Bayesian Optimization

Julien Bect, Emmanuel Vazquez

Bayesian Optimization

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

Julien Bect and Emmanuel Vazquez

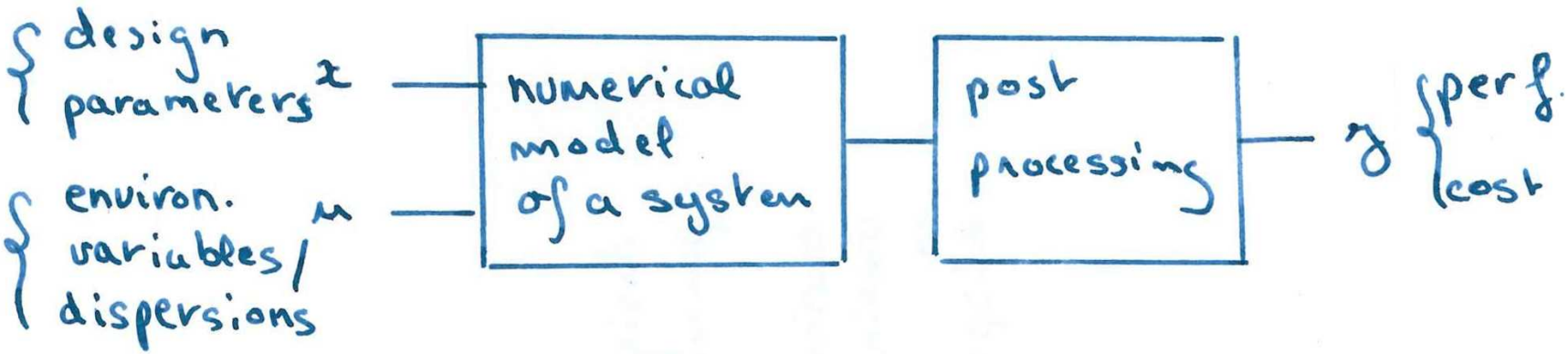
Laboratoire des signaux et systèmes, Gif-sur-Yvette, France

CEA-EDF-INRIA Numerical Analysis Summer School

Université Pierre et Marie Curie (Paris VI)

Paris, 2017, July 3–7

Computer-simulation based design

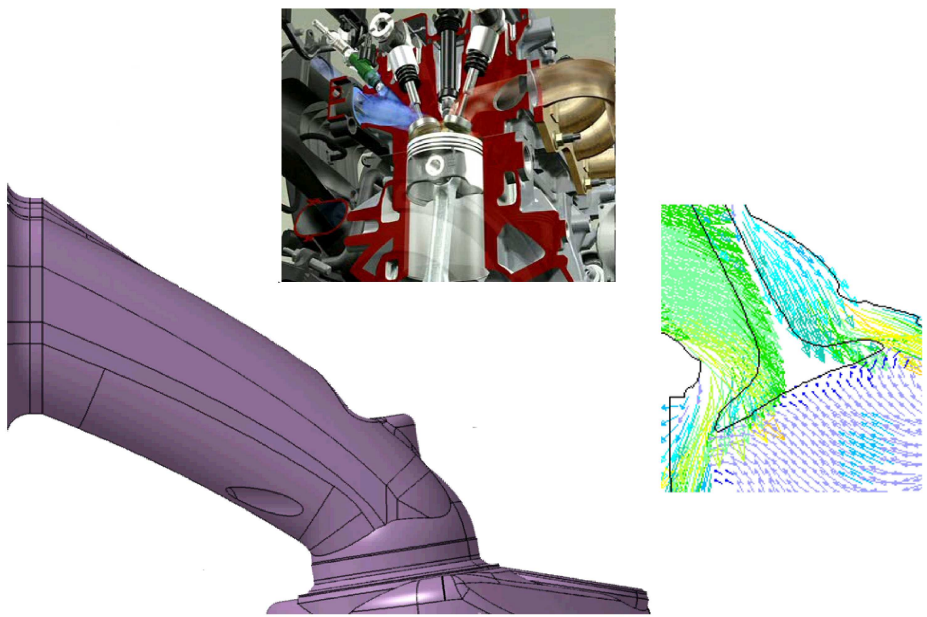


- The numerical model might be time- or resource-consuming
- Design parameters might be subject to dispersions
- The system might operate under unknown conditions

Computer-simulation based design – Example

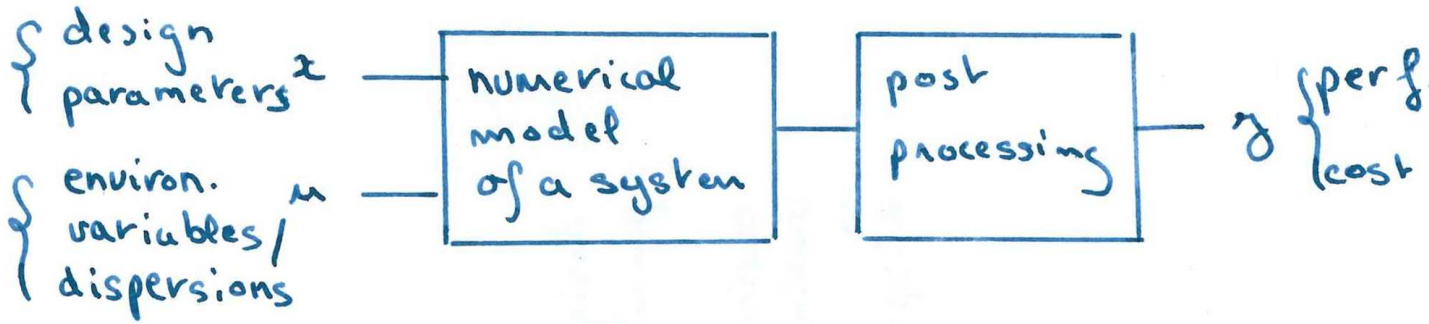
- Computer simulations to design a product or a process, in particular
  - to find the best feasible values for design parameters (optimization problem)
  - to minimize the probability of failure of a product

- 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
- $f : \mathbb{X} \subset \mathbb{R}^d \to \mathbb{R}$ performance as a function of design parameters ($d = 20 \sim 100$)
- Computing $f(x)$ takes $5 \sim 20$ hours
- Objective: estimate $x^\star = \mathrm{argmax}_x f(x)$

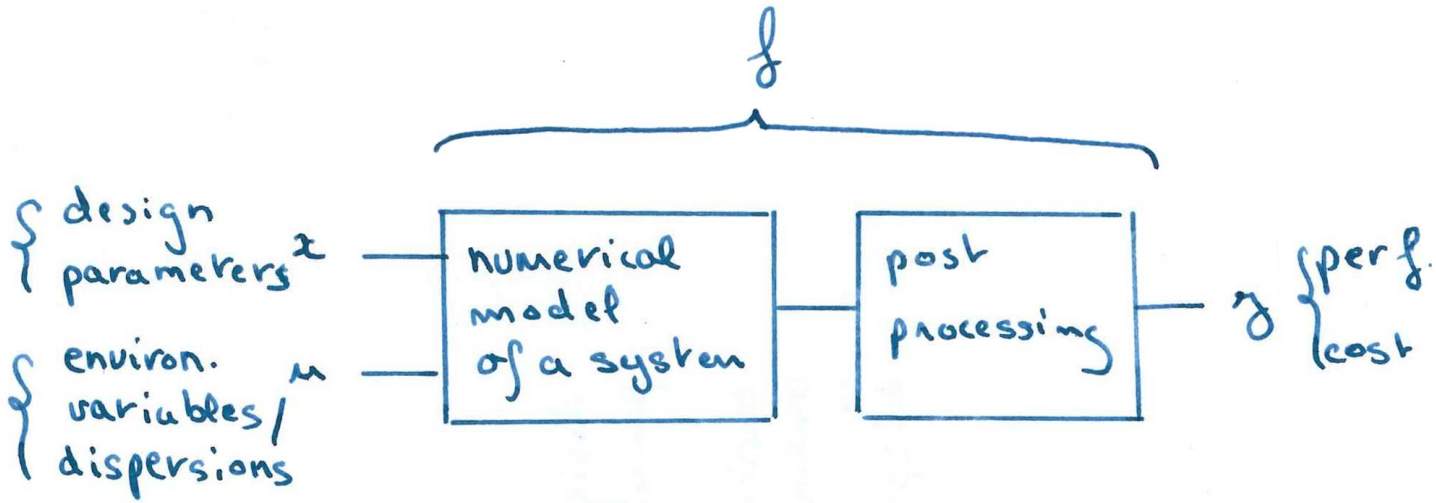


Simulation of an intake port (Navier-Stokes equ.)
(courtesy of Renault)

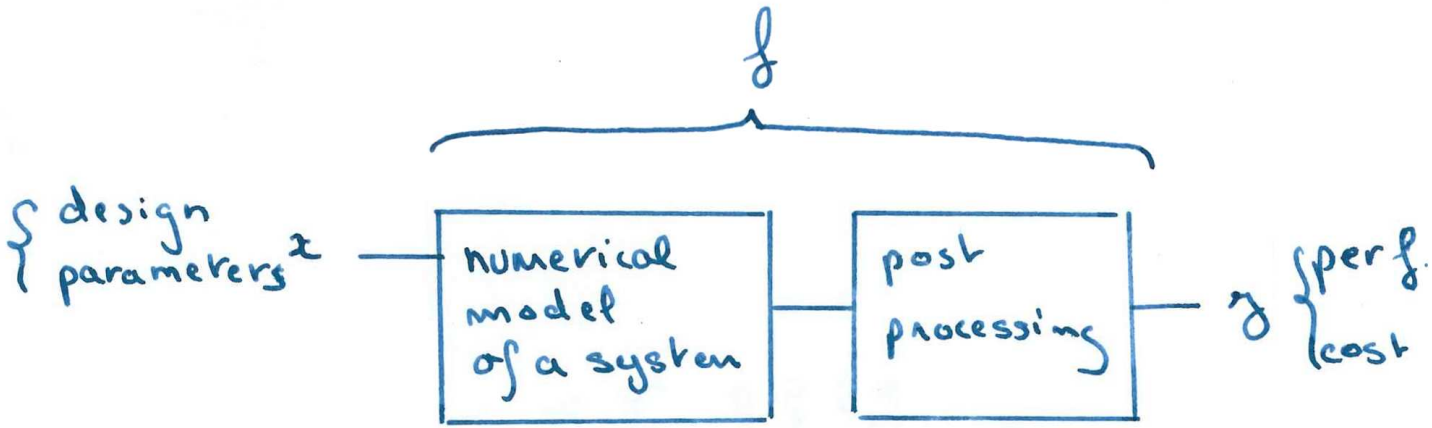
Black-box modeling



Black-box modeling



Black-box modeling



For simplification $\rightarrow$ drop u

Black-box modeling

- Let $f : \mathbb{X} \to \mathbb{R}$ 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 $x_1, \ldots, x_n \in \mathbb{X}$ be n simulations points
- Denote by

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

  the corresp. simulation results (observations/evaluations of f)
- Our objective: use the data $\mathcal{D}_n = (x_i, z_i)_{i=1\ldots n}$ to infer properties about f
- Example: given a new $x \in \mathbb{R}^d$, predict the value $f(x)$

Black-box modeling

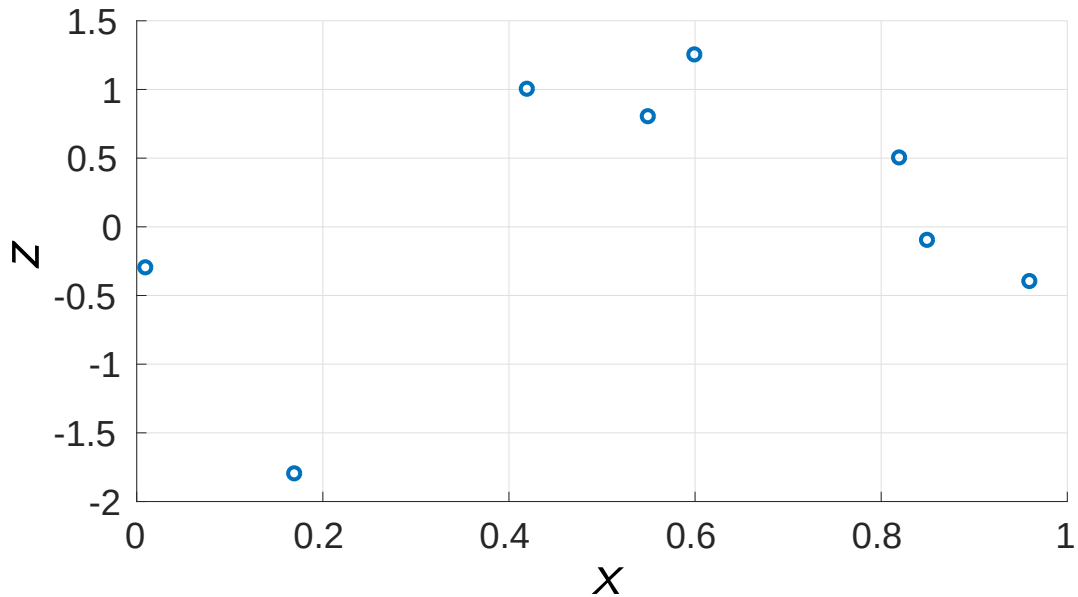
- f is a black-box, only known through evaluation results: query an evaluation at x, observe the result
- Predict the value of f at a given x?

$\rightarrow$ the problem is that of constructing an approximation / an estimator $\widehat{f}_n$ of f from $\mathcal{D}_n$

- Such a $\widehat{f}_n$ 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 $f : [0, 1] \to \mathbb{R}$, at points $x_1, \ldots, x_n$.
- A data set of size $n = 8$:



A simple curve fitting problem

- Any approximation procedure of f consists in building a function $\widehat{f}_n = h(\cdot;\theta)$ 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

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

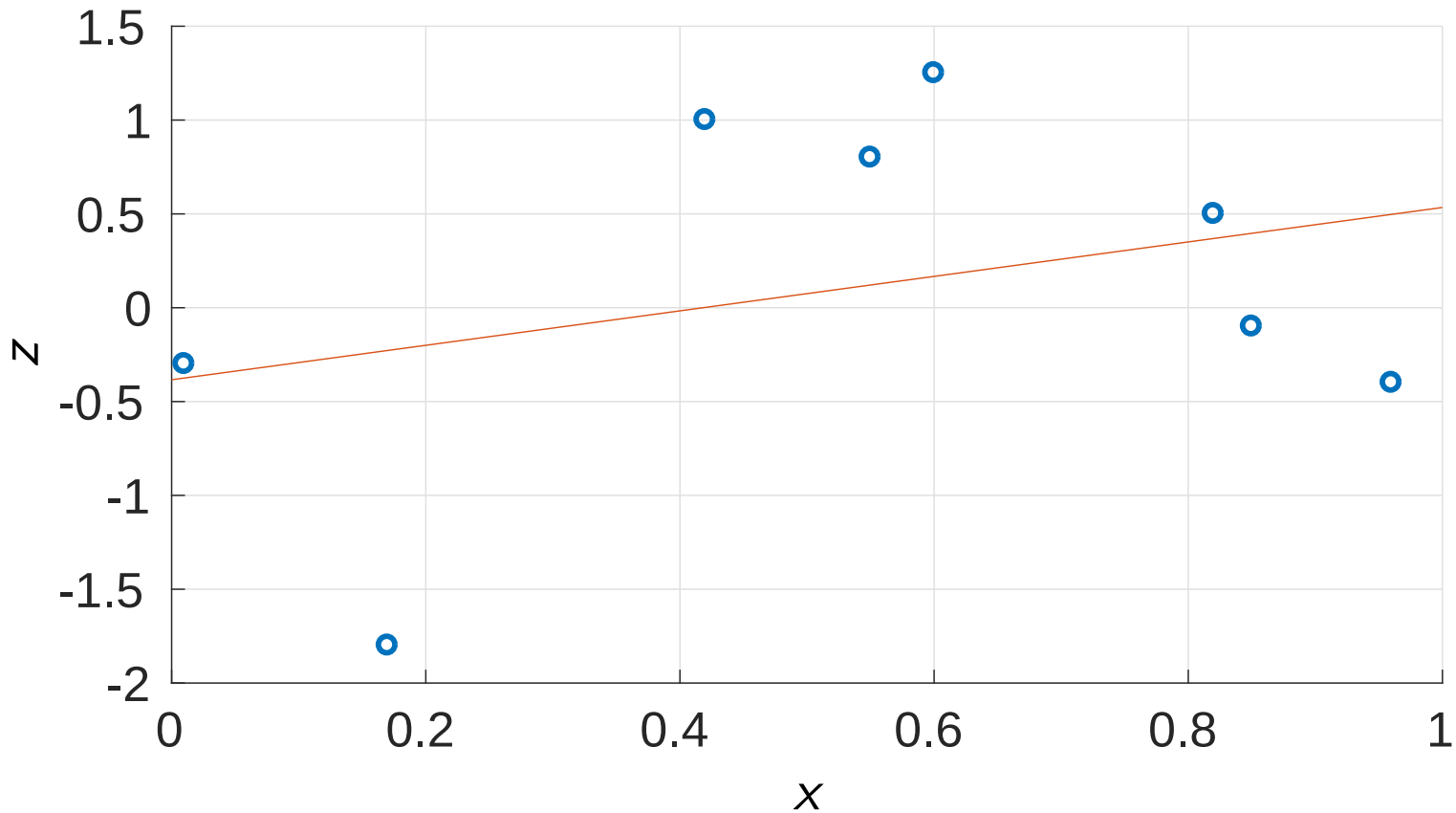
where functions $r_i : \mathbb{X} \to \mathbb{R}$ are called regressors (e.g., $r_1(x) = 1, r_2(x) = x, r_3(x) = x^2 \ldots \to$ polynomial model)

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

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

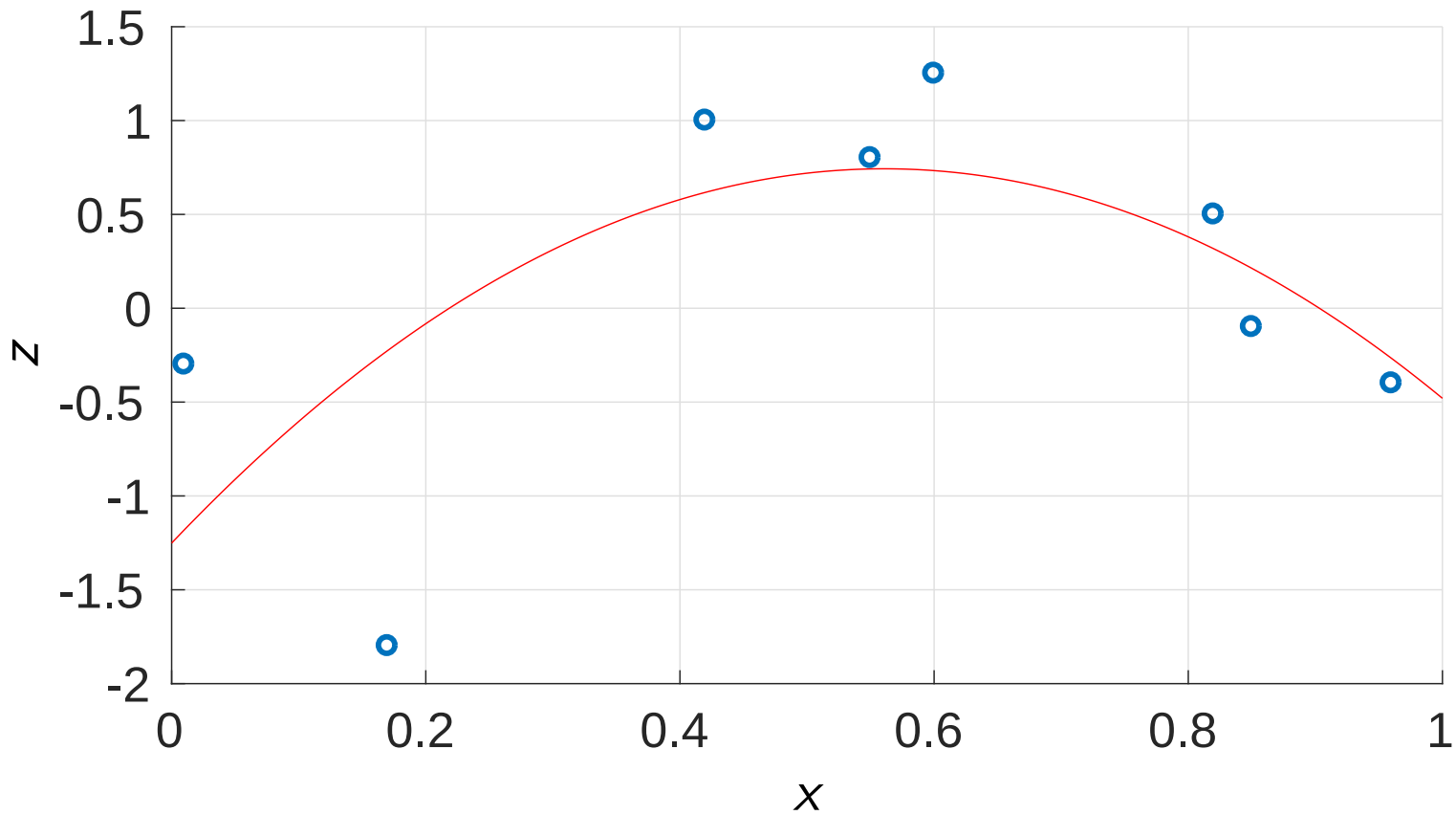
A simple curve fitting problem

- 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

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

with

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

(a truncated Fourier series)

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

A simple curve fitting problem

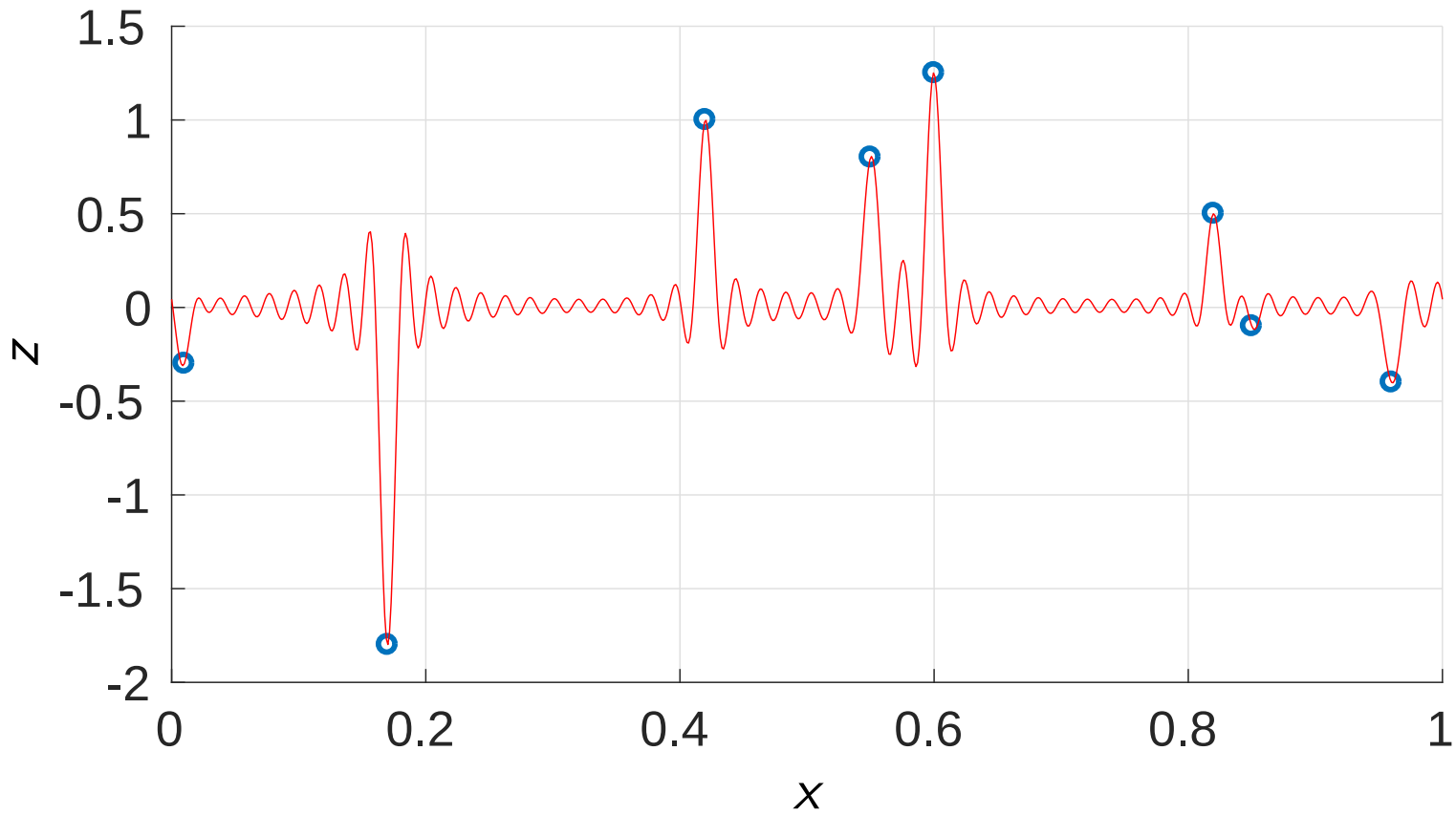
- When the problem becomes ill-defined (as capacity increases), a classical solution for finding a good value of b is to minimize the sum of an approximation error and a regularization term:

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

- $\|\theta\|_2^2$ 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) $\rightarrow$ 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

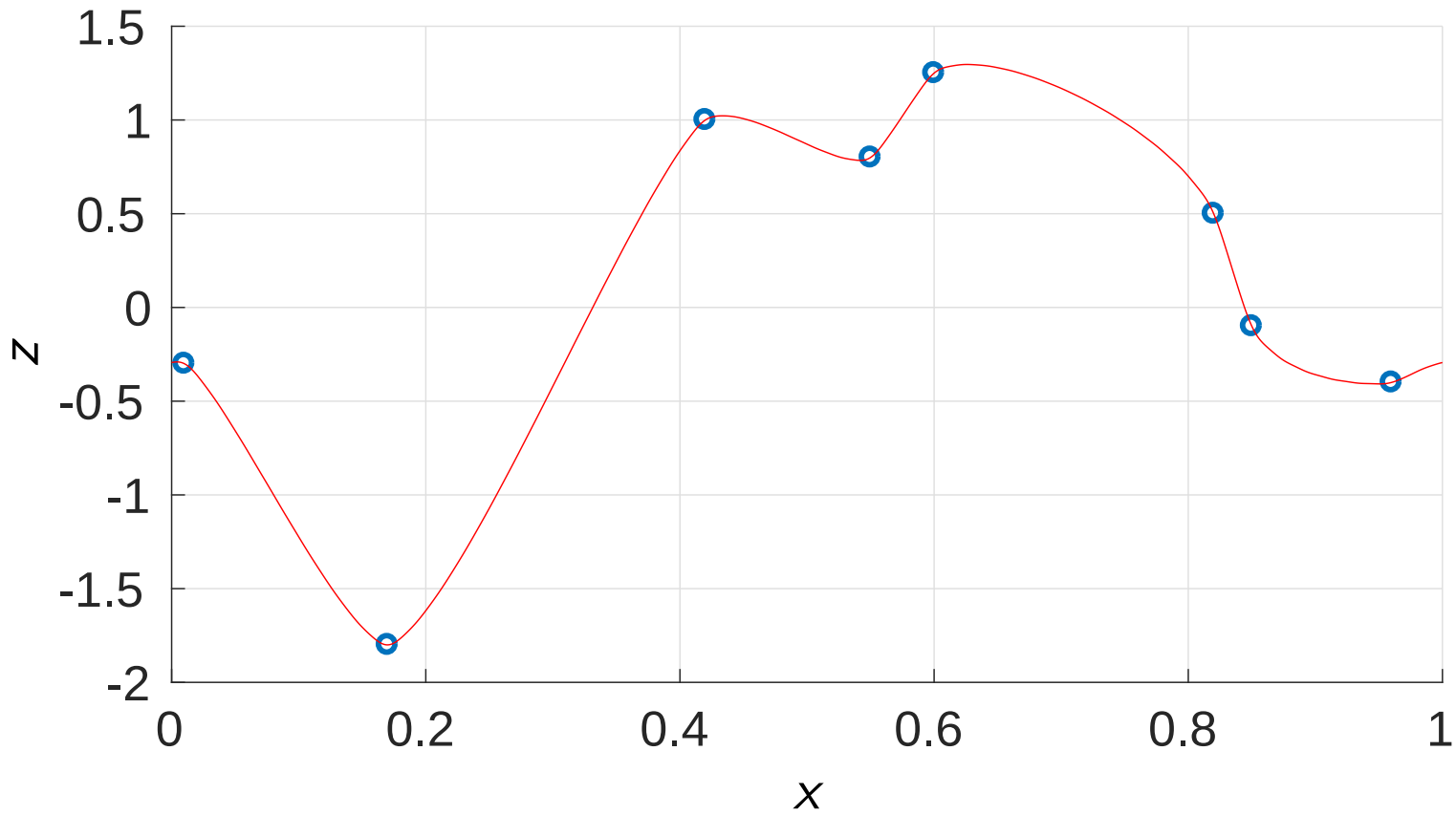
A simple curve fitting problem

- 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

Why a Bayesian approach?

