\hat{F}^{i+l} := \{x : \mu_G(x) + l k \sigma_G(x) \leq 0\}$ 
16:     $\hat{\beta}^{i+l} := \text{ReliabilityAnalysis}(\hat{F}^{i+l})$ 
17:  end for
18:  Refine :=  $\max(\hat{\beta}^{i+1} - \hat{\beta}^i, \hat{\beta}^i - \hat{\beta}^{i-1}) > \epsilon_1$ 
19: end while
    
```

Bayesian RBDO algorithms ?

- ▶ A few GP-based algorithms have been proposed, notably:
 - ▶ Bichon et al (2009): EGO+EGRA algorithm
 - ▶ Dubourg and co-authors (2011a, 2011b): RBDO-N2LA
- ▶ Complex, “weakly Bayesian” algorithms... e.g., RBDO-N2LA:

Algorithm 2 Adaptive surrogate-based nested RBDO strategy

```

1:  $\theta^{(0)}, \theta^L, \theta^U, j := 0$ 
2: for  $i = 1$  to  $n$  do
3:    $\theta_0^i := \min_{\theta \in \mathcal{D}_i(\theta^L, \theta^U)} F_N^{-1}(v_i, \theta)$ 
4:    $\theta_0^i := \max_{\theta \in \mathcal{D}_i(\theta^L, \theta^U)} F_N^{-1}(v_i, \theta)$ 
5: end for
6:  $n := n + 1$ ;  $\mathcal{D}_n := \mathcal{D}_n(v)$ 
7:  $k := \Phi^{-1}(97.5\%)$ ;  $\epsilon_1 := 10^{-1}$ 
8: Refine := true; Optimize := true
9: while Refine and Optimize do
10:  while Refine do
11:     $G := \text{RefineKrigingModel}(n, k, \epsilon_1) \rightarrow \text{Use Algorithm 1}$ 
12:  end while
13:   $\hat{F}^i := \{x : \mu_G(x) \leq 0\}$ 
14:   $\hat{\beta}^i, \nabla_{\mathbf{x}} \hat{\beta}^i := \text{ReliabilityAnalysis}(\hat{F}^i, \theta^{(j)})$ 
15:   $\epsilon^{(j)} := \epsilon(\theta^{(j)}); \nabla_{\mathbf{x}} \epsilon^{(j)} := \nabla_{\mathbf{x}} \epsilon(\theta^{(j)})$ 
16:   $f^{(j)} := f(\theta^{(j)}); \nabla_{\mathbf{x}} f^{(j)} := \nabla_{\mathbf{x}} f(\theta^{(j)})$ 
17:   $d^{(j)} := \text{SolveQuasiSQP}(\epsilon^{(j)}, f^{(j)}, \hat{\beta}^i, \nabla_{\mathbf{x}} \epsilon^{(j)}, \nabla_{\mathbf{x}} f^{(j)}, \nabla_{\mathbf{x}} \hat{\beta}^i)$ 
18:   $s^{(j)} := \text{GoldsteinAmplifyStepSizeRule}(k, f, \hat{\beta}^i, d^{(j)})$ 
19:   $\theta^{(j+1)} := \theta^{(j)} + s^{(j)}$ 
20:  for  $i = -1, 0, +1$  do
21:     $\hat{F}^{i+1} := \{x : \mu_G(x) + ik\sigma_G(x) \leq 0\}$ 
22:     $\hat{\beta}^{i+1} := \text{ReliabilityAnalysis}(\hat{F}^{i+1}, \theta^{(j+1)})$ 
23:  end for
24:  Refine :=  $\max(\hat{\beta}^{+1} - \hat{\beta}^i, \hat{\beta}^i - \hat{\beta}^{-1}) > \epsilon_1$ 
25:  Optimize :=  $|\theta^{(j+1)} - \theta^{(j)}| > \epsilon_0$  or  $|\epsilon^{(j+1)} - \epsilon^{(j)}| > \epsilon_2$ 
    or  $\exists i \mid f_i > 0$  or  $\hat{\beta} < \beta_0$ 
26: end while
    