- Objective: infer properties about $f : \mathbb{X} \to \mathbb{R}$ 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 $(\Omega, \mathcal{A}, \mathrm{P})$ be a probability space, and $(E, \mathcal{E})$ be a measurable outcome space
$\rightarrow$ a random variable X is a measurable function $(\Omega, \mathcal{A}, \mathrm{P}) \rightarrow (E, \mathcal{E})$

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

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

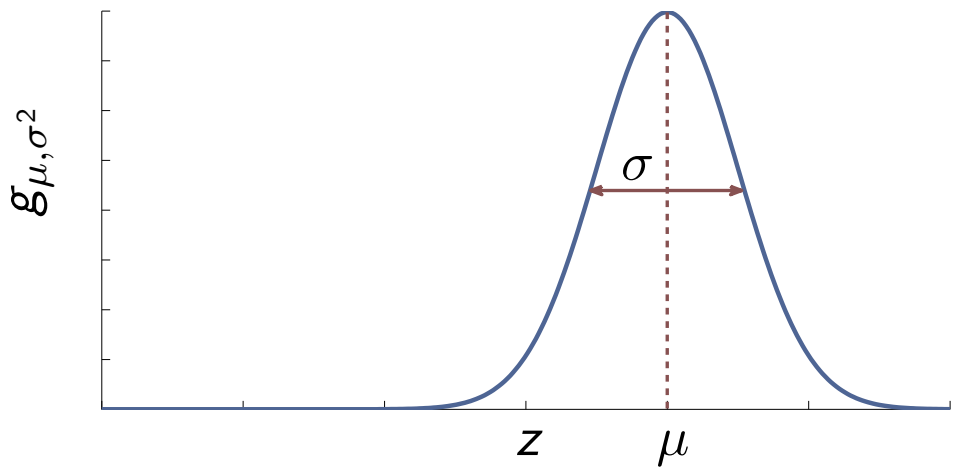
- Case of a random variable with a density

$$\mathrm{P}(X \in [a,b]) = \mathrm{P}^X([a,b]) = \int_a^b p^X(x)\mathrm{d}x$$

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

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

and its second-order moment is defined as

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

- The variance of Z is defined as

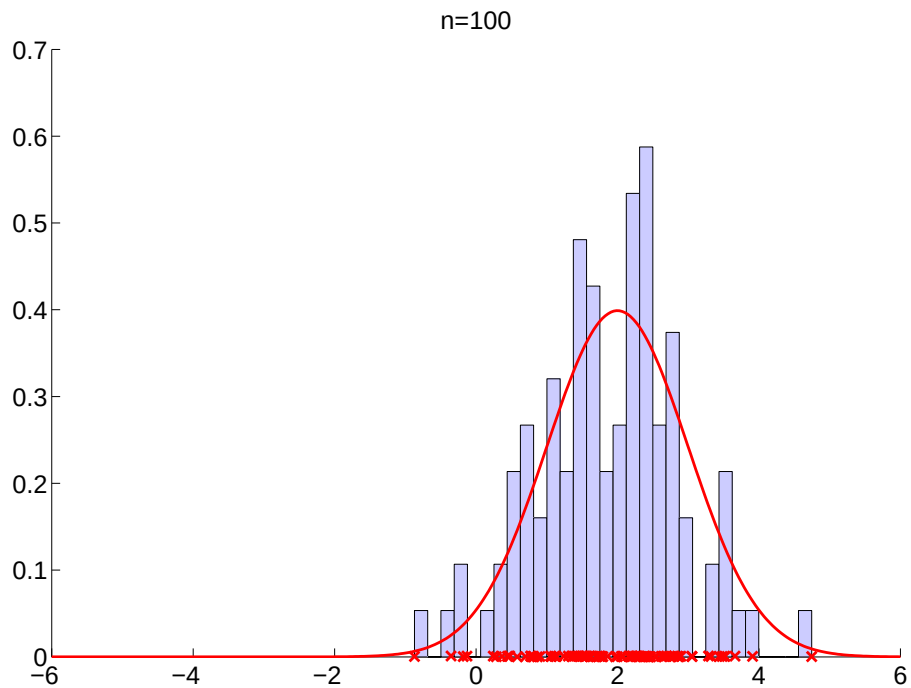
$$\mathrm{var}(Z) = \mathrm{E}\big[(Z - \mathrm{E}(Z))^2\big] = \mathrm{E}\big[Z^2\big] - \mathrm{E}[Z]^2 = \sigma^2$$

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

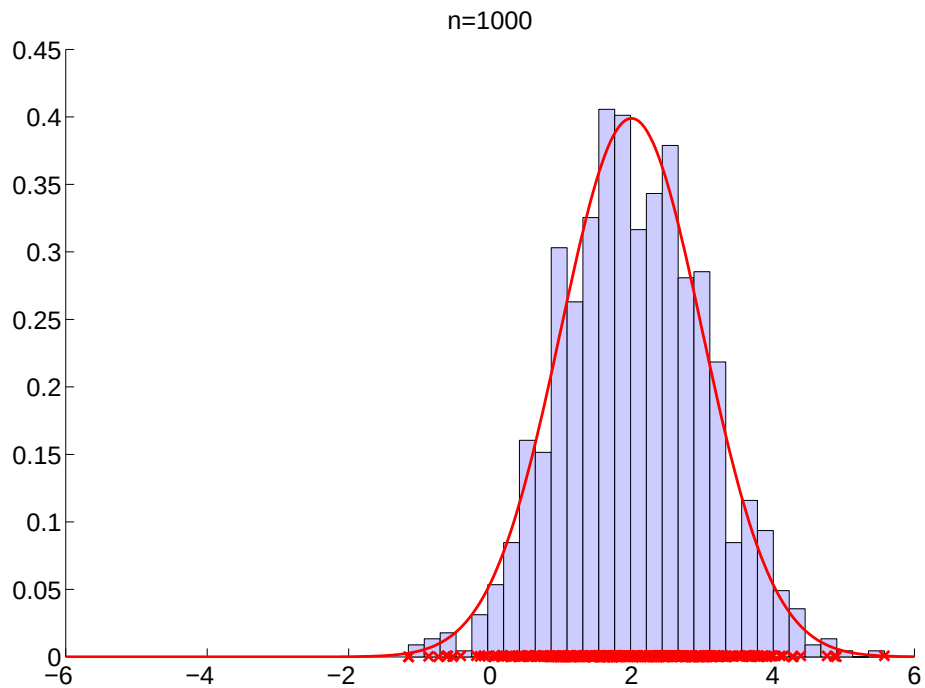
Gaussian random variables

- Using a random generator, it is possible to "generate" sample values $z_1, z_2, \ldots$ of our model $Z \rightarrow$ possible values for our uncertain quantity of interest



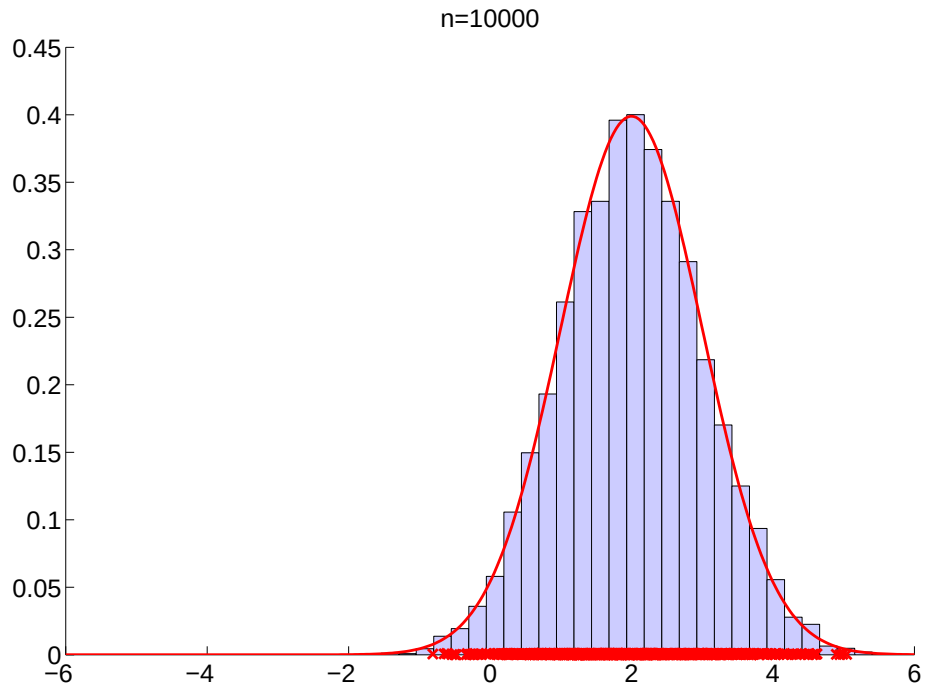
Gaussian random variables

- Using a random generator, it is possible to "generate" sample values $z_1, z_2, \ldots$ of our model $Z \rightarrow$ possible values for our uncertain quantity of interest



Gaussian random variables

- Using a random generator, it is possible to "generate" sample values $z_1, z_2, \ldots$ 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, $\mathcal{Z} = \mathbb{R}^n$)
- $\mathcal{F} \rightarrow \sigma$-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

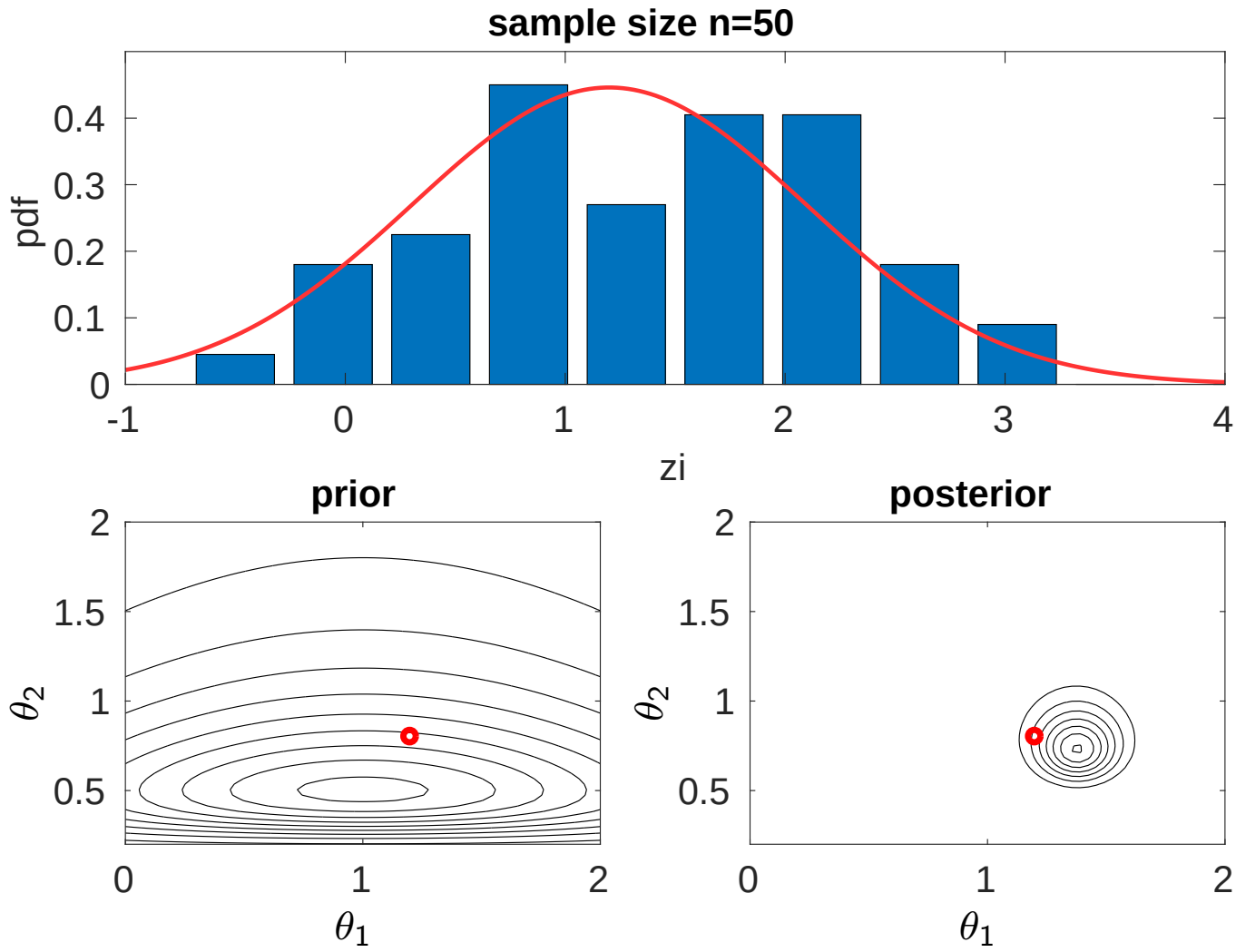
- Suppose we repeat measurements of a quantity of interest: $z_1, z_2, \ldots \in \mathbb{R}$
- Model of observations: $Z_i \overset{iid}{\sim} \mathcal{N}(\theta_1, \theta_2)$, $i = 1, \ldots, n$
- The statistical model can formally be written as the triplet

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

- Moreover, if we a 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 $Z_1, \ldots, Z_n$ (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

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

with

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

- Bayesian model?

- Assume the following statistical model for the observations:

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

  or equivalently,

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

- Moreover, choose a prior distribution for θ:

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

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

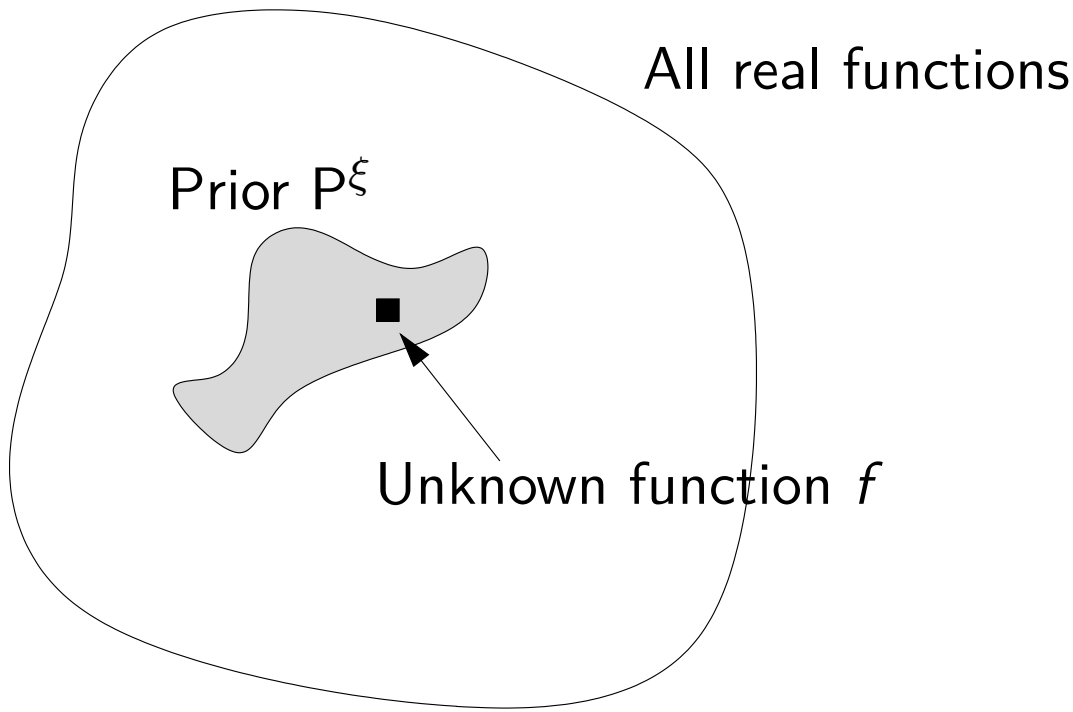
Random process

Def.

A random process $\xi : (\Omega, \mathbb{X}) \to \mathbb{R}$ is a collection of random variables $\xi(\cdot, x) : \Omega \to \mathbb{R}$ 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 $\xi(\omega, \cdot) : \mathbb{X} \to \mathbb{R}$ 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 $\Pi = \mathrm{P}^{\xi}$ is a prior about f

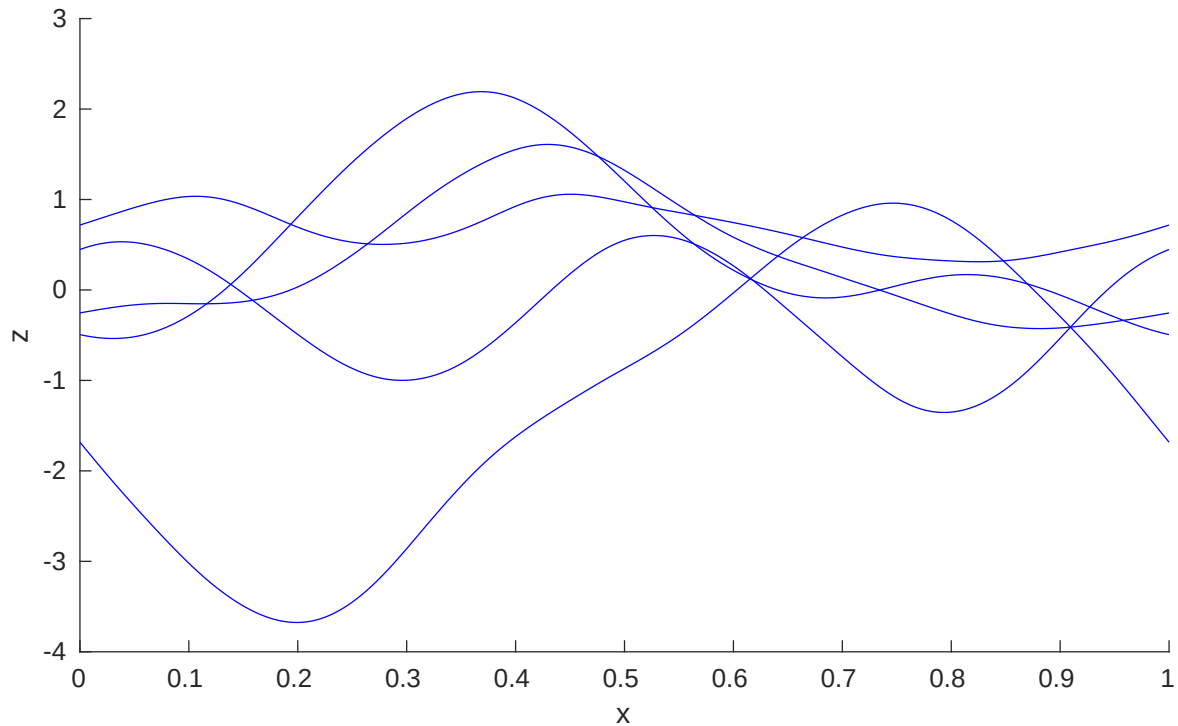


- Here, $\xi(\omega, \cdot) = \theta(\omega)^{\mathsf{t}} r(\cdot)$
- Fixing ω (a sample path) amounts to "choosing" a value for the random vector θ

- Example of sample paths with

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

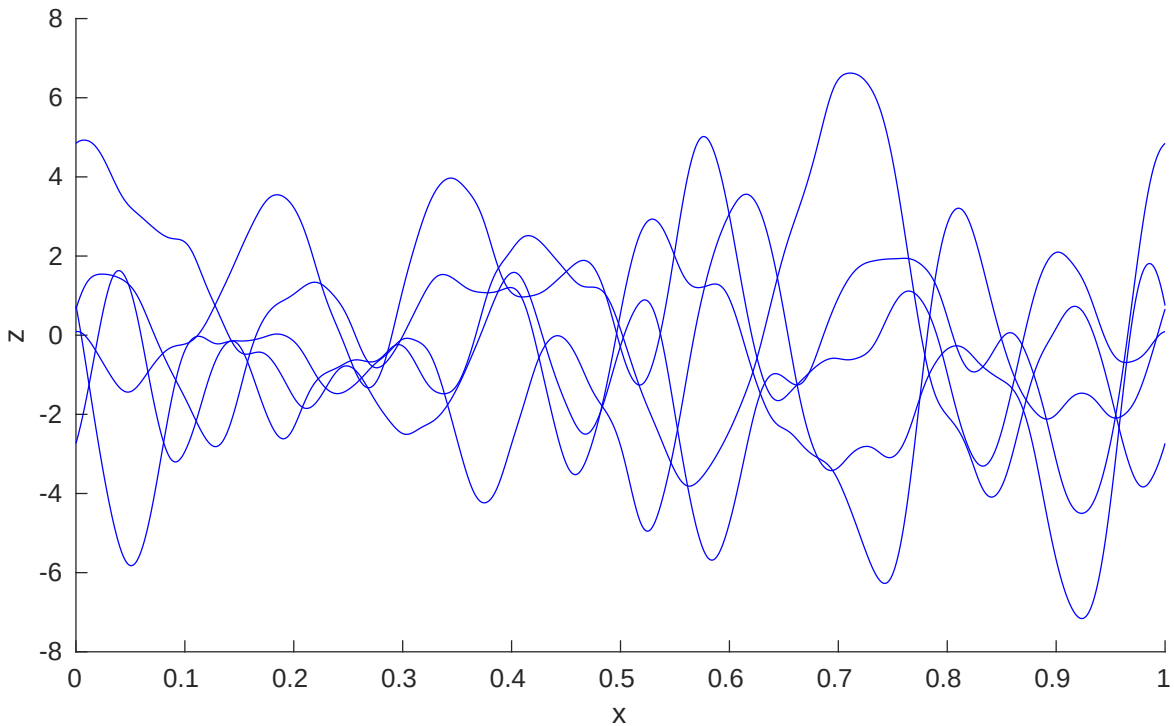
with $\omega_0 = \frac{2\pi}{10}$, $\alpha = 4$



- Example of sample paths with

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

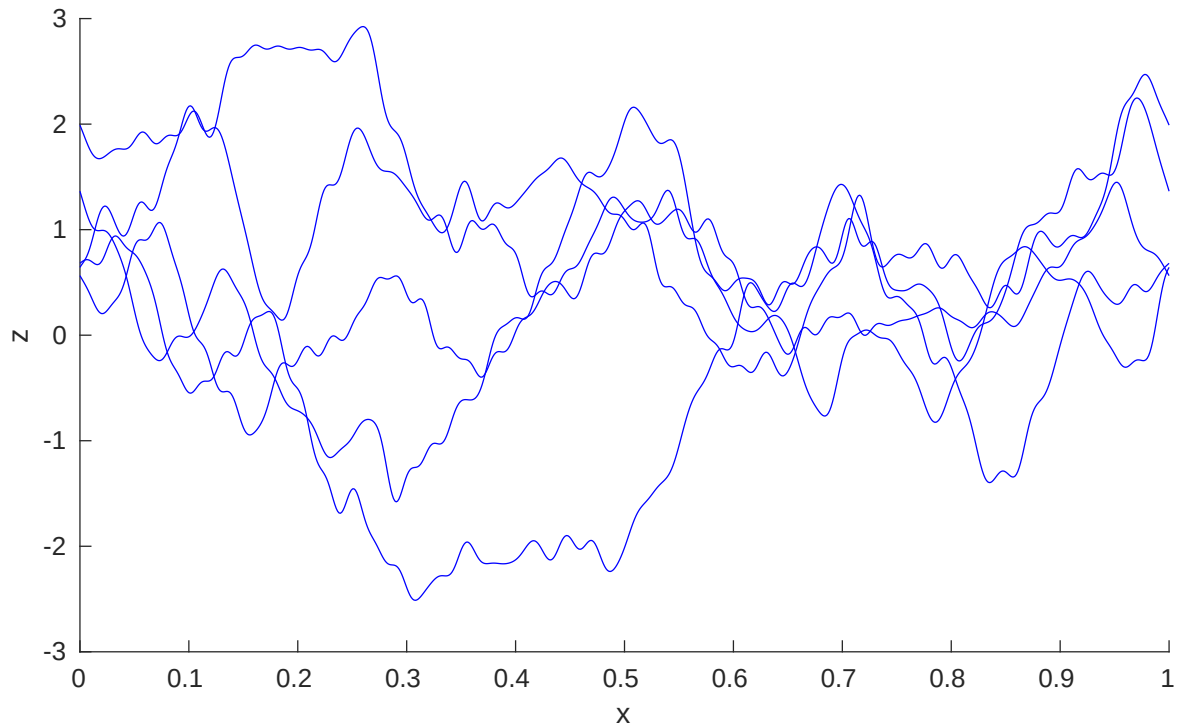
with $\omega_0 = \frac{2\pi}{50}$, $\alpha = 4$



- Example of sample paths with

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

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

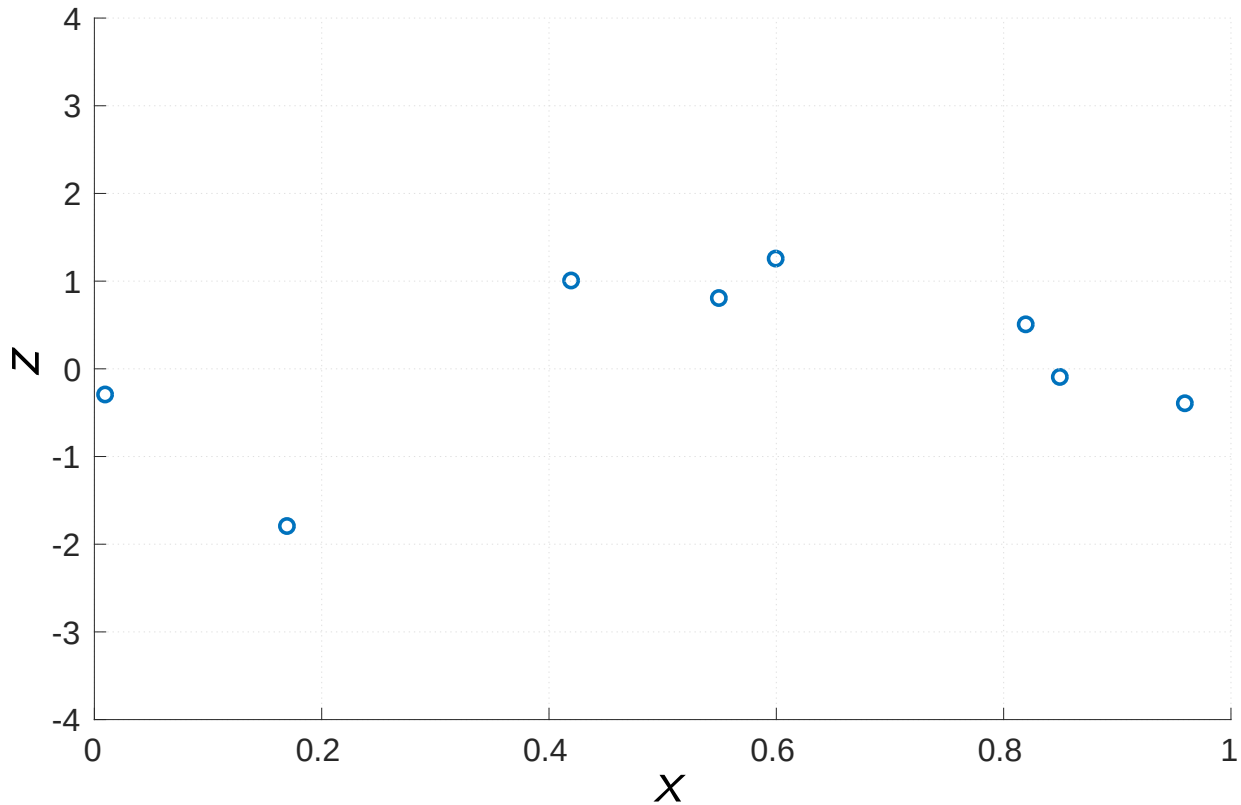


Bayesian approach

- 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

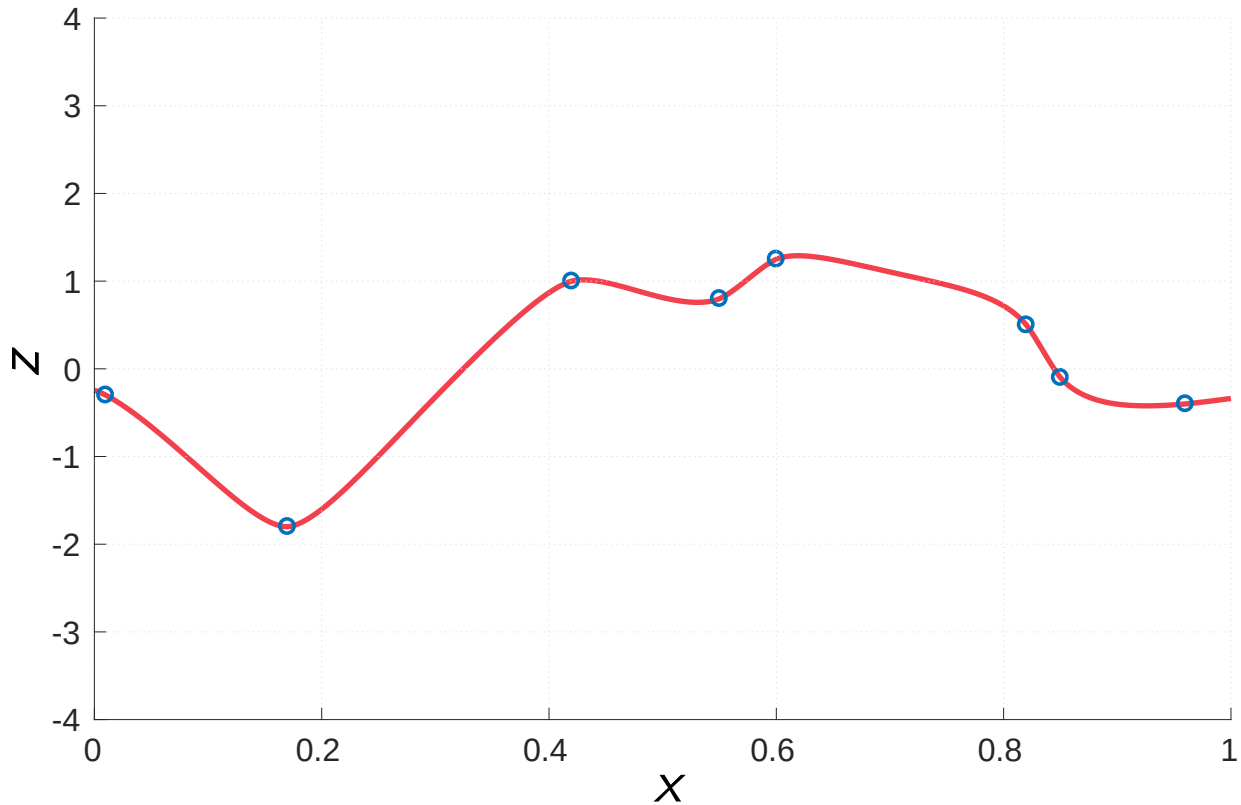
Bayesian approach

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



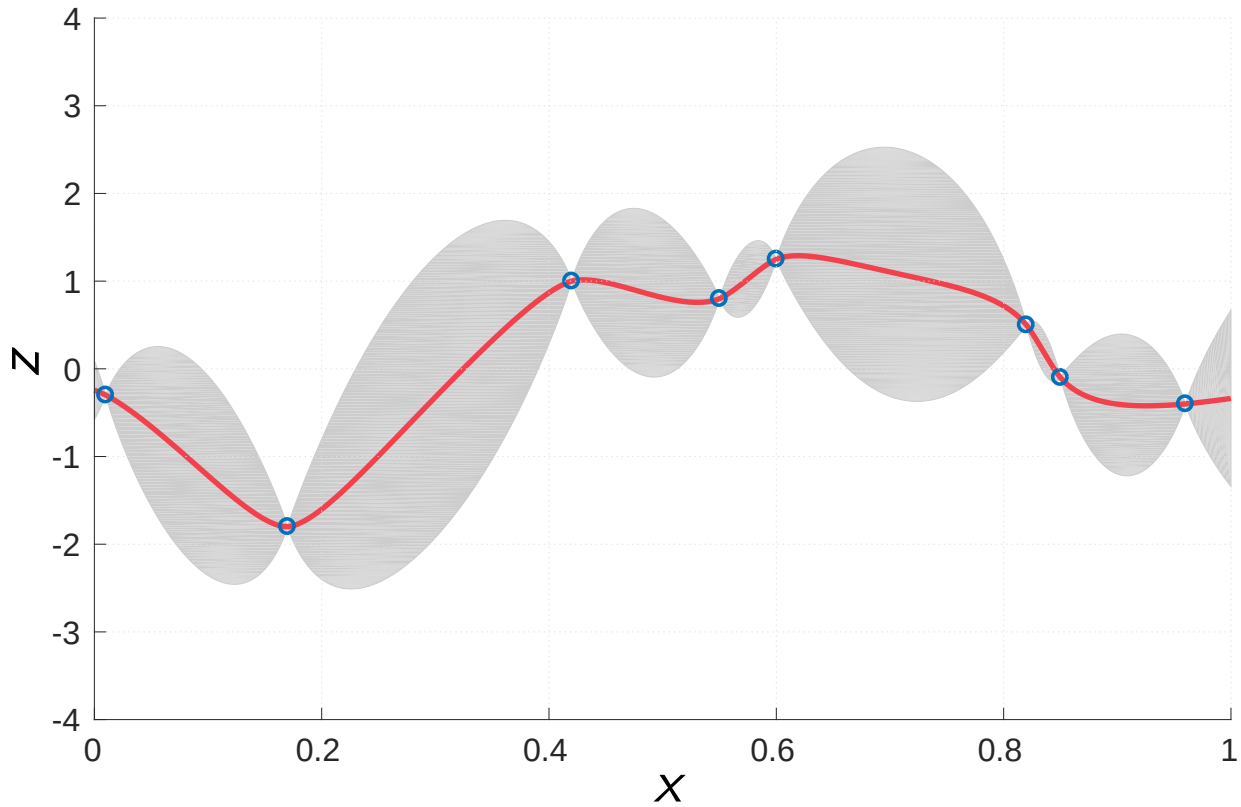
Bayesian approach

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



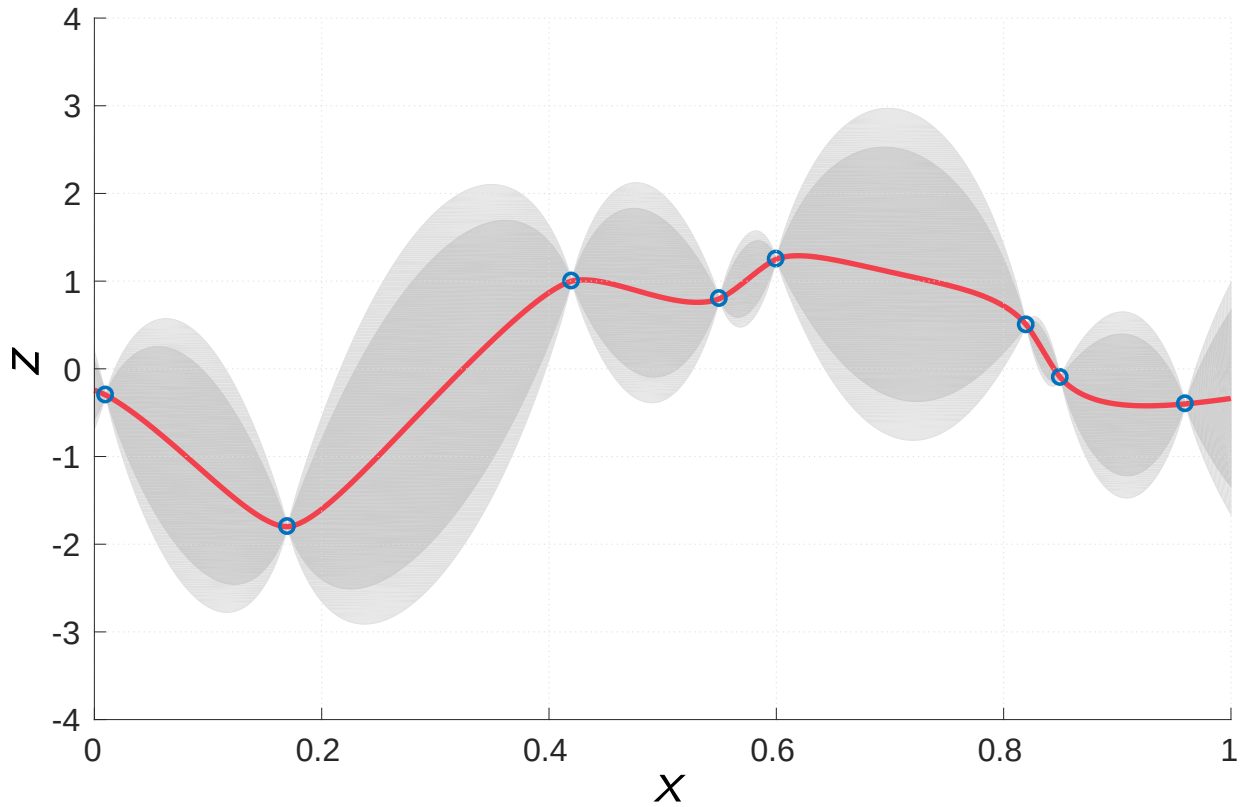
Bayesian approach

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



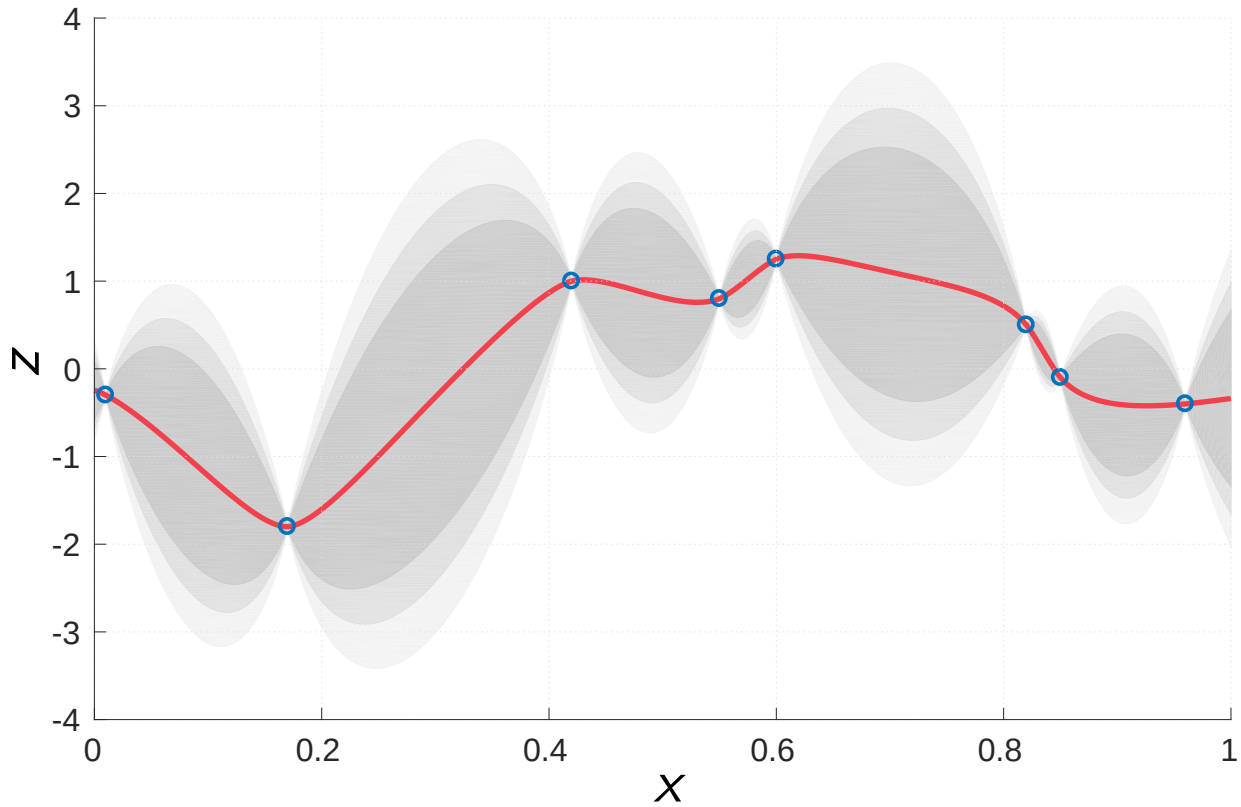
Bayesian approach

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



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

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

Gaussian random vectors

Def.

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

- A Gaussian random vector Z is characterized by its mean vector, $\mu = (\mathrm{E}[Z_1], \ldots, \mathrm{E}[Z_d]) \in \mathbb{R}^d$, and the covariance of the pairs of components (Z_i, Z_j), $i, j \in \{1, \ldots, d\}$, $\mathrm{cov}(Z_i, Z_j) = \mathrm{E}[(Z_i - \mathrm{E}(Z_i))(Z_j - \mathrm{E}(Z_j))]$
- 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 $\mathrm{E}\left(\sum_{i=1}^{d} a_i Z_i\right)$ and $\mathrm{var}\left(\sum_{i=1}^{d} a_i Z_i\right)$

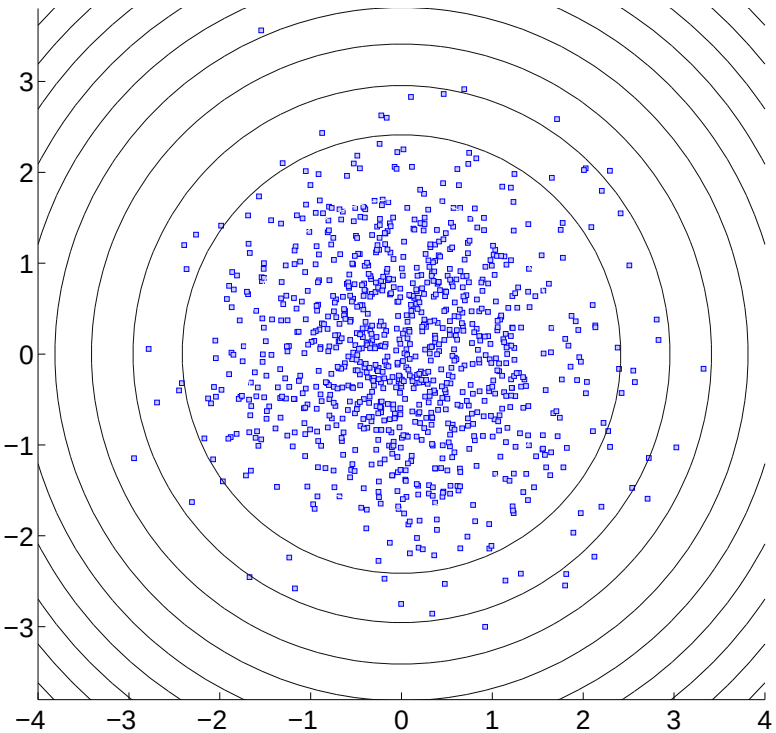
- The correlation coefficient of two components Z_i and Z_j of Z is defined by

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

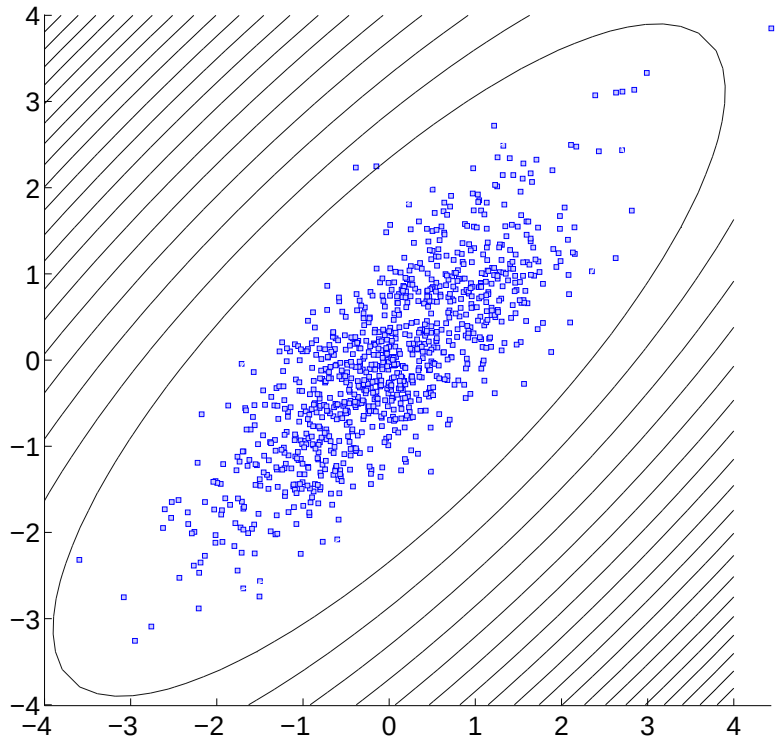
  $\rightarrow$ measures the similarity between Z_i and Z_j

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

  $\rightarrow$ generalization of a Gaussian random vector

Def.

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

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

is Gaussian

Application

- If

$$\begin{cases} \xi(x) = \theta^{\mathrm{t}} r(x), \quad x \in \mathbb{X} \\ \theta_j \overset{\text{indep}}{\sim} \mathcal{N}(0, \sigma^2_{\theta_j}), \quad j = 1, \ldots, 2m+1 \end{cases}$$

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

$$\sum_{i=1}^{n} a_i \xi(x_i) = \sum_i a_i \Big(\sum_j \theta_j r_j(x_i) \Big)$$

$$= \sum_j \Big(\sum_i a_i r_j(x_i) \Big) \theta_j \sim \mathcal{N}\Big(0, \sum_j \Big(\sum_i a_i r_j(x_i) \Big)^2 \sigma^2_{\theta_j} \Big)$$

- Thus, $\xi = \theta^{\mathrm{t}} r$ is a Gaussian process

Gaussian random processes

- A Gaussian process is characterized by
  - its mean function

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

  - and its covariance function

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

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

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

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

$\rightarrow$ 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

$$\begin{cases} \xi(x) = \theta^{\mathsf{t}} r(x), \quad x \in \mathbb{X} \\ \theta_j \overset{\text{indep}}{\sim} \mathcal{N}(0, \sigma^2_{\theta_j}), \quad j = 1, \ldots, 2m+1 \end{cases}$$

then,

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

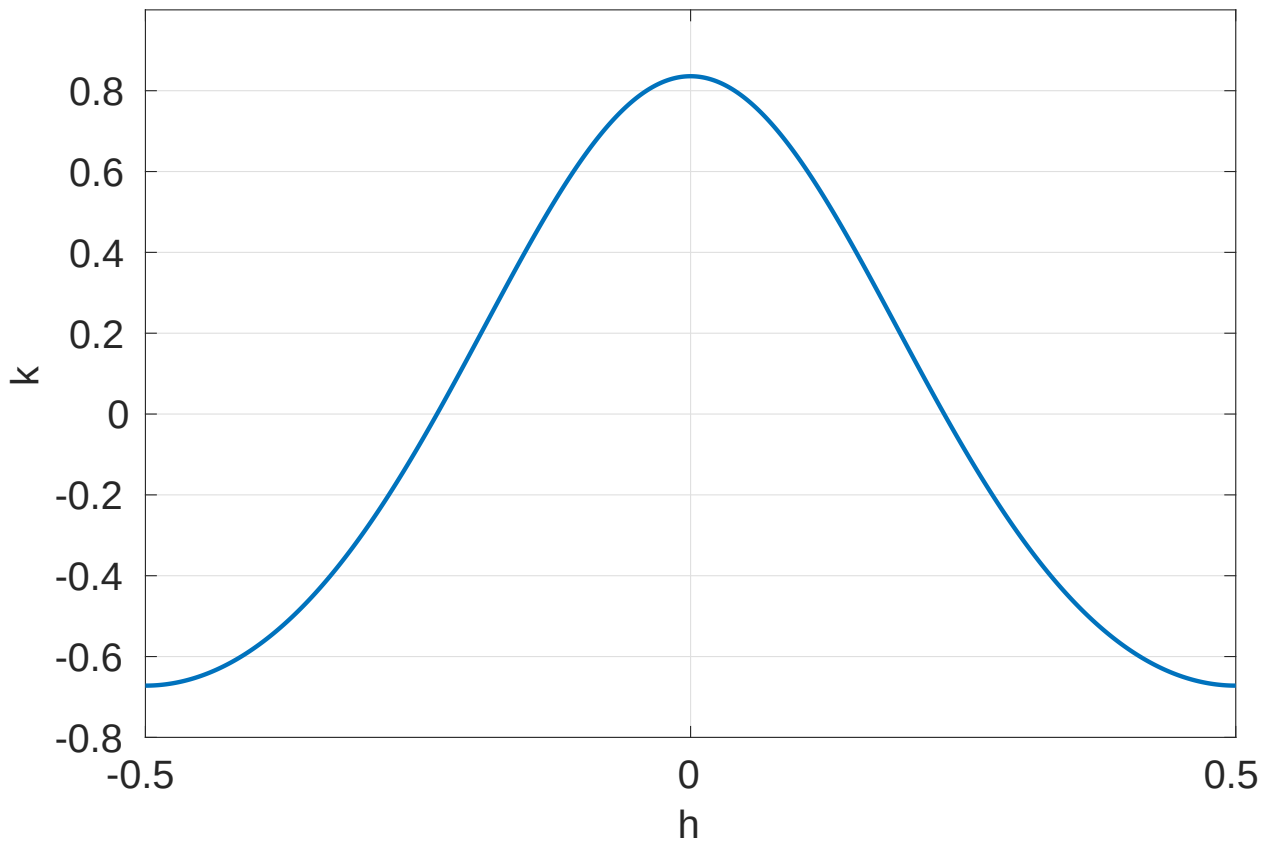
with

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

- Covariance function corresponding to

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

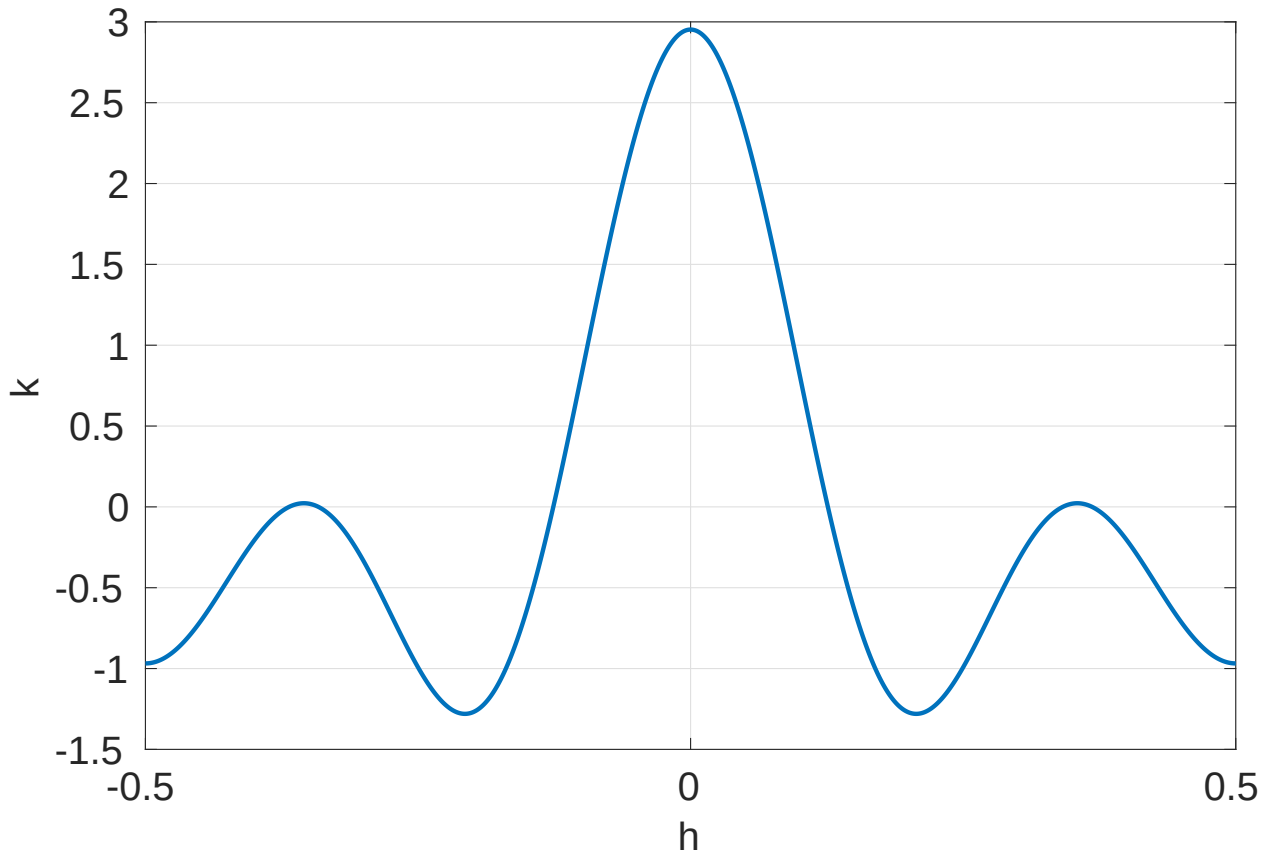
with $\omega_0 = \frac{2\pi}{10}$, $\alpha = 4$