```

Algorithm 1 Population-based adaptive refinement strategy

```

1:  $\mathcal{X} = \emptyset, \mathcal{Y} = \emptyset$ 
2:  $n := n + 1$ ;  $w(x)$ 
3:  $k := \Phi^{-1}(97.5\%)$ ;  $\epsilon_1 := 10^{-1}$ 
4: Refine := true
5:  $\mathcal{D}(x \in \mathcal{M}) := x + 1$ 
6: while Refine do
7:    $\mathcal{P} := \text{MCMCAlgorithm}(\mathcal{D})$ 
8:    $\mathcal{X}_{\text{new}} := \text{KMMeansAlgorithm}(\mathcal{P}, K)$ 
9:    $\mathcal{Y}_{\text{new}} := \mathcal{Y}(\mathcal{X}_{\text{new}})$ 
10:   $\mathcal{X} := \{\mathcal{X}, \mathcal{X}_{\text{new}}\}$ ;  $\mathcal{Y} := \{\mathcal{Y}, \mathcal{Y}_{\text{new}}\}$ 
11:   $G := \text{MaximumLikelihoodKrigingModel}$ 
    ( $\mathcal{X}, \mathcal{Y}, f(\bullet), R(\bullet, \ell), \ell_1, \ell_2$ )
12:   $\mathbb{P}\{x \in \mathcal{M}\} := x + \Phi\left(\frac{k\sigma_G(x)}{\sigma_G(x)}\right) - \Phi\left(\frac{-k\sigma_G(x) - \mu_G(x)}{\sigma_G(x)}\right)$ 
13:   $\mathcal{Y} := x + \mathbb{P}\{x \in \mathcal{M}\} w(x)$ 
14:  for  $j = -1, 0, +1$  do
15:     $\hat{F}^{j+1} := \{x : \mu_G(x) + ik\sigma_G(x) \leq 0\}$ 
16:     $\hat{\beta}^{j+1} := \text{ReliabilityAnalysis}(\hat{F}^{j+1})$ 
17:  end for
18:  Refine :=  $\max(\hat{\beta}^{+1} - \hat{\beta}^0, \hat{\beta}^0 - \hat{\beta}^{-1}) > \epsilon_1$ 
19: end while
    
```

- ▶ RBDO-N2LA is available in FERUM (Bourrinet et al, 2009)

RBDO and other formulations: alternative approach

- ▶ A general alternative approach in two steps
 1. Explore the design space **efficiently** using **multi-objective** BO,
 2. Evaluate probabilities of failure, quantiles, etc. **a posteriori** for non-dominated (and possibly other) solutions,

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 - ▶ i.e., the constraint $P_U(f_{c,j}(x, U) > 0) \leq p_j^{\text{tol}}$
 - ▶ becomes: **$\min_x f_{c,j}(x, u_0)$ u.c. $f_{c,j}(x, u_0) \leq 0$**

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- ▶ In step 1. constraints can be taken into account as objectives
 - ▶ i.e., the constraint $P_U(f_{c,j}(x, U) > 0) \leq p_j^{\text{tol}}$
 - ▶ becomes: $\min_x f_{c,j}(x, u_0)$ u.c. $f_{c,j}(x, u_0) \leq 0$
- ▶ In step 2. no new evaluations need to be carried out
 - ▶ the posterior distribution of ξ is used to **assess uncertainties**

RBDO and other formulations: alternative approach

STK demo

... Robust design through multi-objective optimization ...

Lecture 1 : From meta-models to UQ

- 1.1 Introduction
- 1.2 Black-box modeling
- 1.3 Bayesian approach
- 1.4 Posterior distribution of a quantity of interest
- 1.5 Complements on Gaussian processes

Lecture 2 : Bayesian optimization (BO)

- 2.1. Decision-theoretic framework
- 2.2. From Bayes-optimal to myopic strategies
- 2.3. Design under uncertainty

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