- Covariance function corresponding to

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

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:

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

- 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 $k_{\text{sta}} : \mathbb{R}^d \to \mathbb{R}$ 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

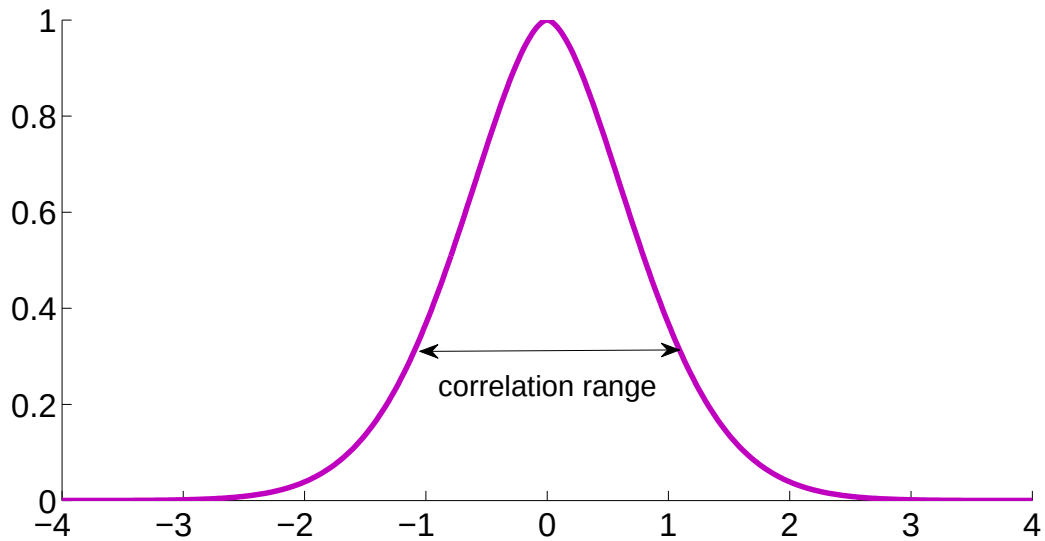
- The covariance function can be written as

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

  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,

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

- Recall, Bochner's spectral representation theorem

Theorem

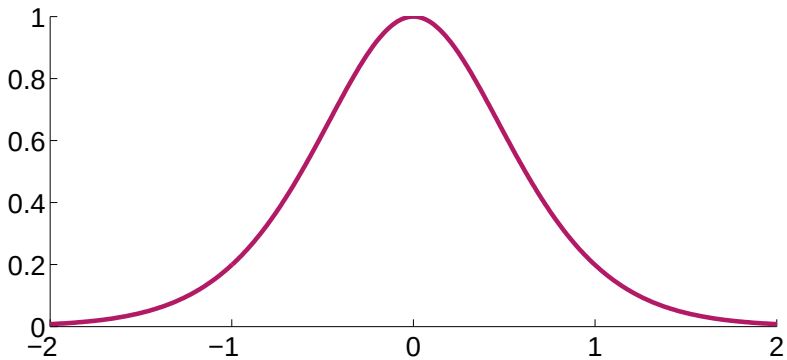
A real function $k(h)$, $h \in \mathbb{R}^d$ is symmetric positive iff it is the Fourier transform of a finite positive measure, i.e.

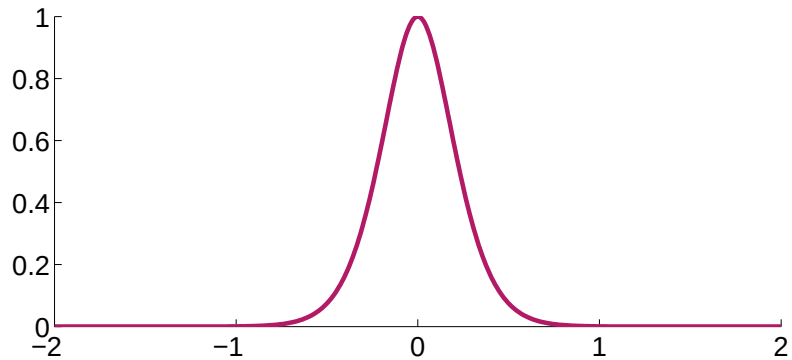
$$k(h) = \int_{\mathbb{R}^d} e^{\imath(u,h)} d\mu(u)\,,$$

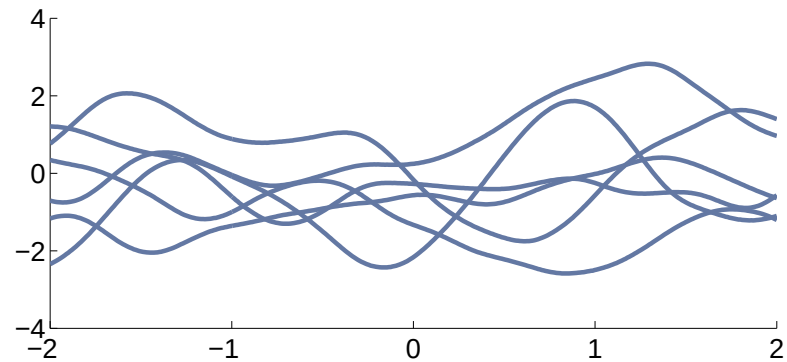
where μ is a finite positive measure on $\mathbb{R}^d$.

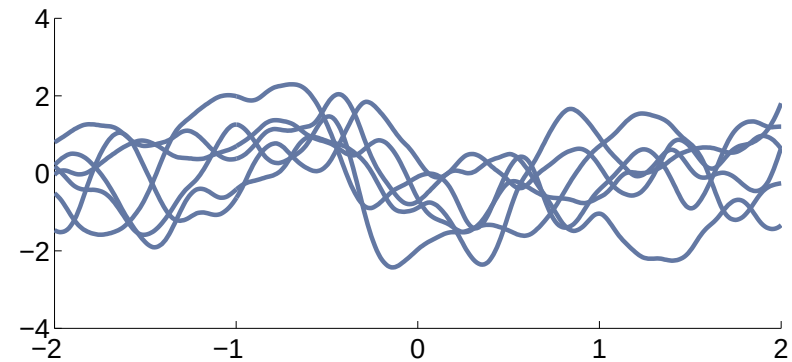
Gaussian process simulation

- Using a random generator, it is possible to "generate" sample paths $f_1, f_2, \ldots$ 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 $\underline{\xi} = (\xi(x_1), \dots, \xi(x_n))^{\mathrm{t}}$ (NB: $\underline{\xi} \sim \mathcal{N}(0, K)$)
- Consider the Cholesky factorization of K

$$K = CC^{\mathrm{t}},$$

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

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

"Simplification" of the Bayesian model for the simple curve fitting problem

- Instead of choosing the model

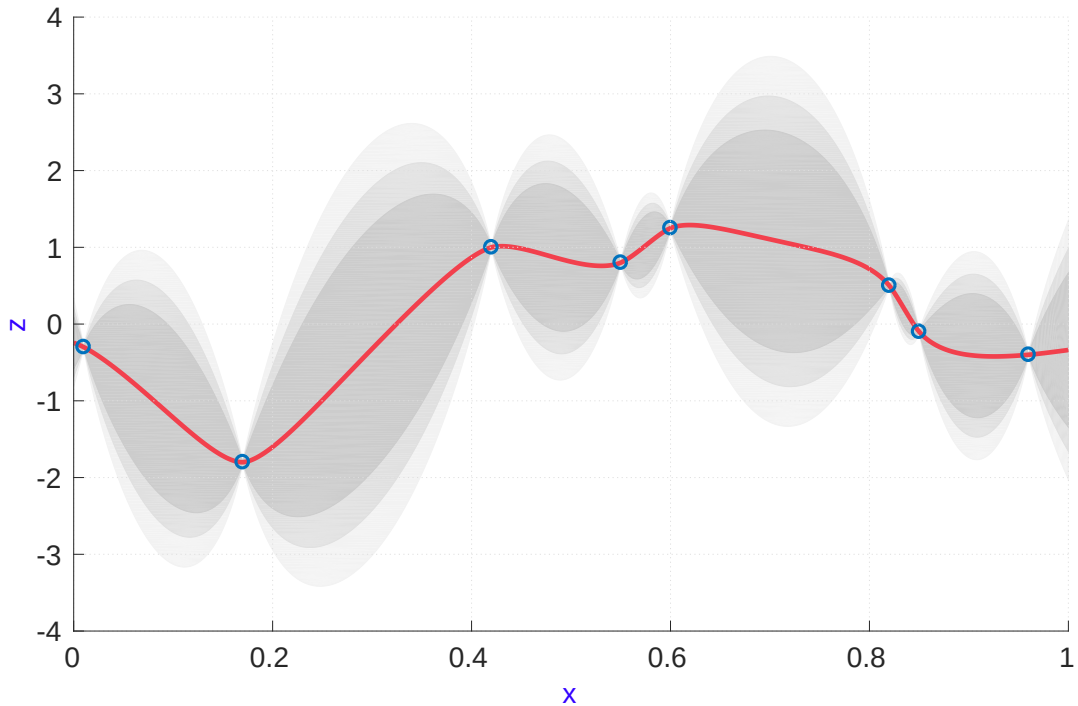
$$\begin{cases} \xi(x) = \theta^{\mathrm{t}} r(x), \quad x \in \mathbb{X} \\ \theta_j \overset{\text{indep}}{\sim} \mathcal{N}(0, \sigma_{\theta_j}^2), \quad j = 1, \ldots, 2m+1 \end{cases}$$

  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

Posterior

- How to compute a posterior distribution, given the Gaussian-process prior ξ and data?



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 $T = (T_1, \ldots, T_n)$
- 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 $(\Omega, \mathcal{A}, \mathrm{P})$ be a probability space. Given two events $A, B \in \mathcal{A}$ such that $\mathrm{P}(B) \neq 0$, define the probability of A given B (or conditional on B) by

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

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

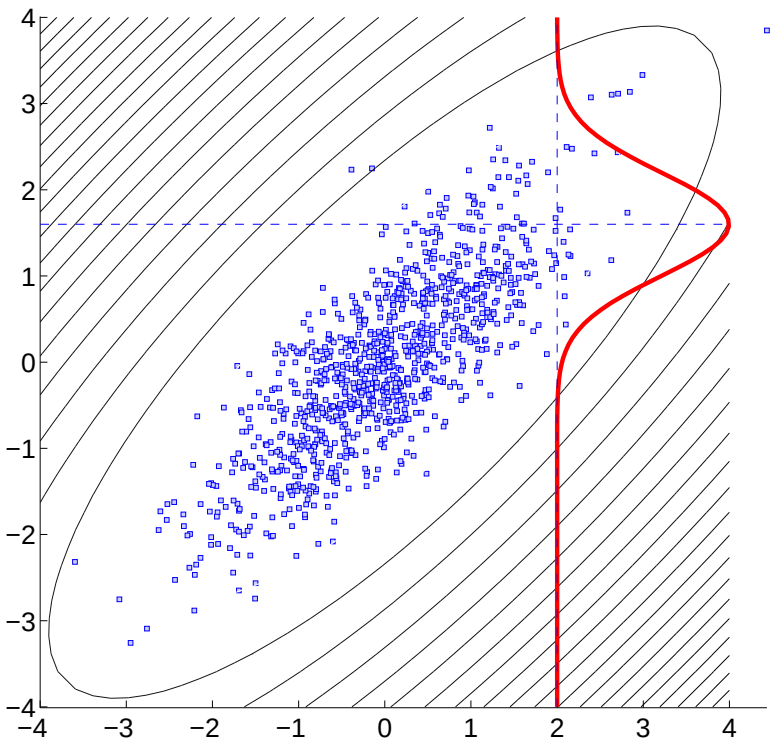
$$p^{X|T}(x \mid t) = \begin{cases} \dfrac{p^{(X,T)}(x,t)}{p^T(t)} = \dfrac{p^{(X,T)}(x,t)}{\int p^{X,T}(x,t)dx} & \text{if } p^T(t) > 0 \\ \text{arbitrary density} & \text{if } p^T(t) = 0. \end{cases}$$

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

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

$\rightarrow$ Gaussian distribution!



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

$$\mathrm{E}(X \mid T = t) \stackrel{\Delta}{=} \int_{\mathbb{R}} x\, p^{X|T}(x|t)dx = h(t)$$

Def.

The random variable $\mathrm{E}(X \mid T) = h(T)$ 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

$$\widehat{X} = \operatorname{argmin}_Y \mathrm{E}\left[(X - Y)^2\right]$$

where the minimum is taken over all functions of T is given by $\widehat{X} = \mathrm{E}(X \mid T)$

- In other words, $\mathrm{E}(X \mid T)$ is the best approximation (in the sense of the quadratic mean) of X by a function of T

Important properties of conditional expectation

(1) $\mathrm{E}(X \mid T)$ is a random variable depending on $T \rightarrow$ there exists a function h such that $\mathrm{E}(X \mid T) = h(T)$

(2) The operator $\pi_H : X \mapsto \mathrm{E}(X \mid T)$ 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) $\forall \alpha \in \mathbb{R}$, $\mathrm{E}(\alpha X + Y \mid T) = \alpha \mathrm{E}(X \mid T) + \mathrm{E}(Y \mid T)$ a.s.

ii) $\mathrm{E}(\mathrm{E}[X \mid T]) = \mathrm{E}(X)$

iii) If $X \perp\!\!\!\perp T$, $\mathrm{E}(X \mid T) = \mathrm{E}(X)$

Conditional expectation: Gaussian random variables

- Recall that the space of second-order random variables $L^2(\Omega, \mathcal{A}, \mathrm{P})$ 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 $L^2(\Omega, \mathcal{A}, \mathrm{P})$ is Gaussian iff $\forall X_1, \ldots, X_n \in G$ and $\forall a_1, \ldots, a_n \in \mathbb{R}$ 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

Theorem (Projection theorem in centered Gaussian spaces)

Let G be a centered Gaussian space. Let $X, T_1, \ldots, T_n \in G$. Then $\mathrm{E}(X \mid T_1, \ldots, T_n)$ is the orthogonal projection (in L^2) of X on $\mathcal{T} = \mathrm{span}\{T_1, \ldots, T_n\}$.

proof Let $\widehat{X} \in G$ be the orthogonal projection of X on $\mathcal{T}$.

- we have $X = \widehat{X} + \varepsilon$ where $\varepsilon \in G$ is orthogonal to $\mathcal{T}$.
  In G, orthogonality $\Leftrightarrow$ independence. Thus, $\varepsilon \perp\!\!\!\perp T_i$, $i = 1, \ldots, n$.
- Then,

$$\begin{aligned}\mathrm{E}(X \mid T_1, \ldots, T_n) &= \mathrm{E}(\widehat{X} \mid T_1, \ldots, T_n) + \mathrm{E}(\varepsilon \mid T_1, \ldots, T_n) \\ &= \widehat{X} + \mathrm{E}(\varepsilon) = \widehat{X}\end{aligned}$$

The result follows.

∎

- 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 $\mathrm{E}(Z_1 \mid Z_2)$ is the orthogonal projection of Z_1 onto Z_2. Thus

$$\mathrm{E}(Z_1 \mid Z_2) = \lambda Z_2$$

with

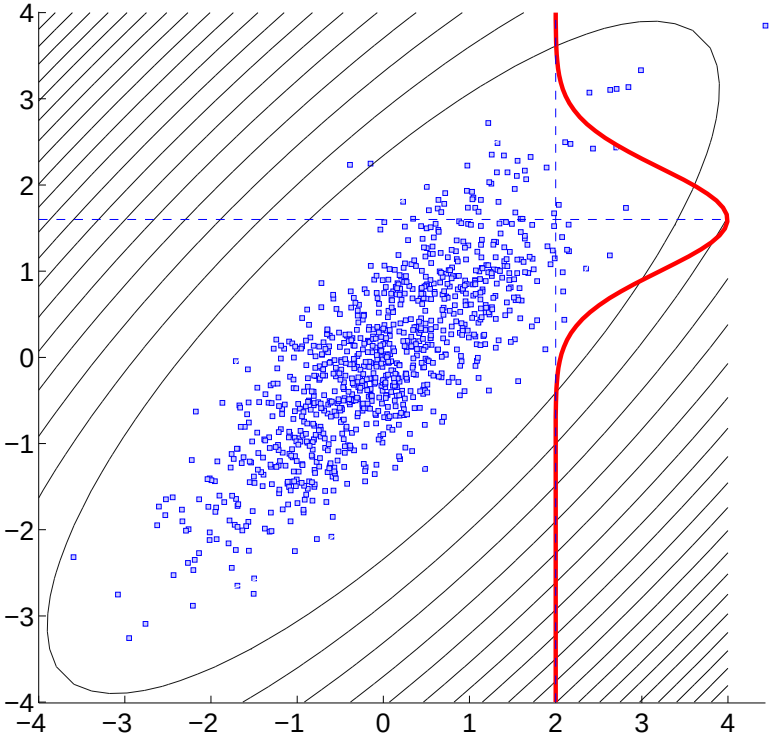
$$(Z_1 - \lambda Z_2, Z_2) = (Z_1, Z_2) - \lambda(Z_2, Z_2) = 0\,.$$

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 $Z_2 \mid Z_1 \sim \mathcal{N}(\mu(Z_1), \sigma(Z_1)^2) \rightarrow \mu$? σ ?



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

$$\begin{aligned}
\sigma^2 &= \mathrm{E}\big((Z_2 - \mathrm{E}(Z_2 \mid Z_1))^2 \mid Z_1\big) \\
&\overset{\perp}{=} \mathrm{E}\left((Z_2 - E(Z_2 \mid Z_1))^2\right) \\
&= \mathrm{E}\left((Z_2 - \lambda Z_1)^2\right) \\
&\overset{\perp}{=} \mathrm{E}\left((Z_2 - \lambda Z_1) Z_2\right) \\
&= \sigma_2^2 - \lambda \sigma_{1,2}
\end{aligned}$$

Generalization

Exercise: Let $(Z_0, Z_1, \ldots, Z_n)$ be a centered Gaussian vector.

Determine $E(Z_0 \mid Z_1, \ldots, Z_n)$.

Application: computation of the posterior distrib. of a GP

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

$$\xi(x_0) \mid \xi(x1), \ldots, \xi(x_n)\,?$$

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

$$\xi(\cdot) \mid \xi(x1), \ldots, \xi(x_n)\,?$$

Computation of the posterior distribution of a GP

Prop.

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

- *mean* $\quad \widehat{\xi}_n : x \mapsto \mathrm{E}(\xi(x) \mid \xi(x_1), \ldots, \xi(x_n))$
- *covariance* $\quad k_n : x, y \mapsto \mathrm{E}\left((\xi(x) - \widehat{\xi}_n(x))(\xi(y) - \widehat{\xi}_n(y))\right)$

Computation of the posterior distrib. of a GP

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

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

- Moreover, the posterior mean $\widehat{\xi}_n(x)$ is the orthogonal projection of $\xi(x)$ onto $\mathrm{span}\{\xi(x_i), i = 1, \ldots, n\}$, such that
  - $\widehat{\xi}_n(x) = \mathrm{argmin}_Y \, \mathrm{E}\left[(\xi(x) - Y)^2\right] \rightarrow$ the variance of the prediction error is minimum
  - $E(\widehat{\xi}_n(x)) = \mathrm{E}[\mathrm{E}\left(\xi(x) \mid F_n\right)] = \mathrm{E}(\xi(x)) = 0 \rightarrow$ unbiased estimation
- $\widehat{\xi}_n(x)$ is the best linear predictor (BLP) of $\xi(x)$ from $\xi(x_1), \ldots, \xi(x_n)$, 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

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

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

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

- $\sigma_n^2(x)$ 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

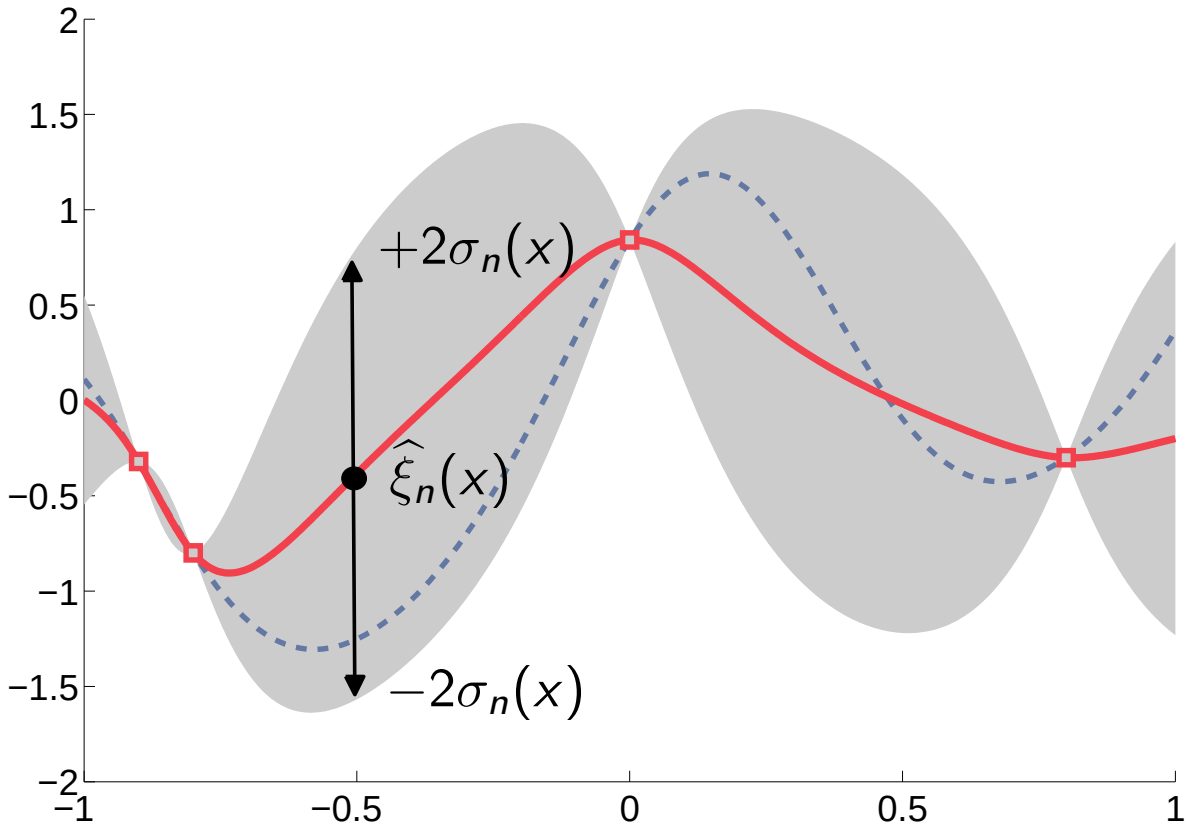
  - $\lambda(x) = (\lambda_1(x), \ldots, \lambda_n(x))^{\mathrm{t}}$
  - K: $n \times n$ covariance matrix of the observation vector
  - $k(x)$: $n \times 1$ vector with entries $k(x_i, x)$

Kriging equations

proof

Posterior distrib. of a GP

- For all $x \in \mathbb{X}$, the random variable $\xi(x) \mid F_n$ with distrib. $\mathcal{N}(\widehat{\xi}_n(x), \sigma_n^2(x))$ represents the residual uncertainty about $\xi(x)$ when $\xi(x_1), \ldots, \xi(x_n)$ 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 $\xi \sim \mathrm{GP}(0, k)$
- For $i = 1, \ldots, n$, we observe $Z_i = \xi(x_i) + \varepsilon_i$ at points x_i, where the random variables ε_i model an observation noise:
  - $\varepsilon_i \overset{\text{i.i.d}}{\sim} \mathcal{N}(0, \sigma^2)$
  - independent from ξ
- As above, the posterior mean $\widehat{\xi}_n(x)$ of $\xi(x)$ is obtained as the orthogonal projection of $\xi(x)$ on the linear subspace $\mathrm{span}\{Z_i, i = 1, \ldots, n\}$:

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

with $\lambda_i(x)$ such that

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

Generalization: prediction from noisy observations

- Thus, $\forall i$

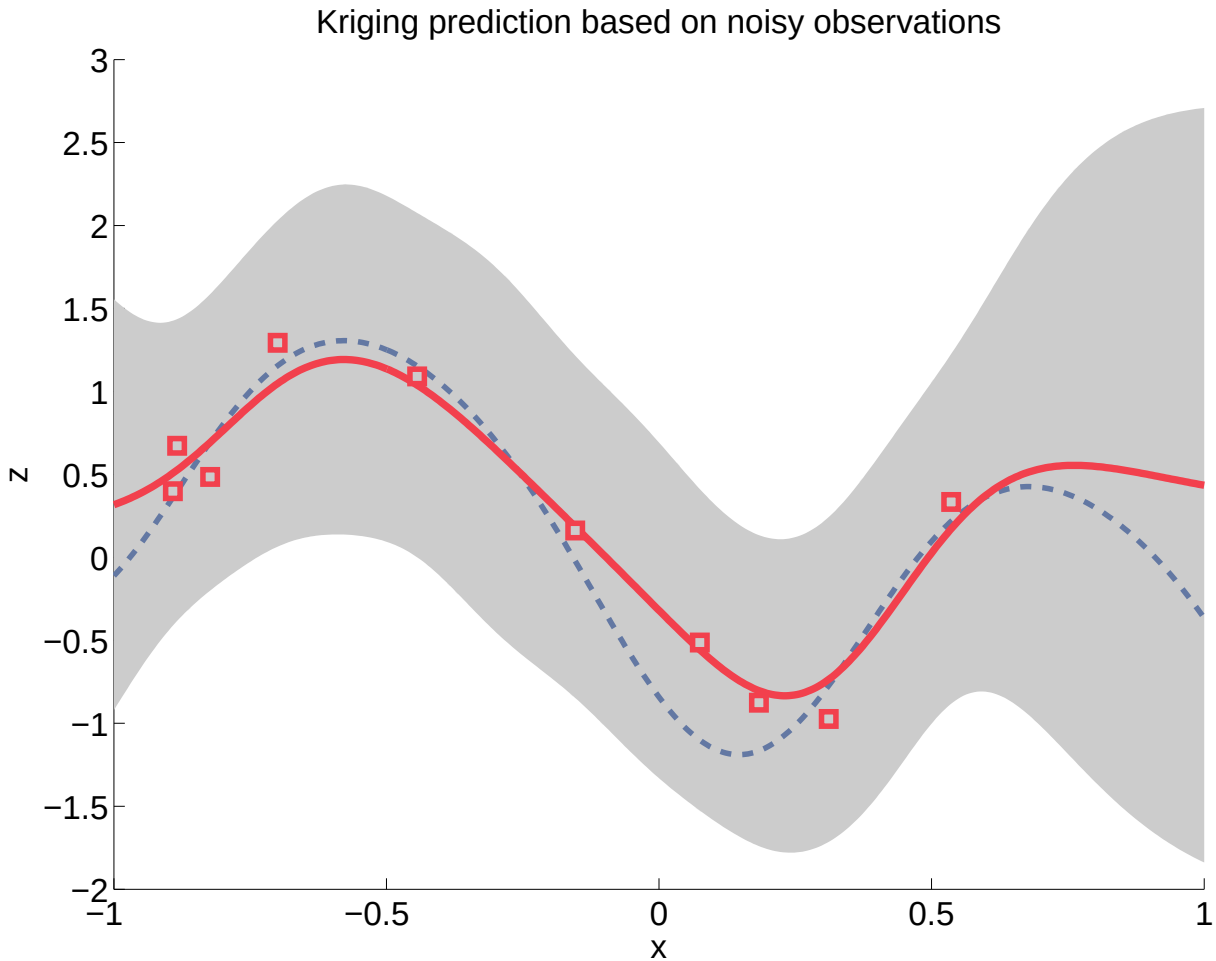
$$\mathsf{E}\left[(\xi(x) - \widehat{\xi}_n(x))Z_i\right]$$

$$= \mathsf{E}\left[\xi(x)(\xi(x_i) + \varepsilon_i)\right] - \sum_{j=1}^{n} \lambda_j(x)\mathsf{E}\left[(\xi(x_j) + \varepsilon_j)(\xi(x_i) + \varepsilon_i)\right]$$

$$= k(x, x_i) - \sum_{j=1}^{n} \lambda_j(x)\left(k(x_j, x_i) + \sigma^2\delta_{i,j}\right)$$

- 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 $\rightarrow$ a smooth approximation is preferred

iii) The covariance matrix is ill-conditioned $\rightarrow$ adding a small observation noise will regularize the solution of the linear system (why?)

Posterior of a quantity of interest

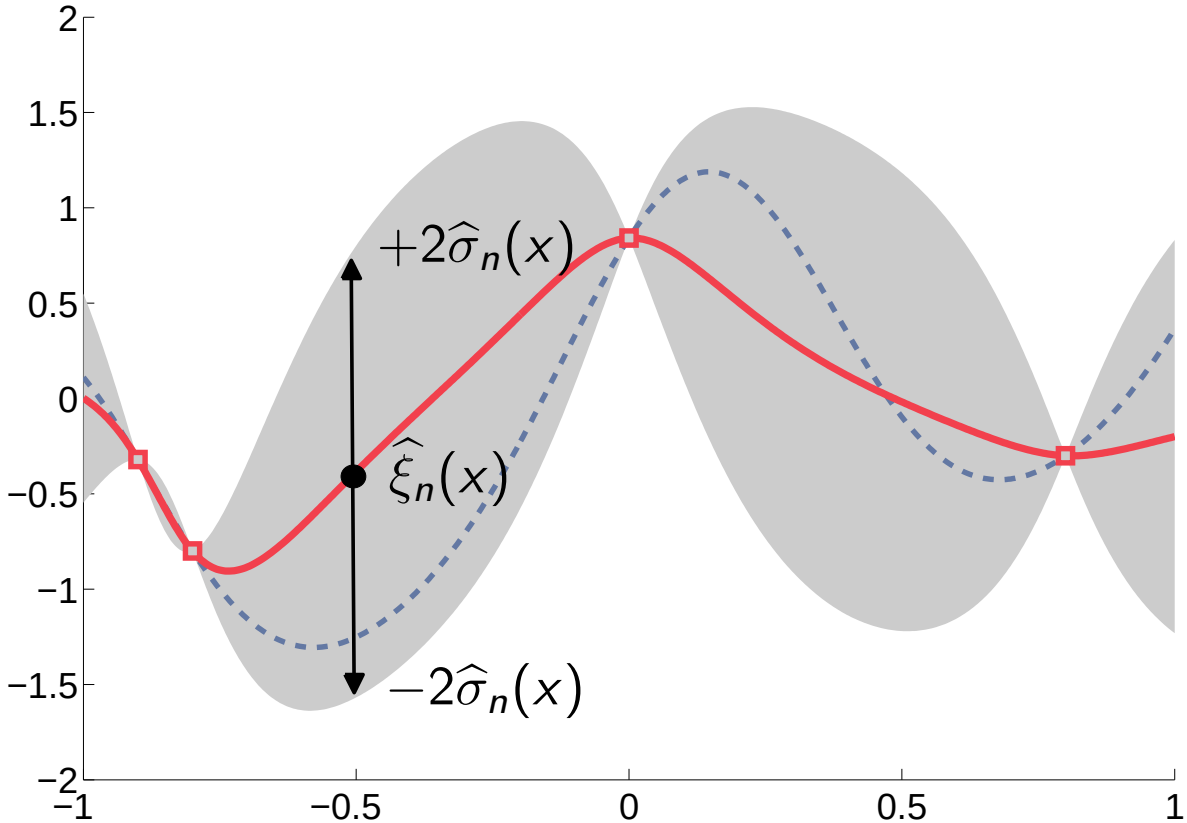
- Using the posterior distribution of ξ, we can address questions like
  - What are plausible values for $\xi(x)$ at a given x? (obviously)
  - What are plausible values for $\int g(\xi(x))\,\mathrm{d}\mu(x)$ for given g and μ?
  - What are plausible values for the minimum $M = \min_x \xi(x)$?
  - Where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

Example of a quantity of interest: the improvement

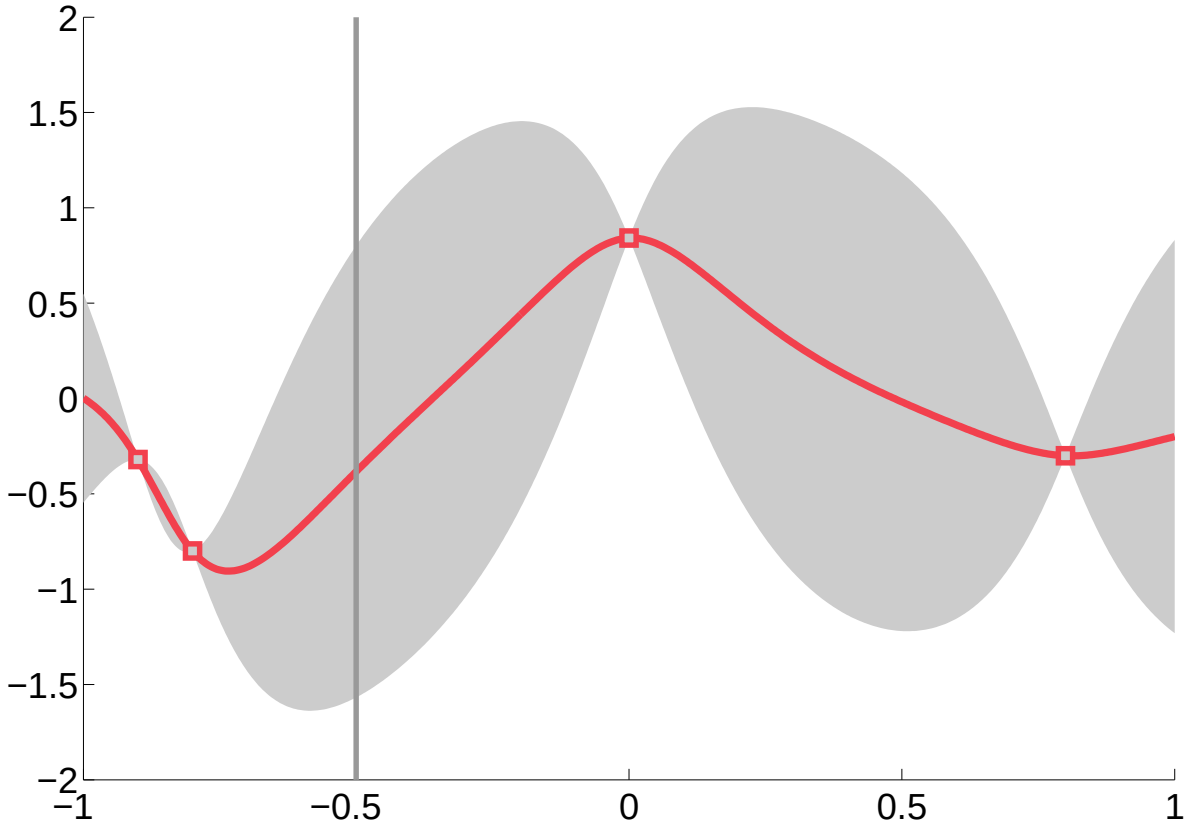
- Suppose that our objective is to minimize an unknown function $f : \mathbb{X} \to \mathbb{R}$
- In our Bayesian approach, we choose a GP prior ξ for f (in other words, ξ is a model of f)
- Objective: construct a sequence $(X_1, X_2, \ldots) \in \mathbb{X}$ that converges to $X^\star = \operatorname{argmin}_x \xi(x)$
- Given $X_1, \ldots, X_{n+1}$, 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:

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

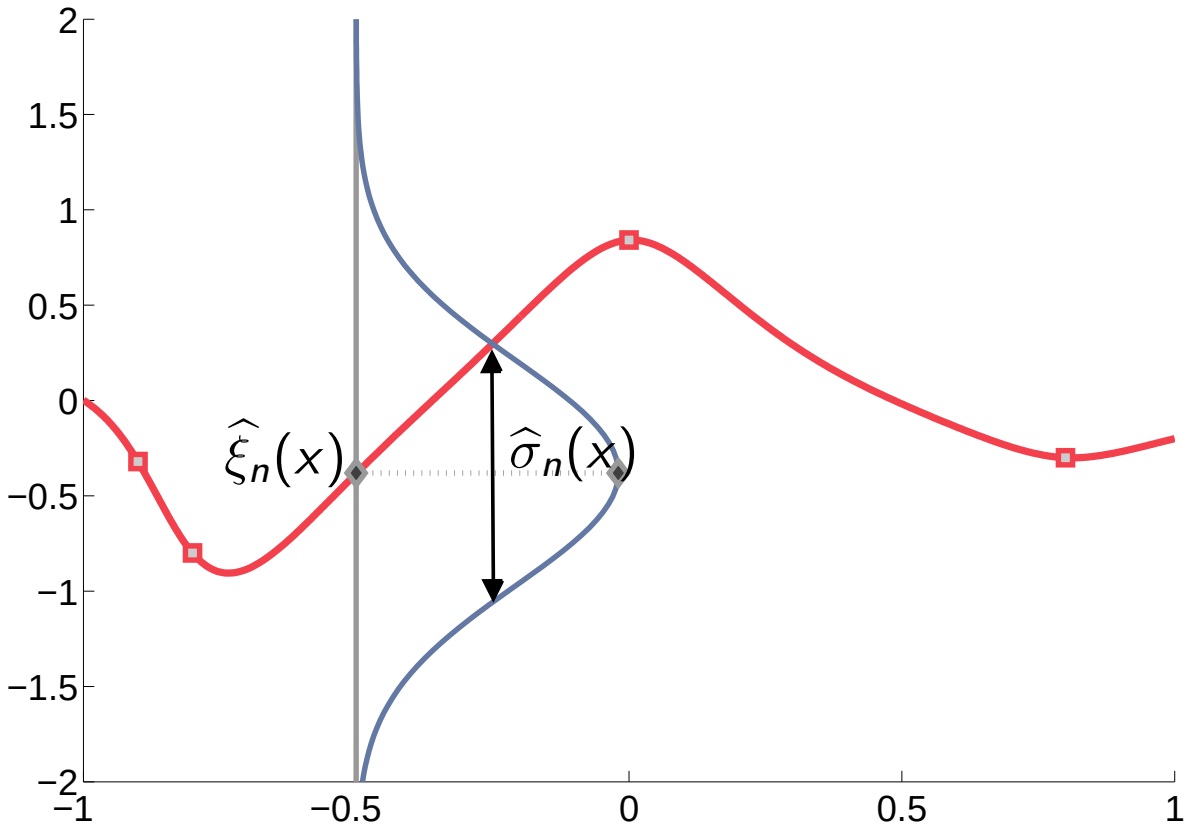
Example of a quantity of interest: the improvement



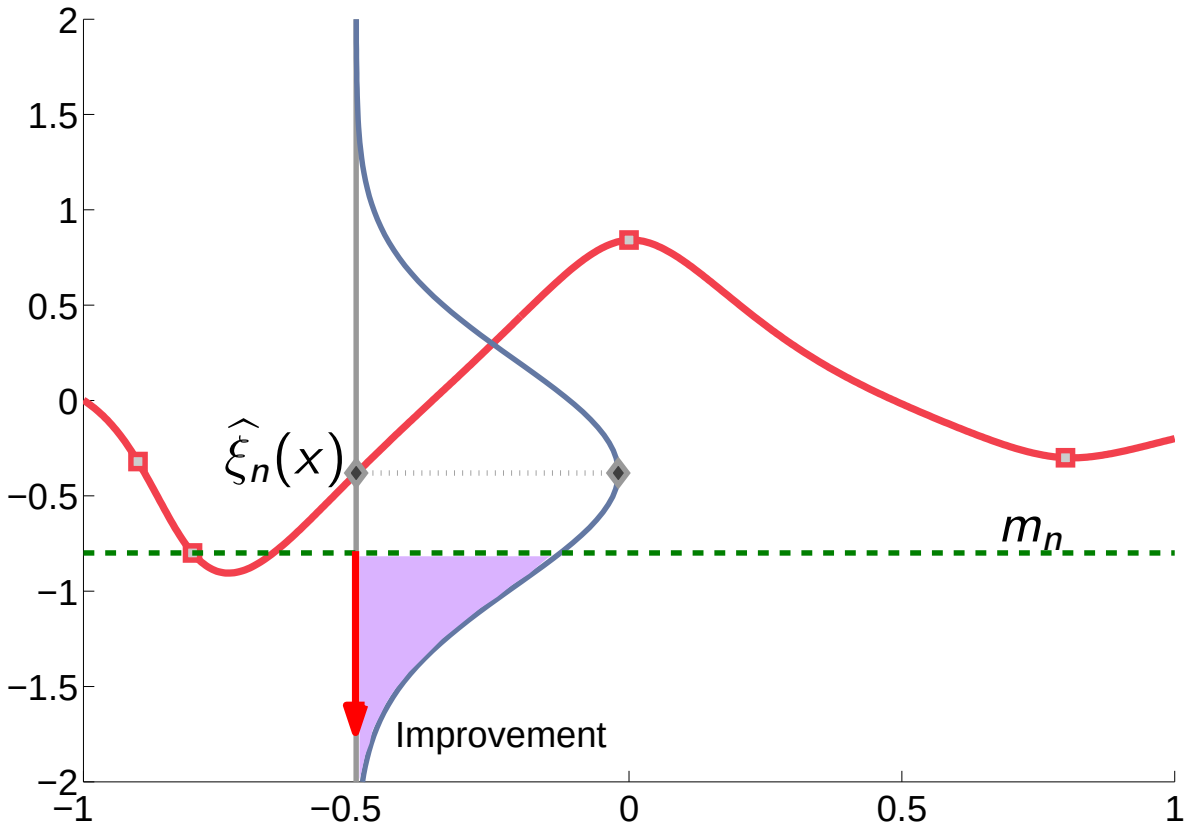
Example of a quantity of interest: the improvement



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

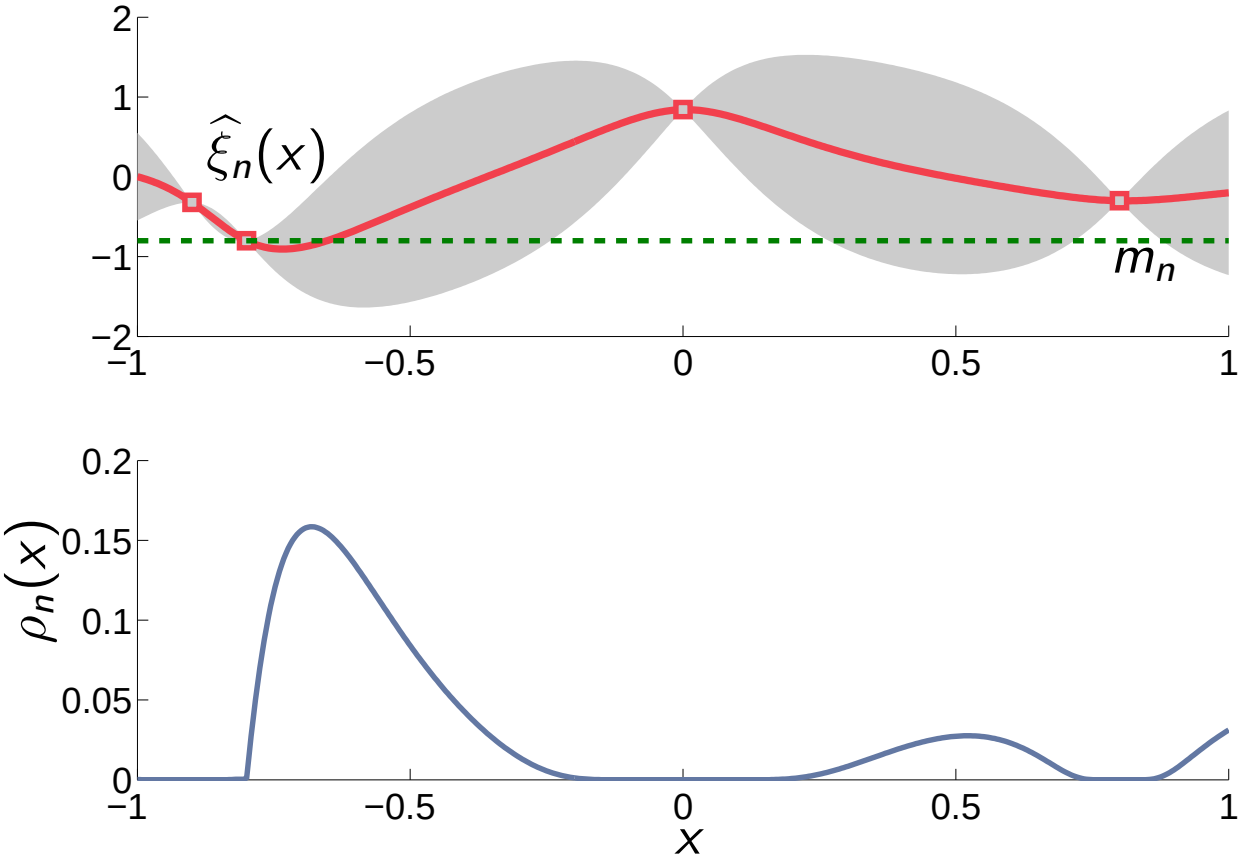
$$\begin{aligned}\rho_n(x) &= E(I_n \mid \xi(X_1), \ldots, \xi(X_n)) \\ &= \int_{z=-\inf}^{m_n} (m_n - z)\, p^{\xi(x)|\xi(X_1),\ldots,\xi(X_n)}(z)\, \mathrm{d}z \\ &= \gamma(m_n - \widehat{\xi}_n(x), \sigma_n^2(x))\end{aligned}$$

with

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

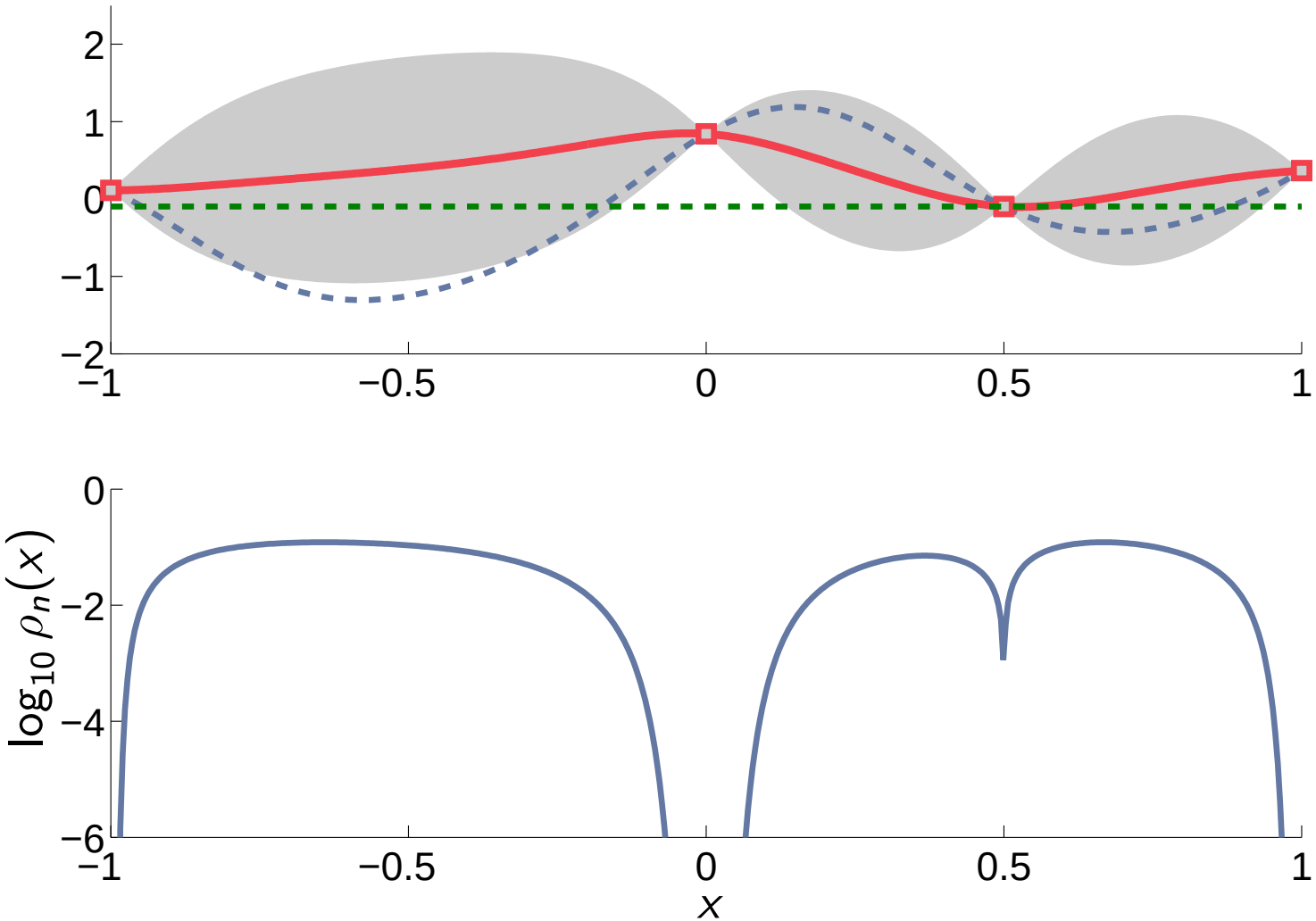
- ρ_n is called the expected improvement [Mockus 78, Schonlau et al. 96, Jones et al. 98]

Example of a quantity of interest: the improvement



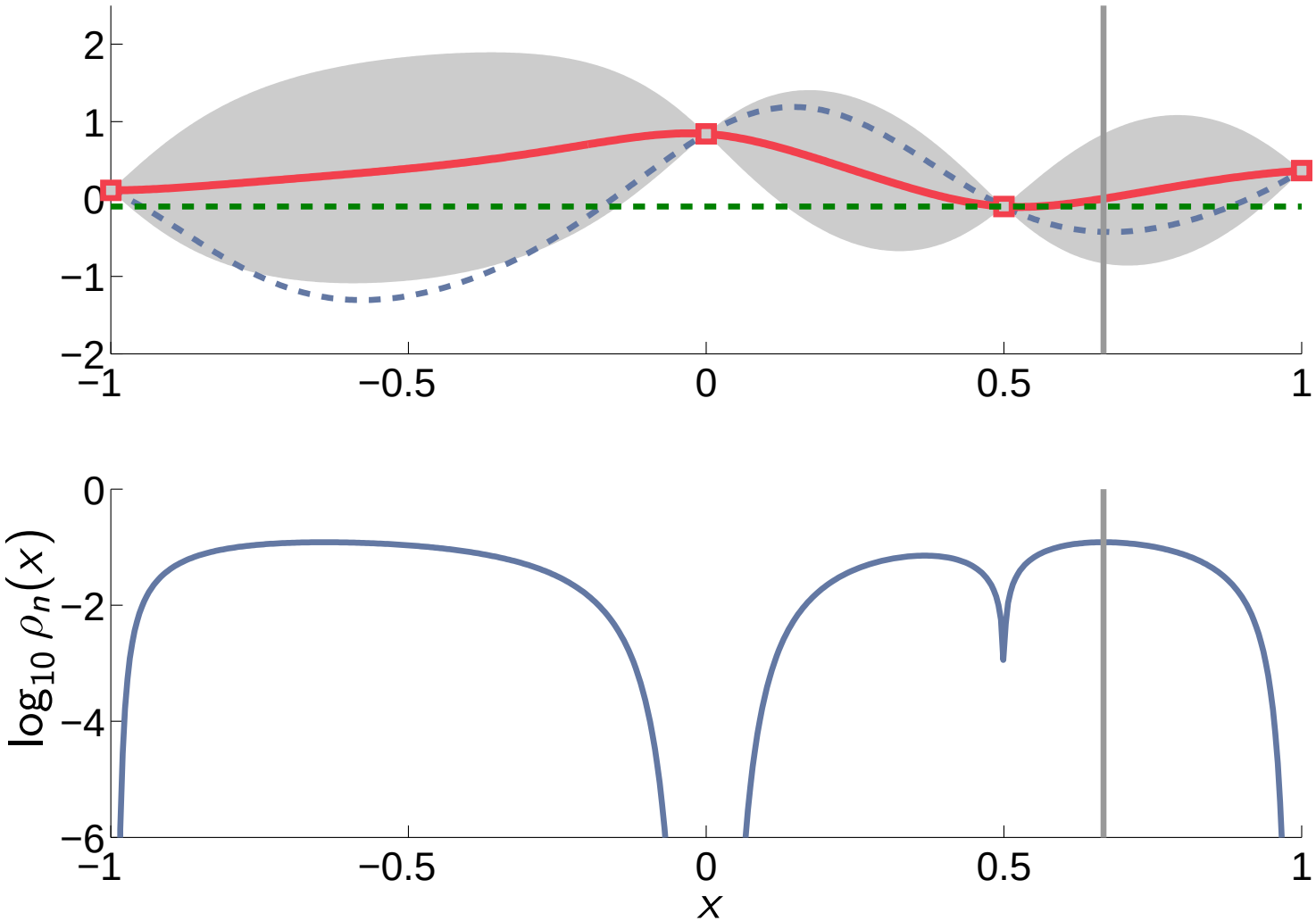
Insertion into an optimization algorithm

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



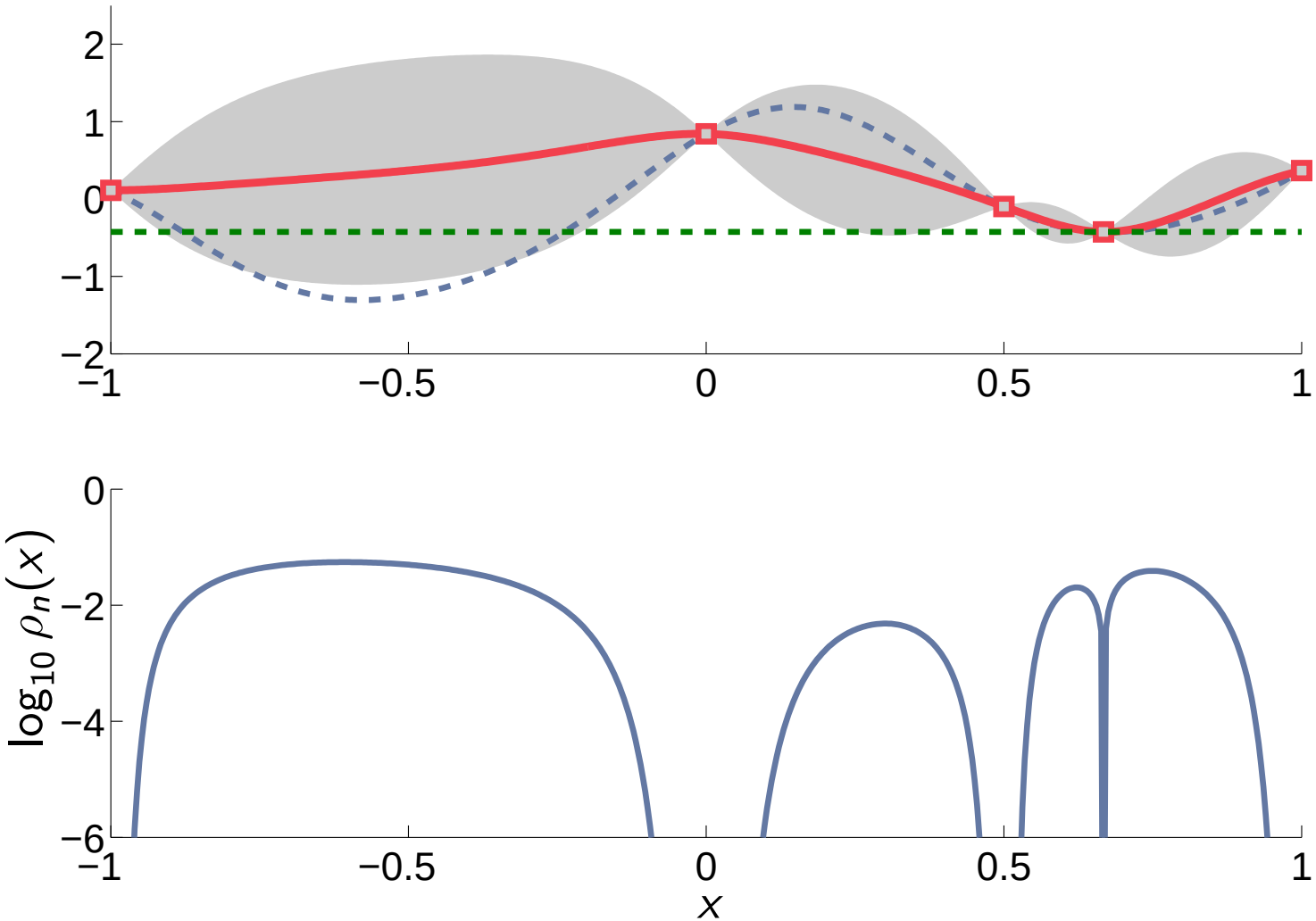
Insertion into an optimization algorithm

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



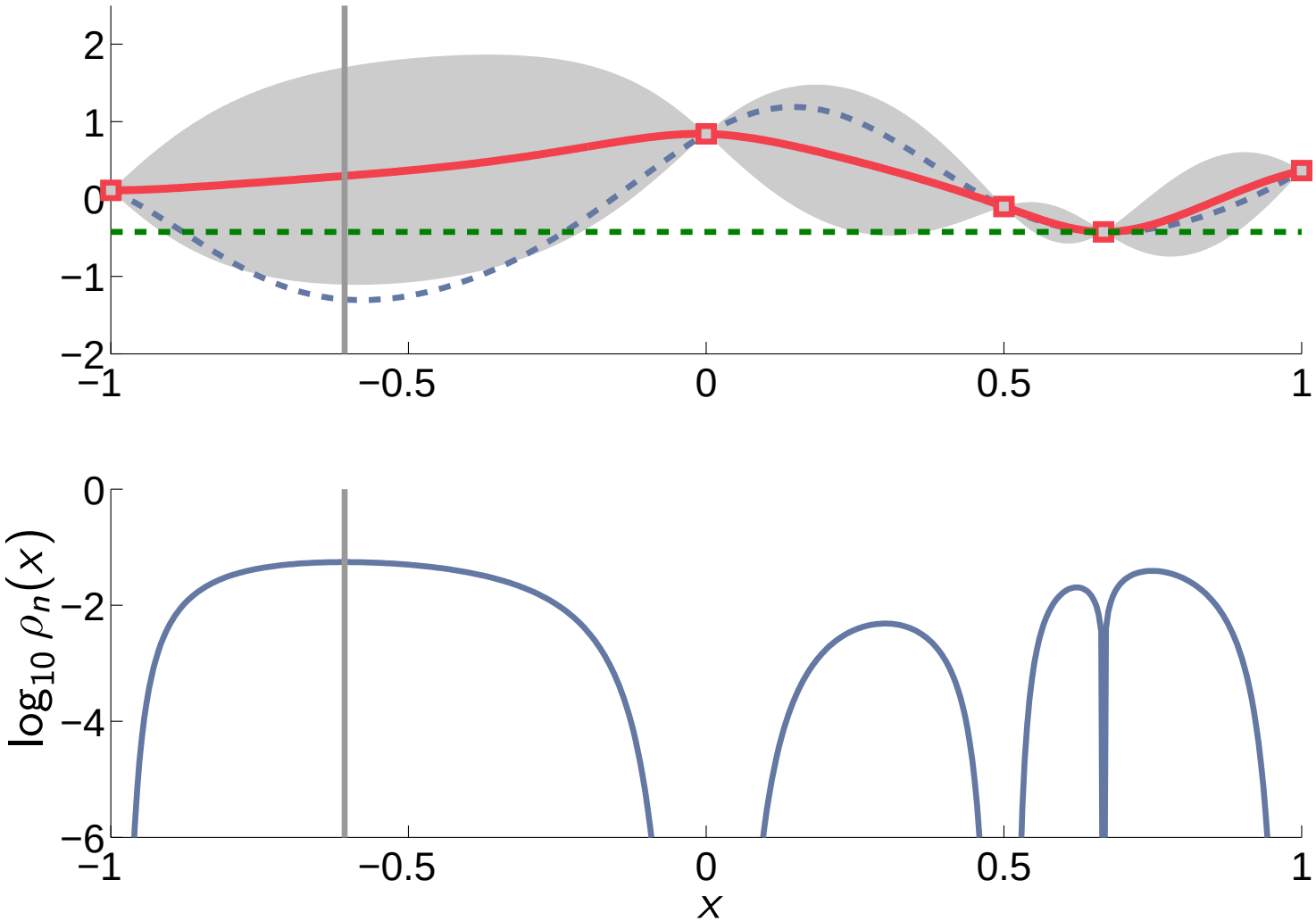
Insertion into an optimization algorithm

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



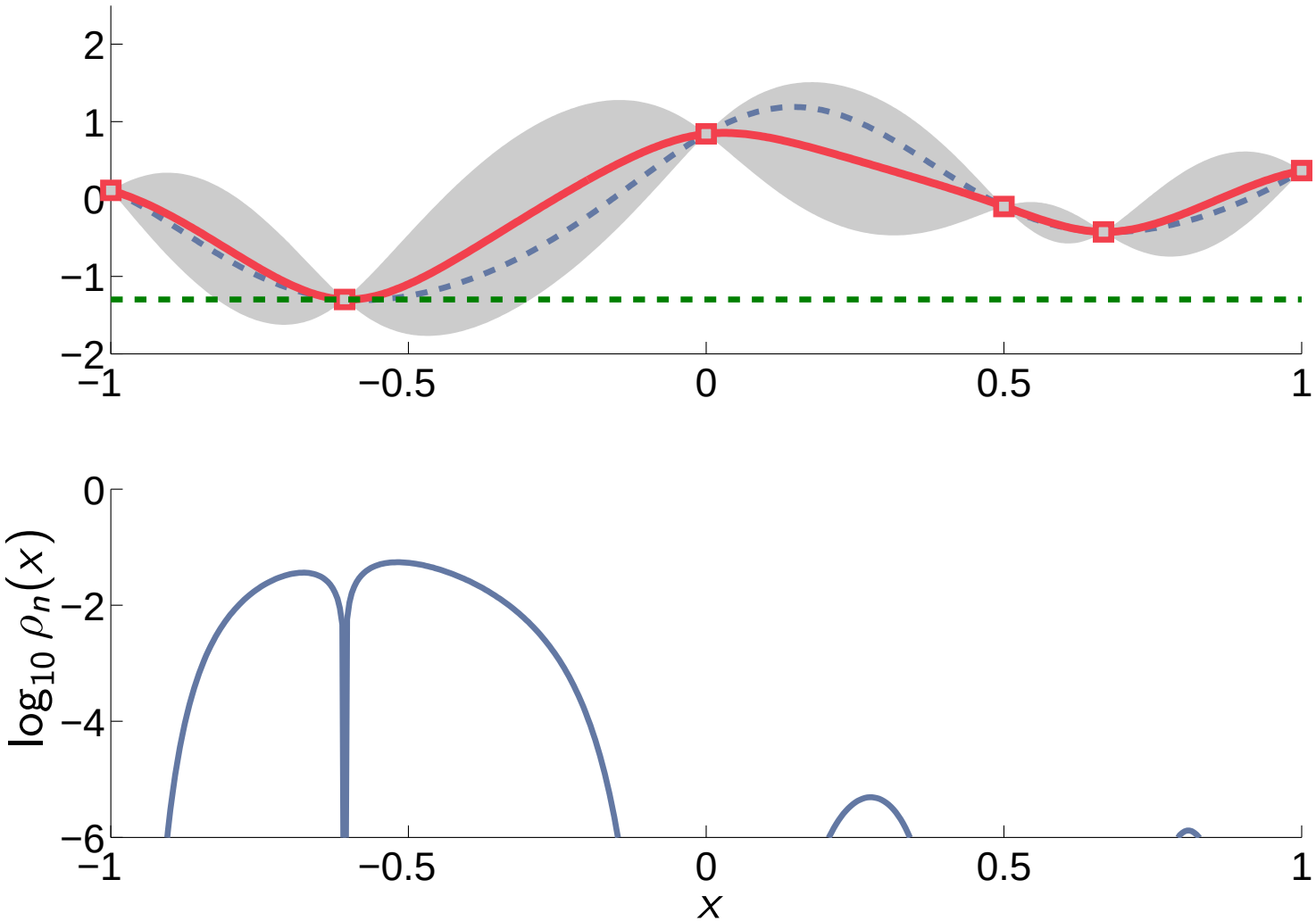
Insertion into an optimization algorithm

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



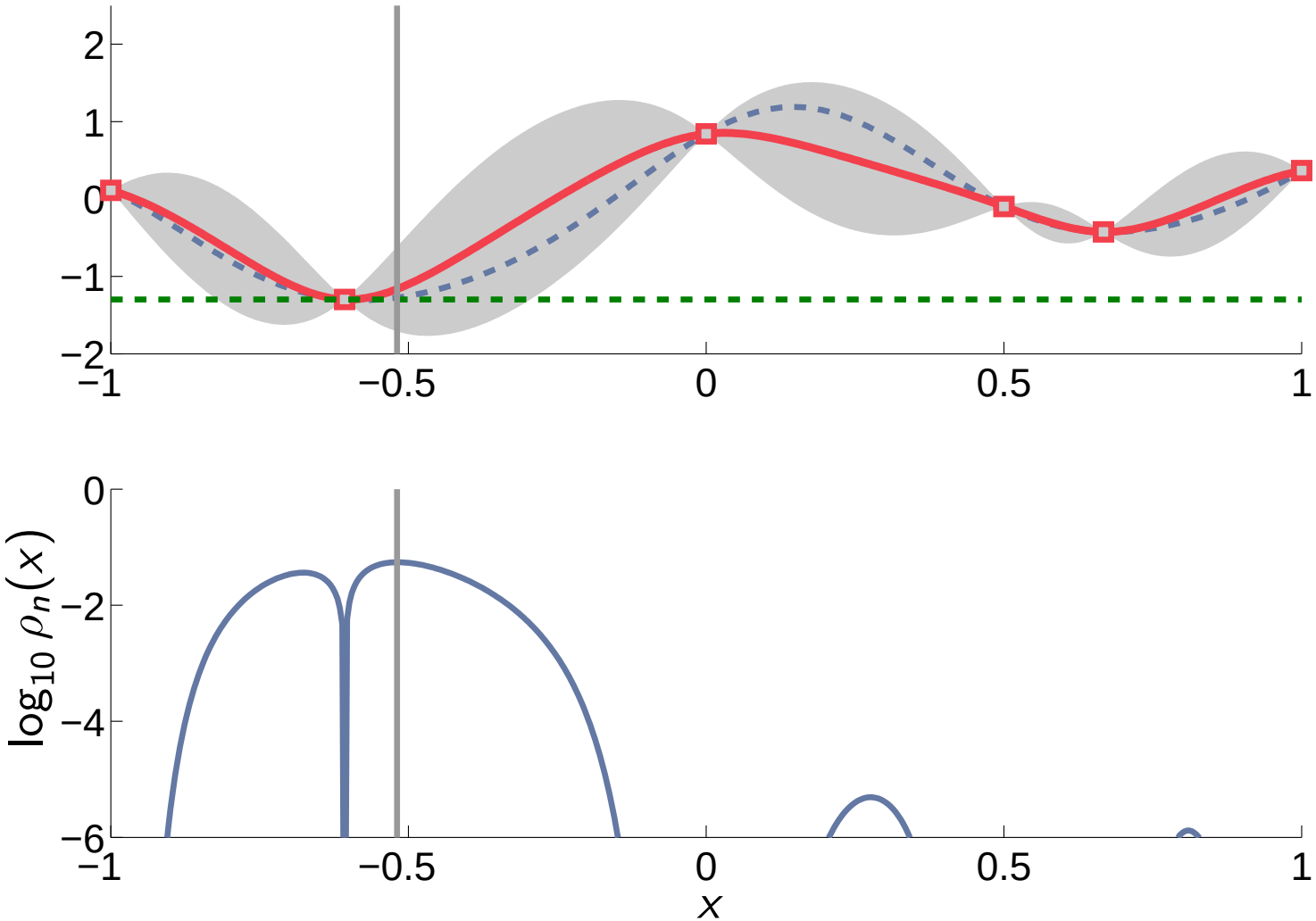
Insertion into an optimization algorithm

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



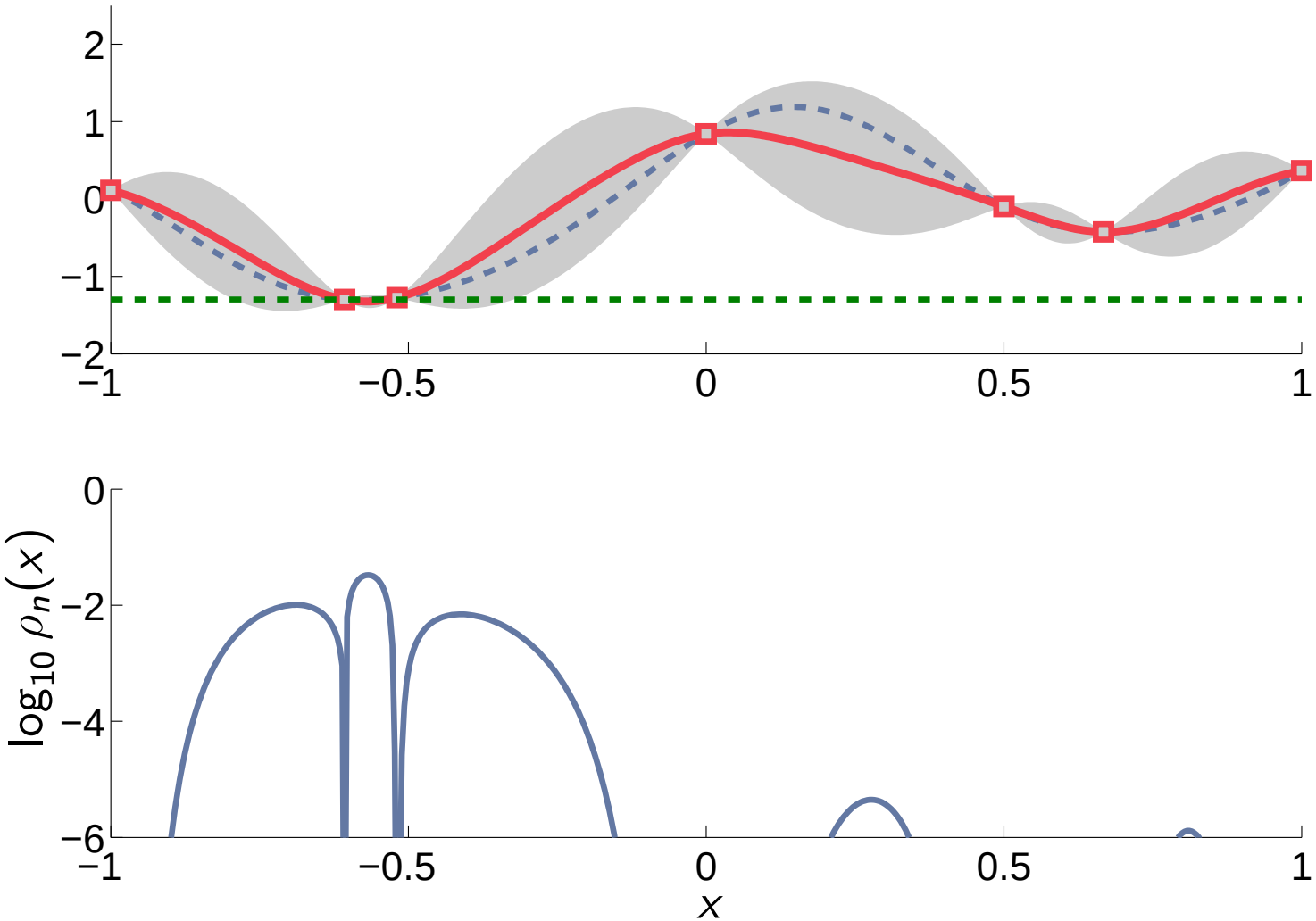
Insertion into an optimization algorithm

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



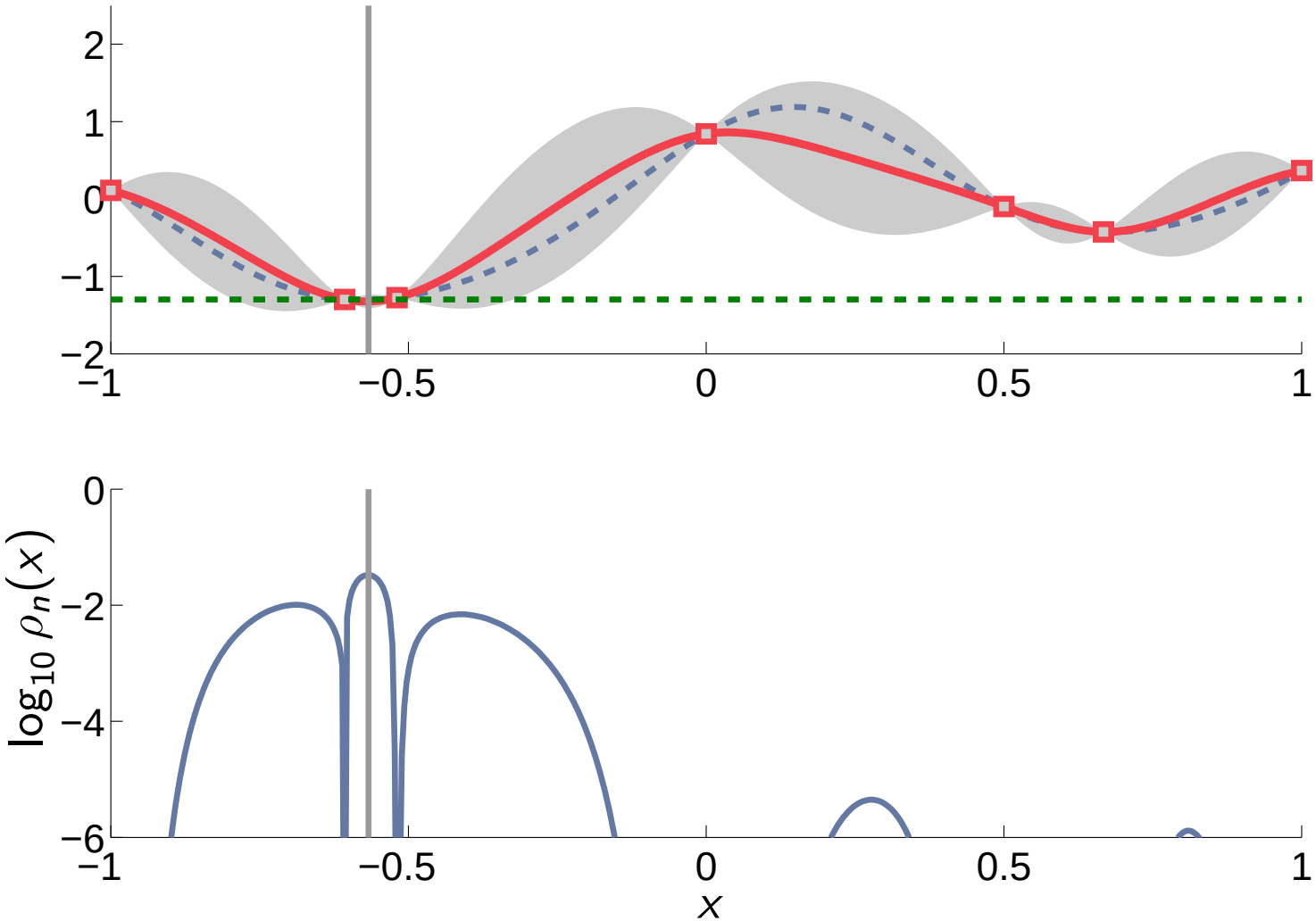
Insertion into an optimization algorithm

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



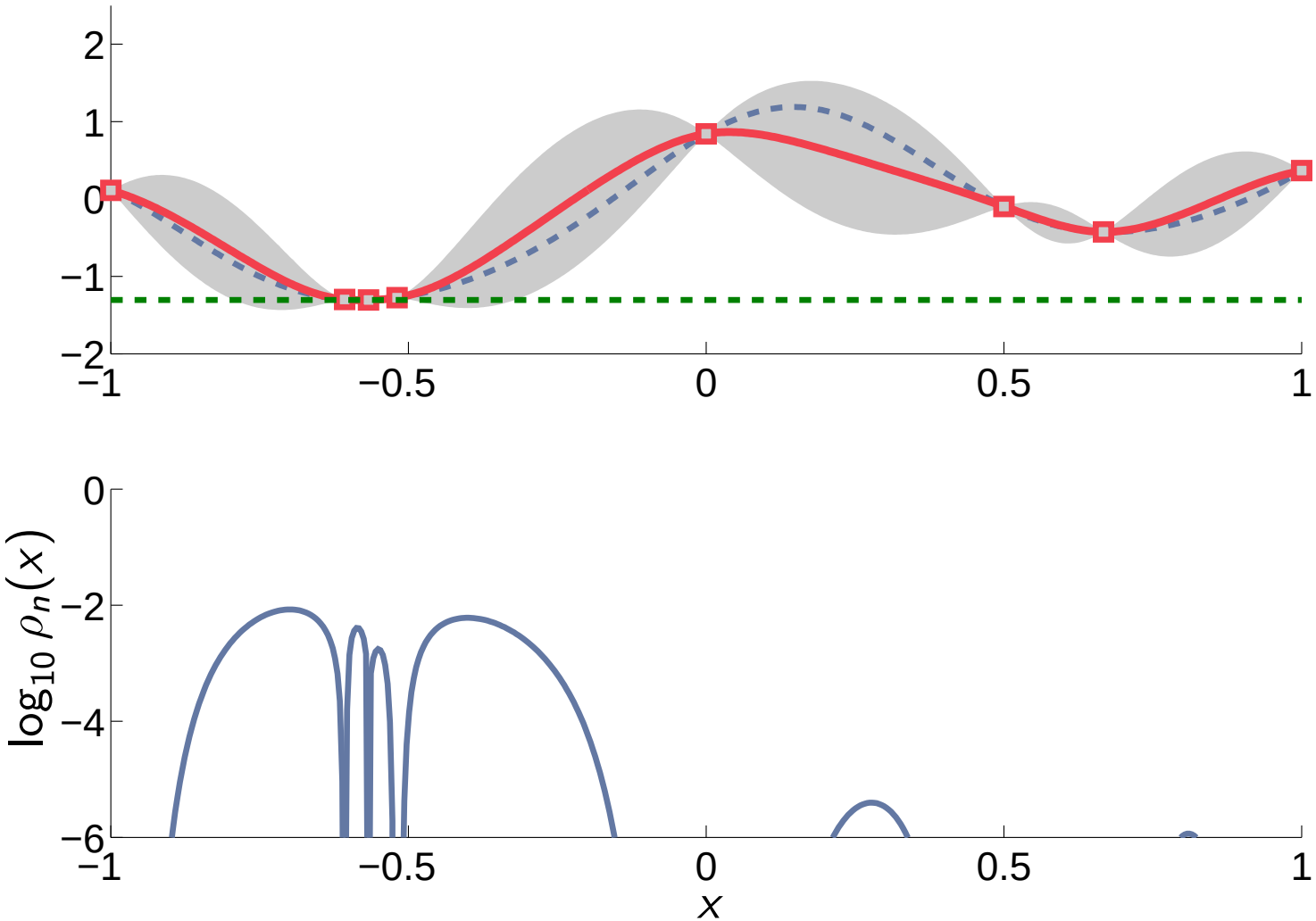
Insertion into an optimization algorithm

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



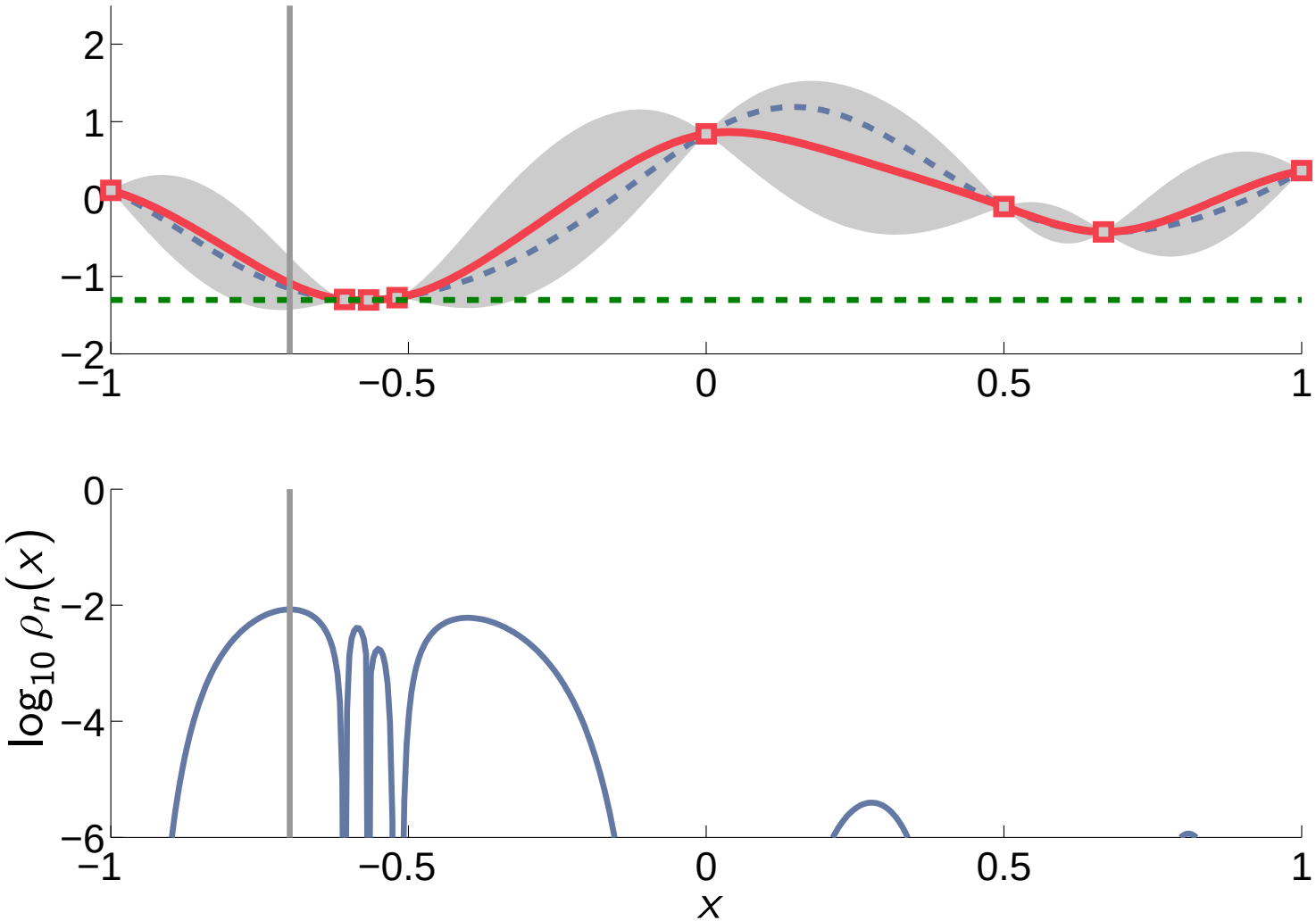
Insertion into an optimization algorithm

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



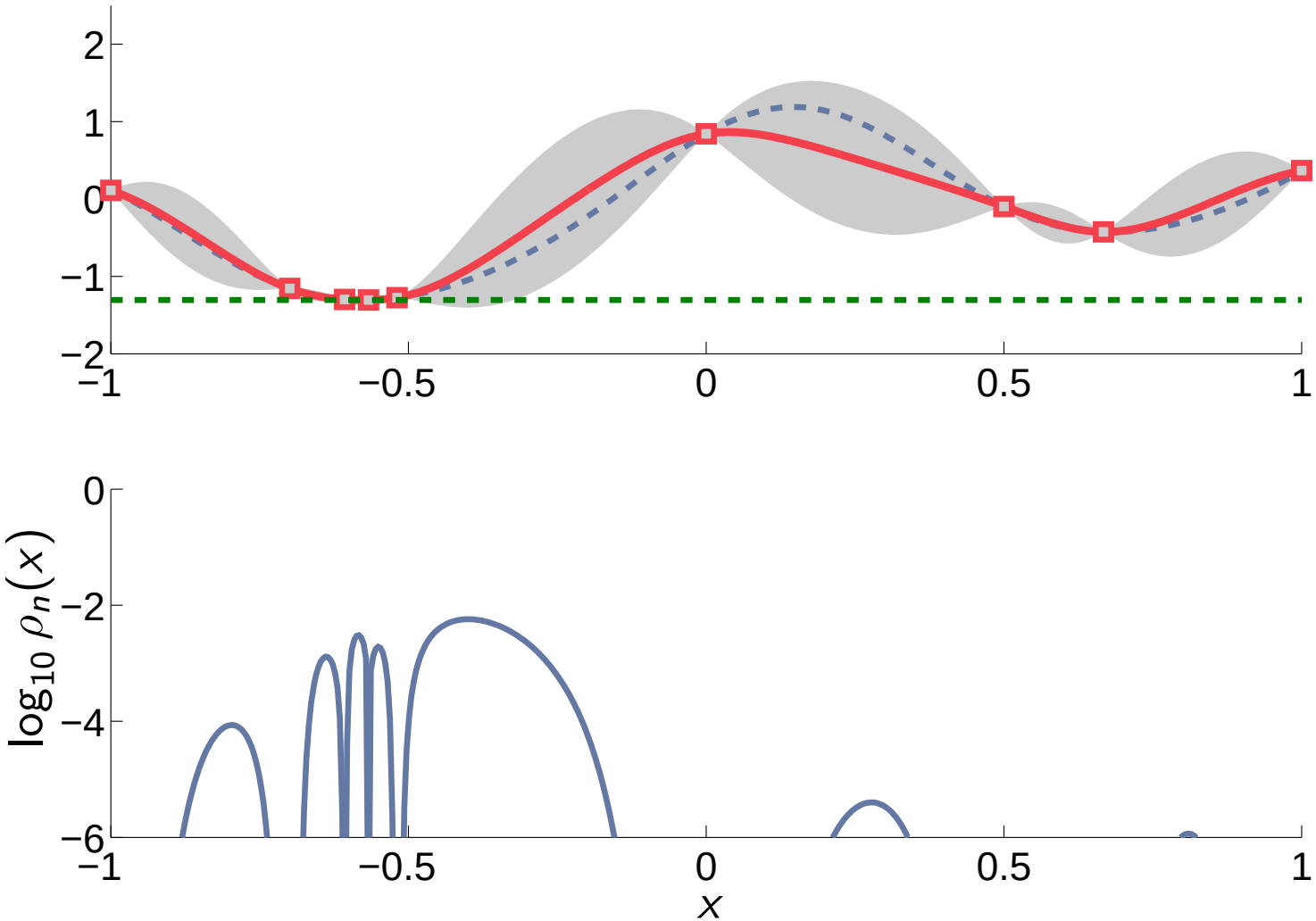
Insertion into an optimization algorithm

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



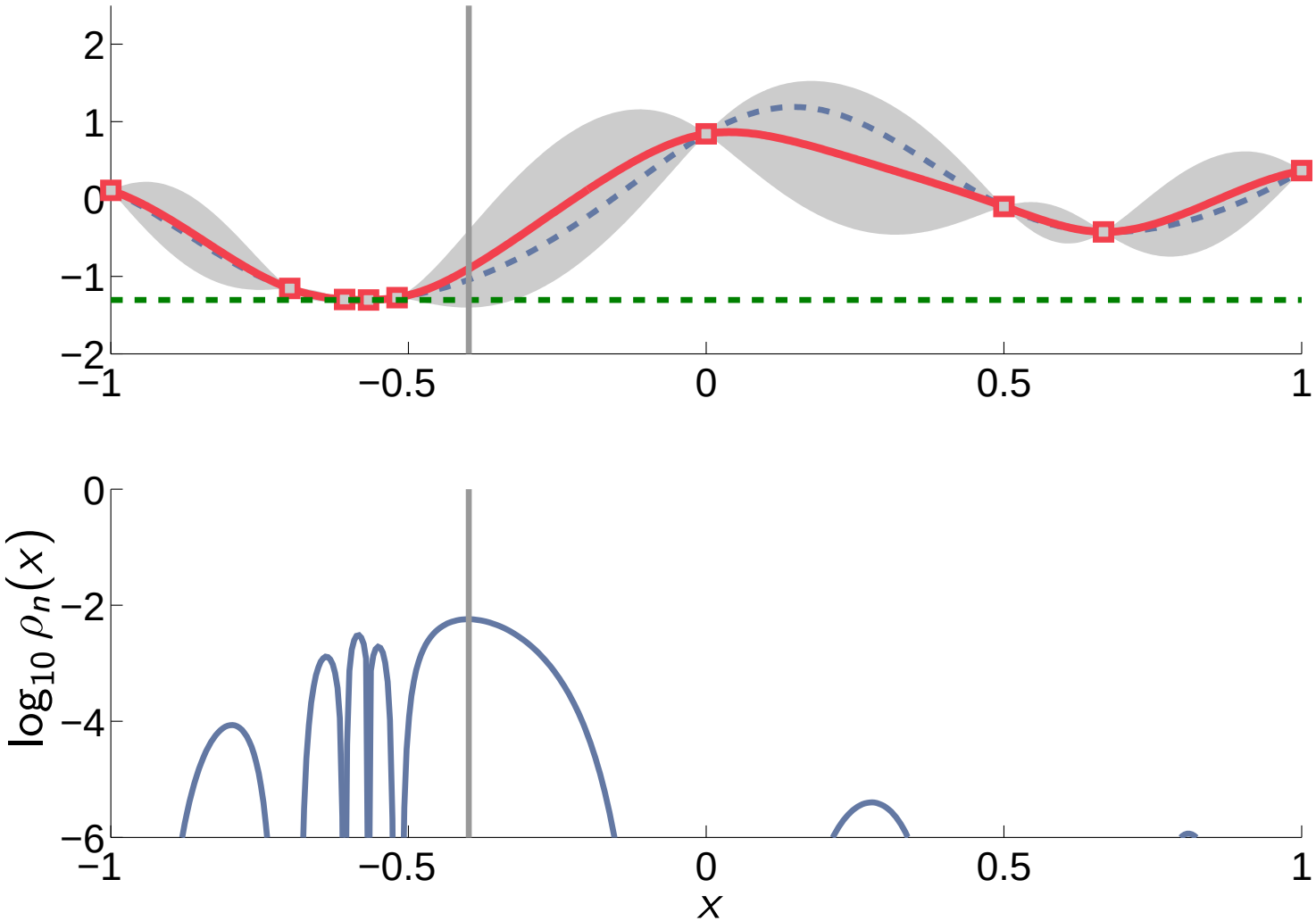
Insertion into an optimization algorithm

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



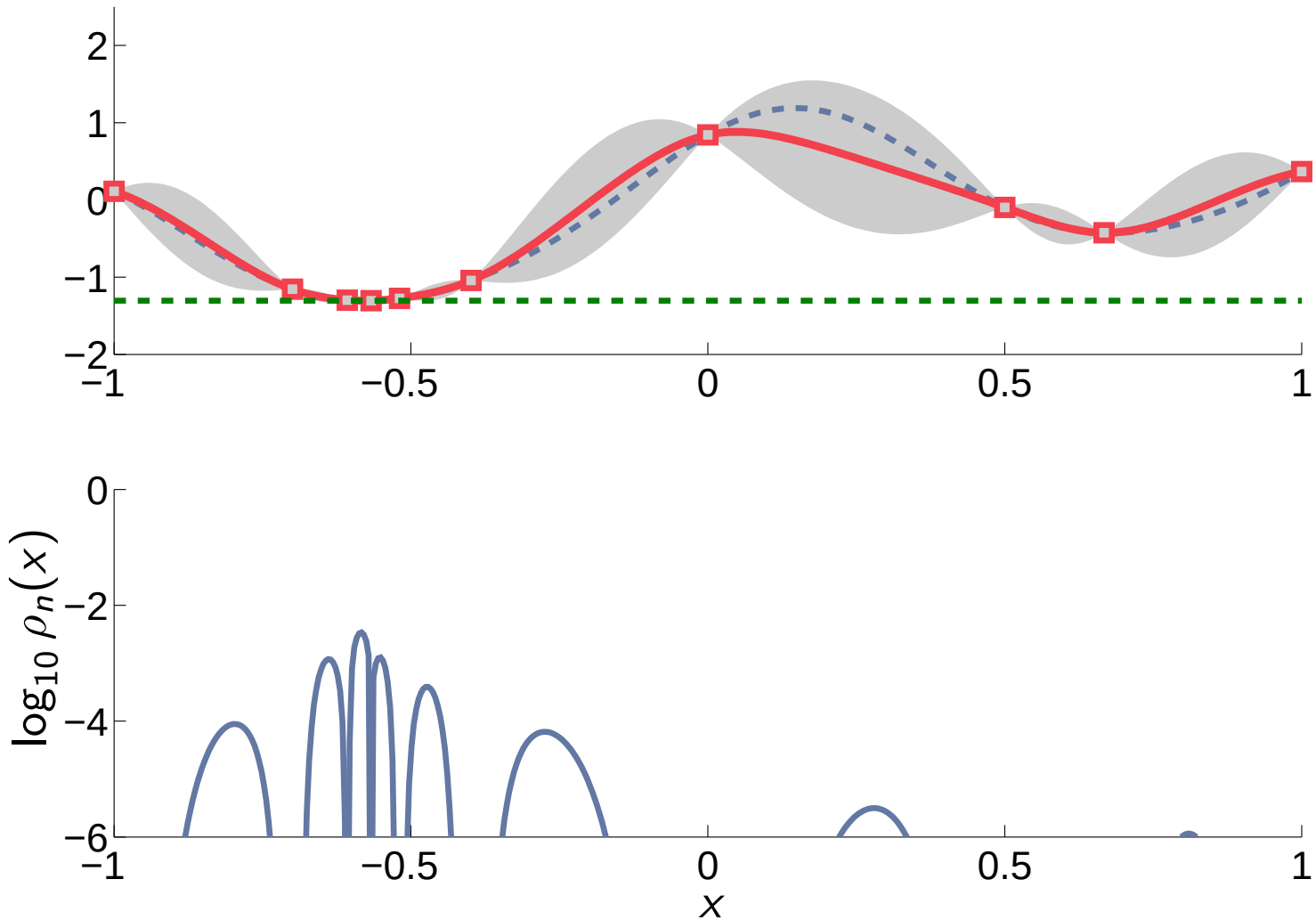
Insertion into an optimization algorithm

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



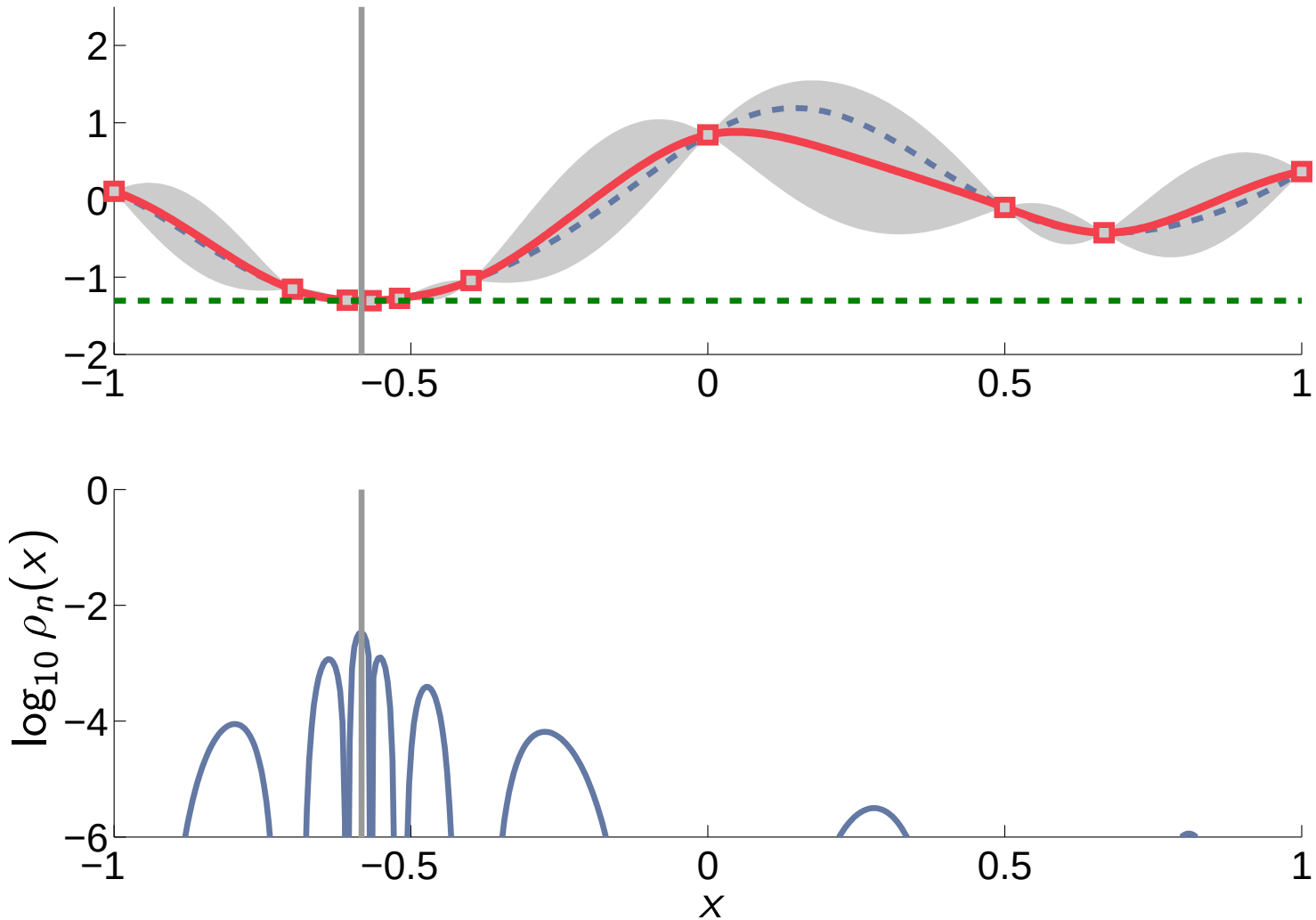
Insertion into an optimization algorithm

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



Insertion into an optimization algorithm

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



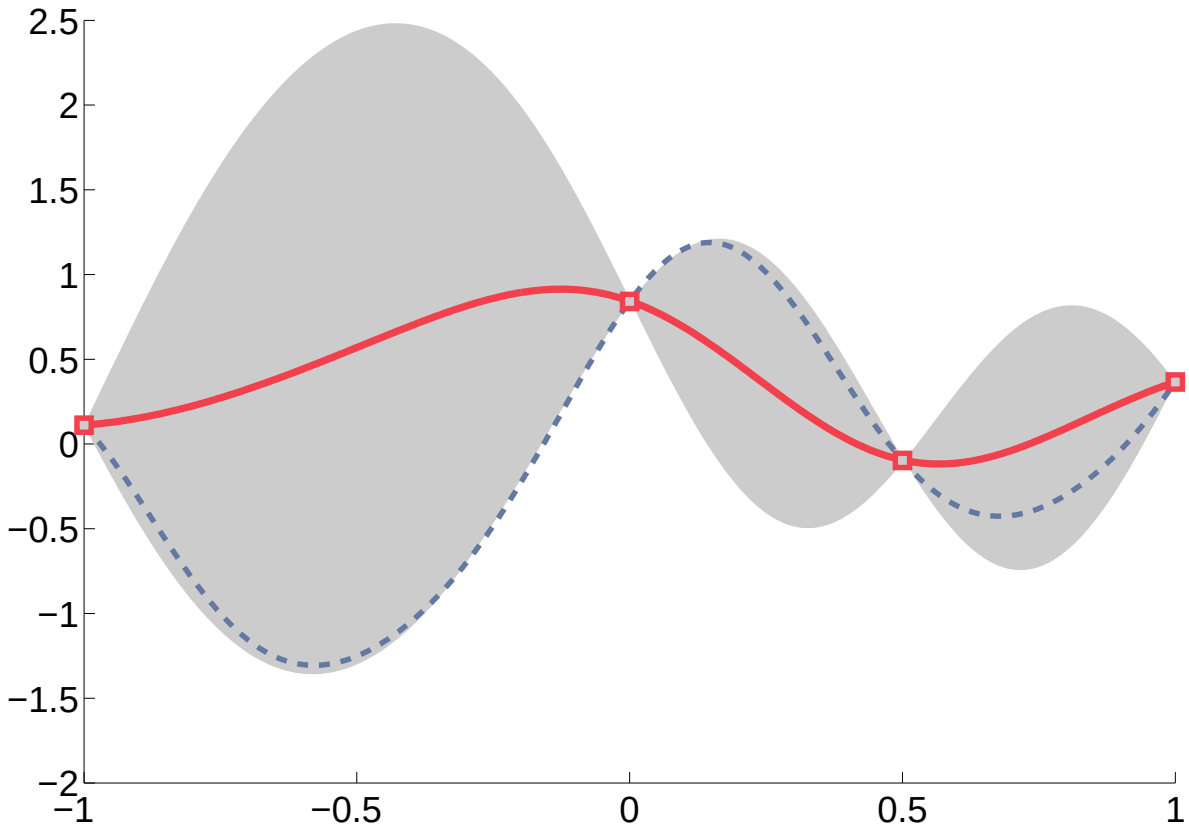
Example of quantity of interest: the minimizer

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

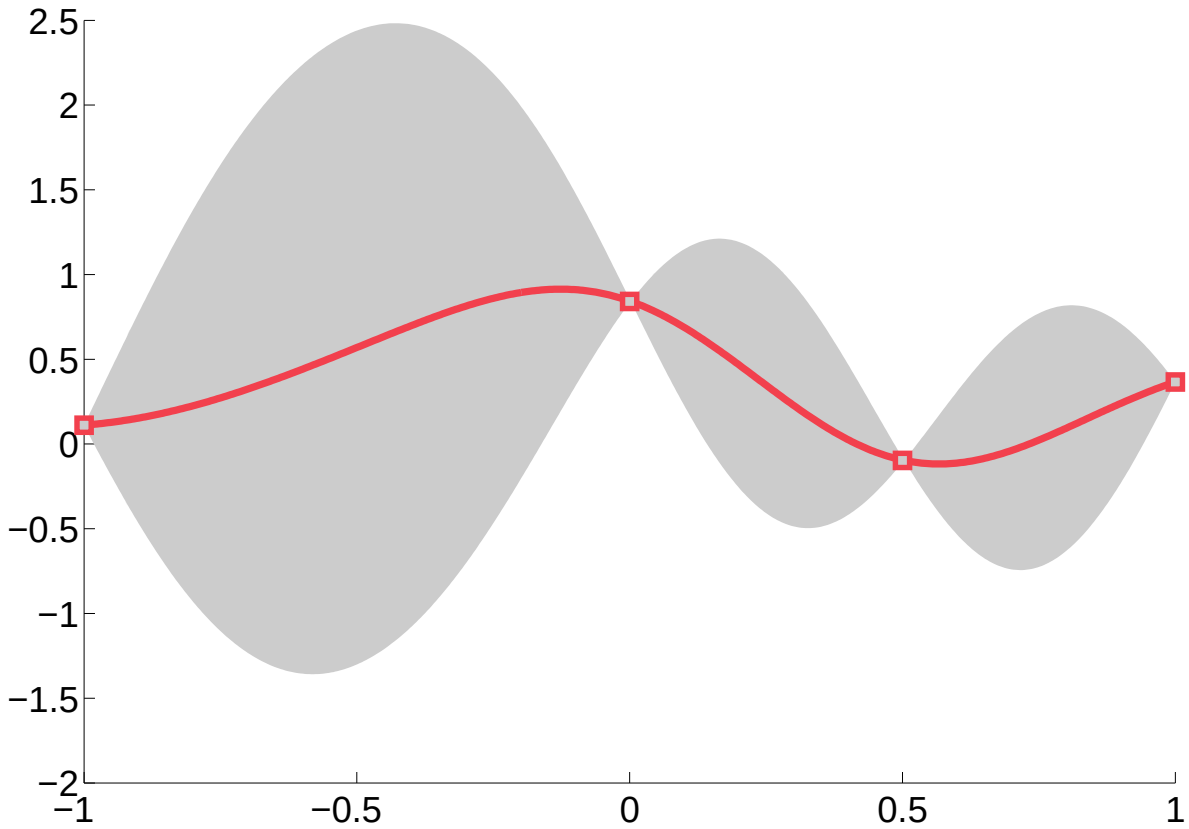
$$x^\star = \text{argmin}_x \, f(x)$$

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

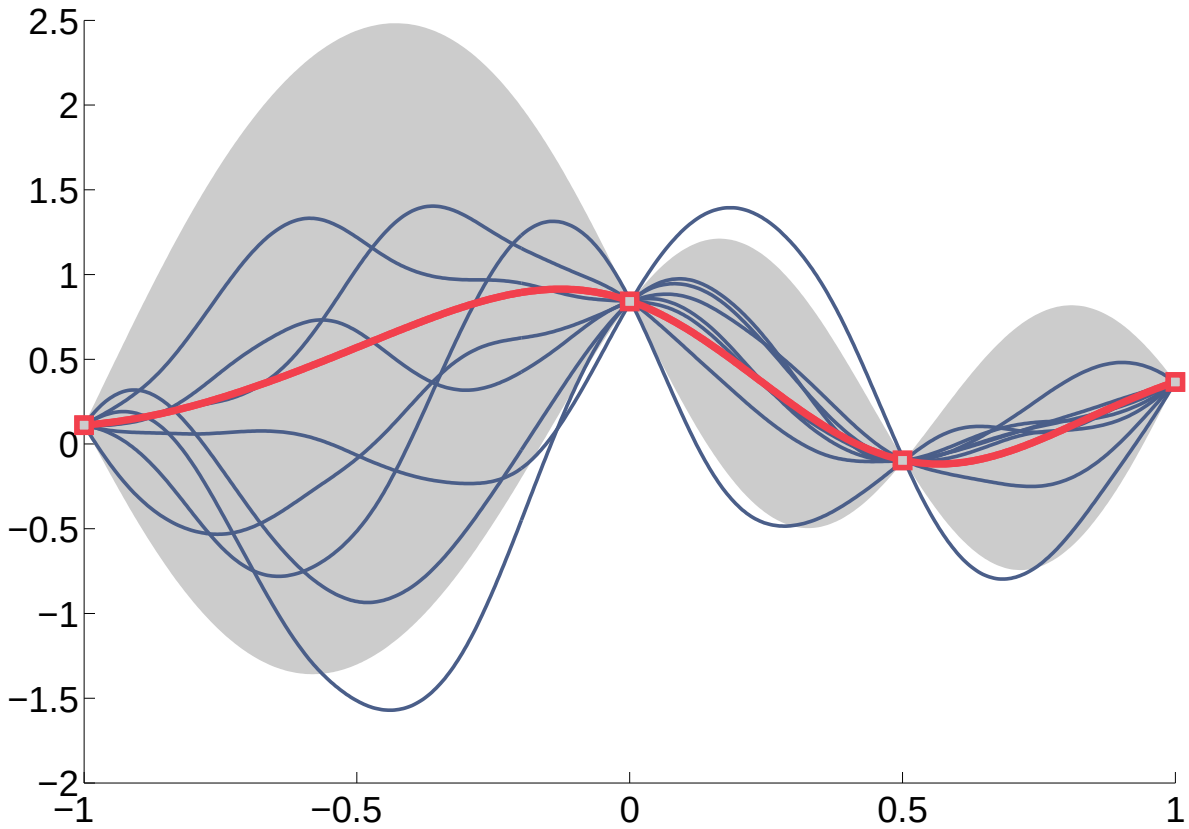
Empirical posterior density of the minimizer



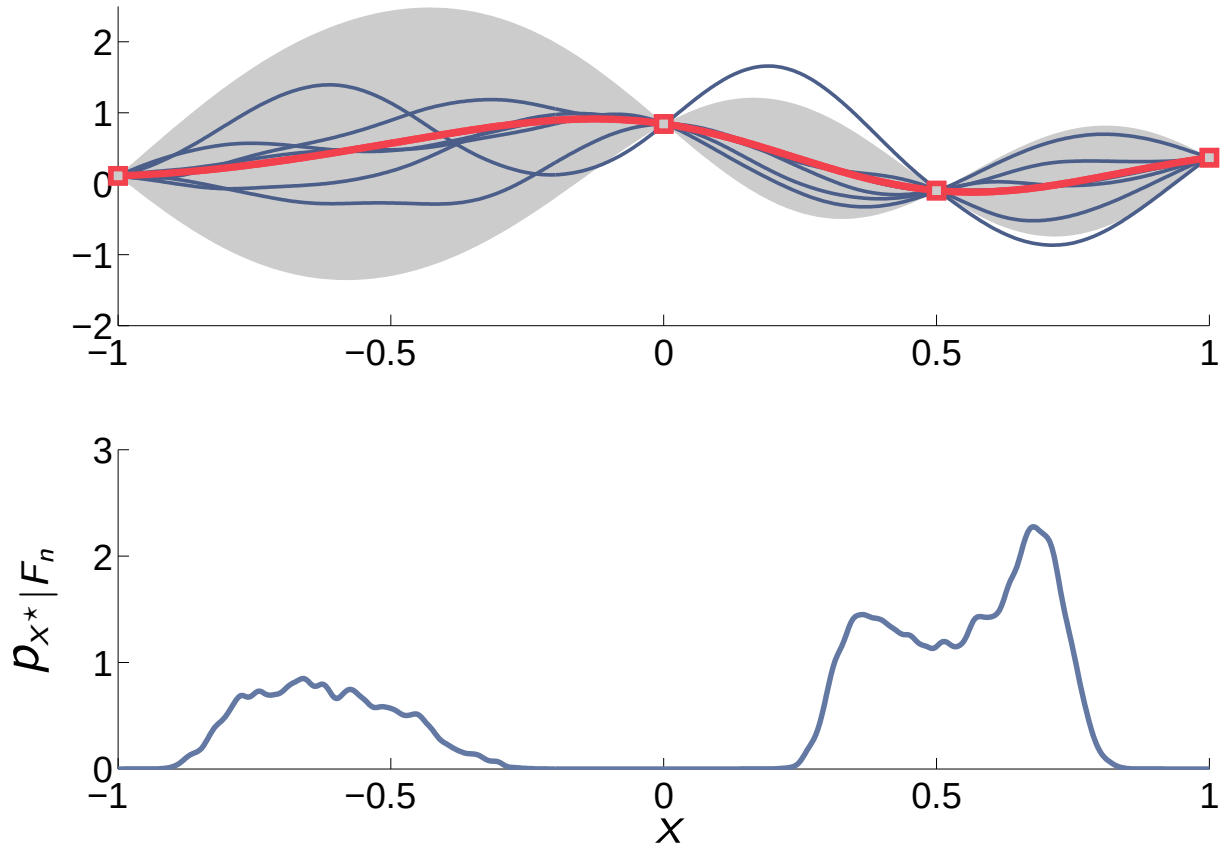
Empirical posterior density of the minimizer



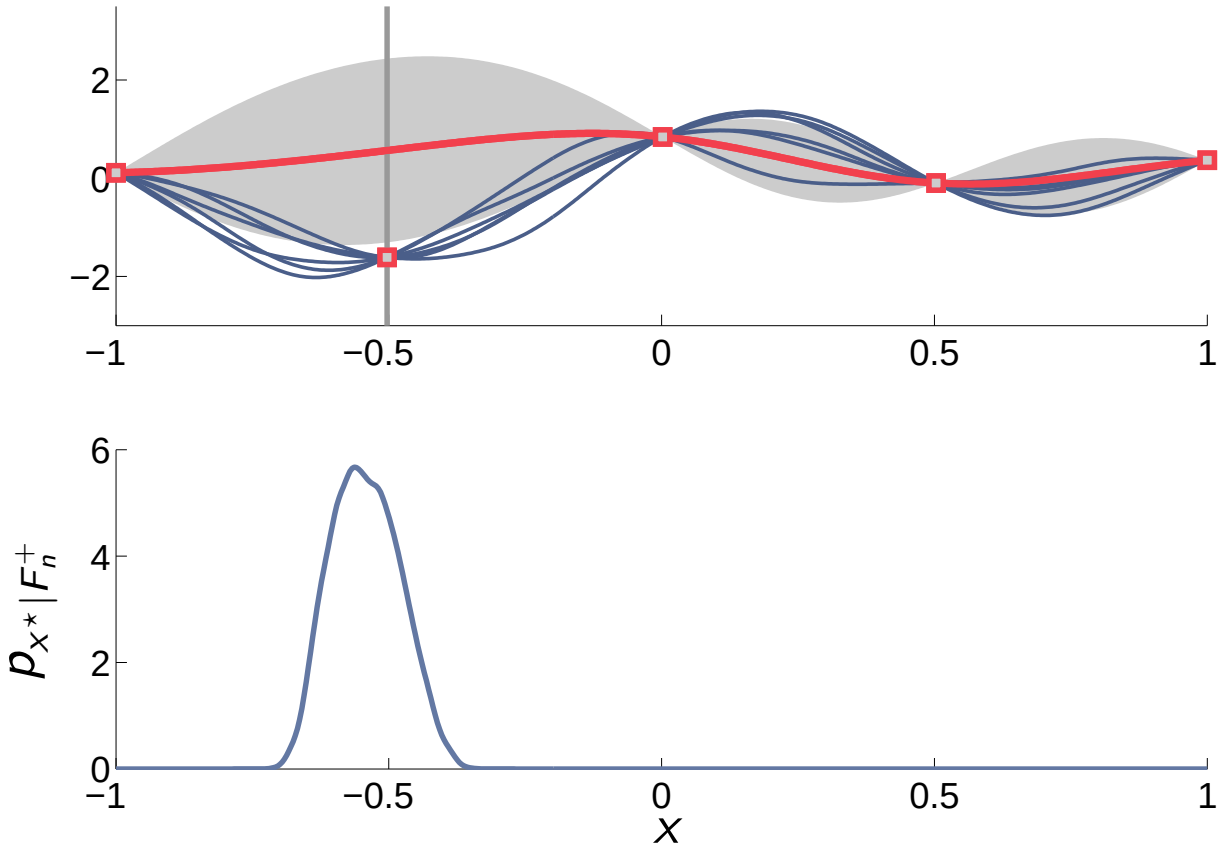
Empirical posterior density of the minimizer



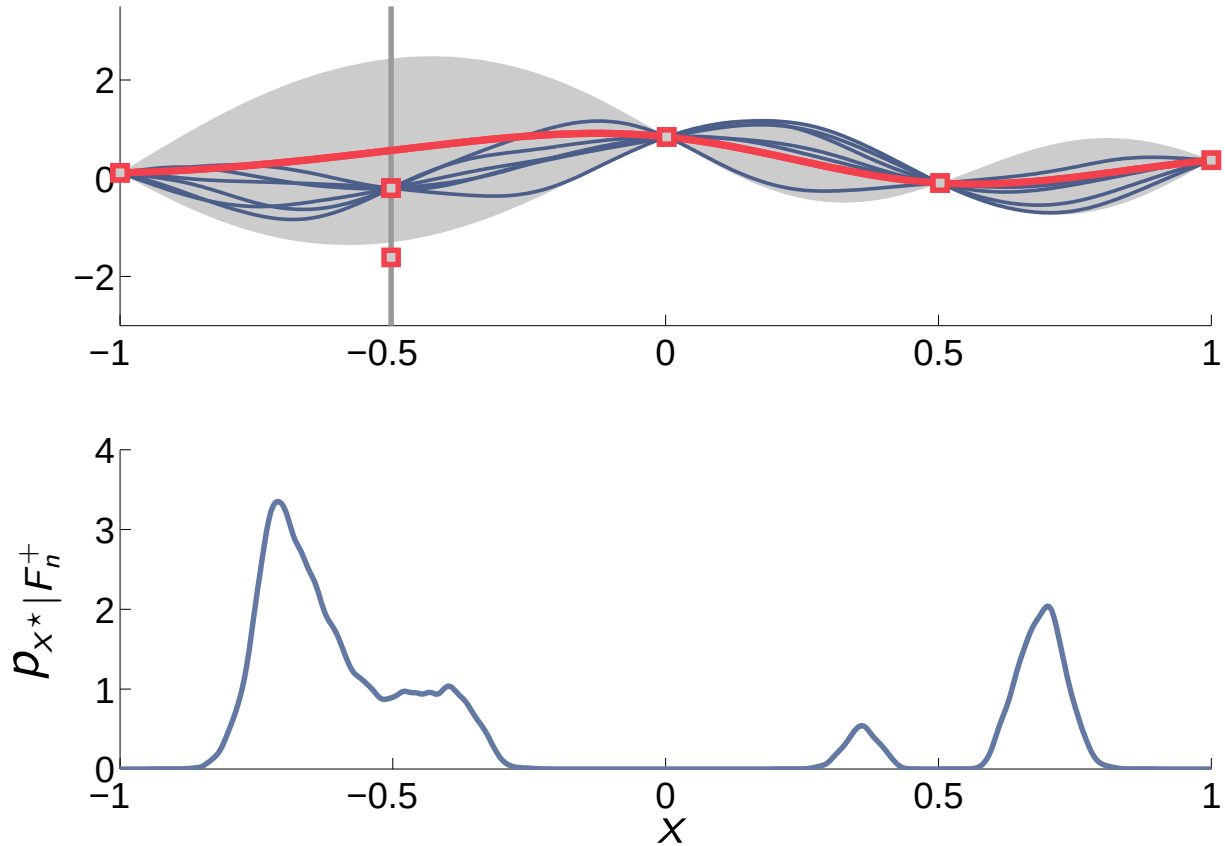
Empirical posterior density of the minimizer



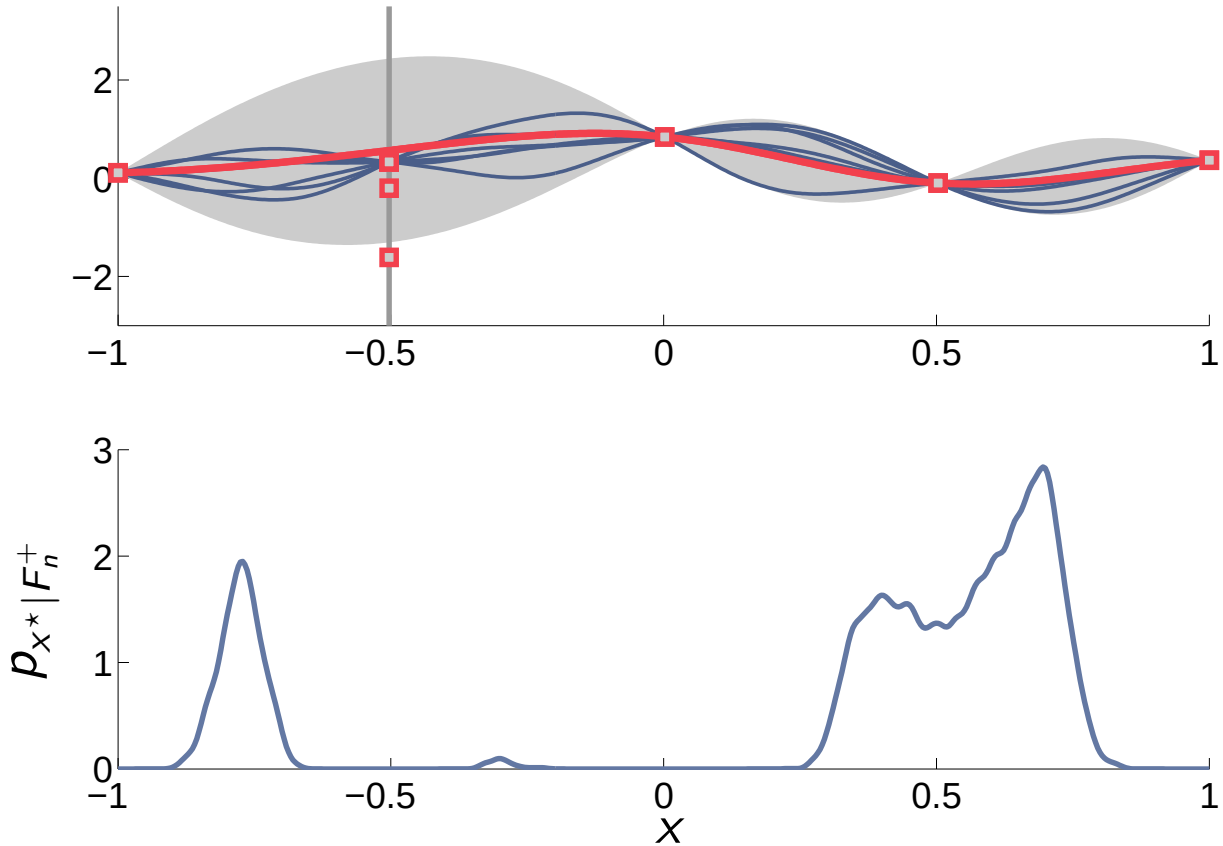
Empirical posterior density of the minimizer



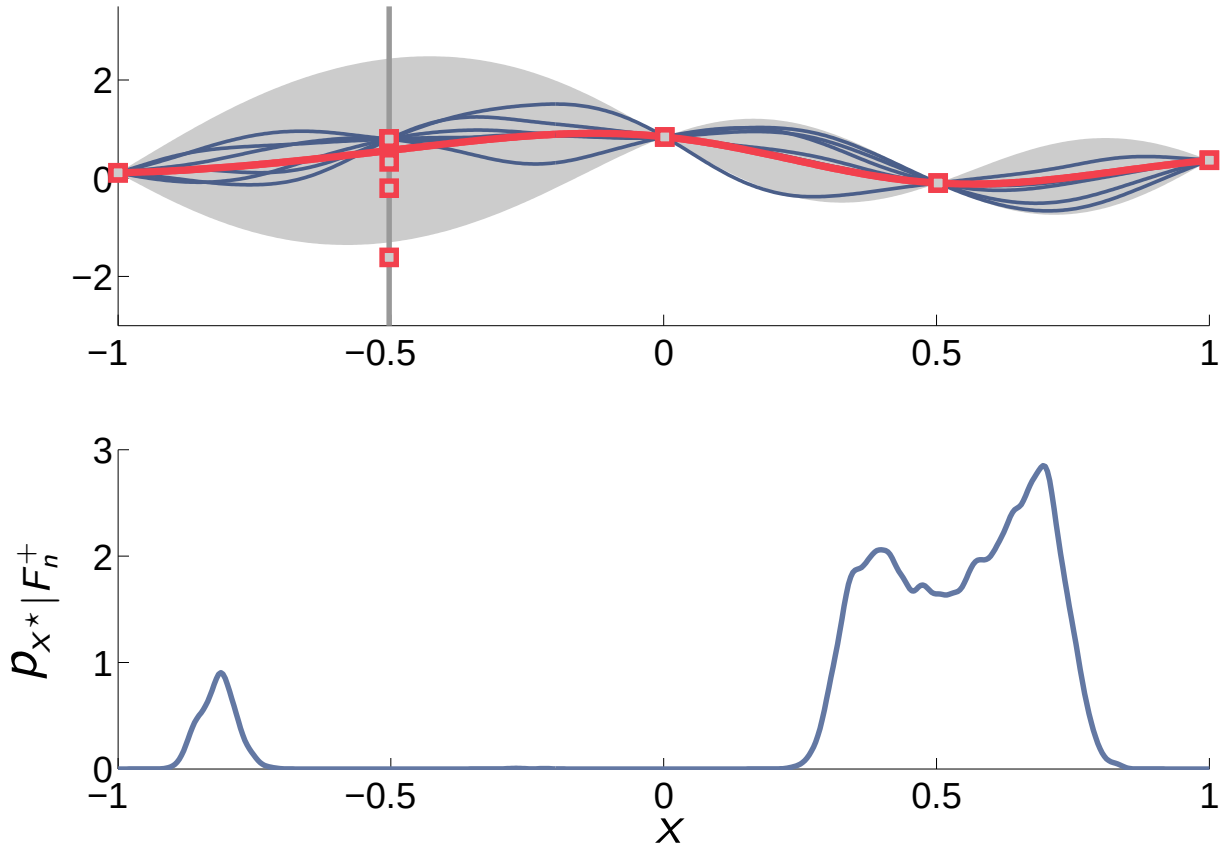
Empirical posterior density of the minimizer



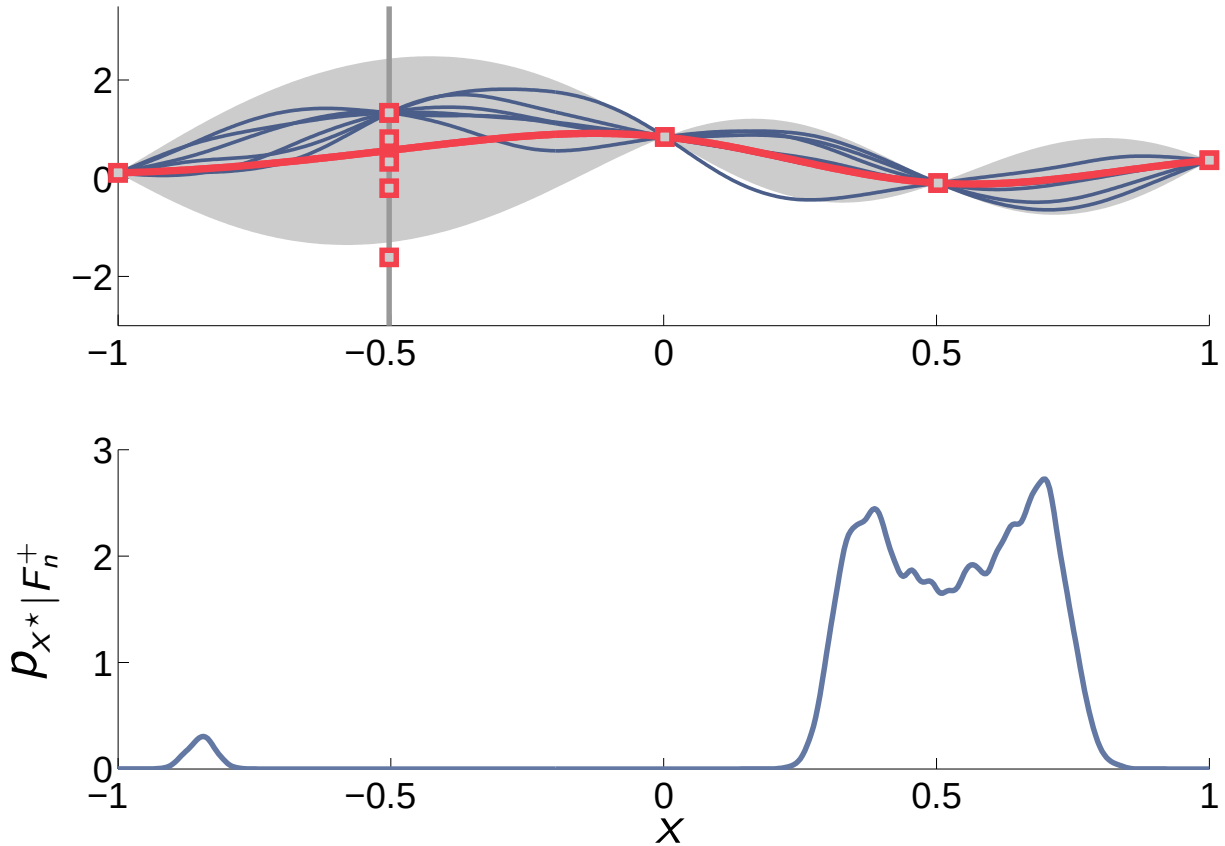
Empirical posterior density of the minimizer



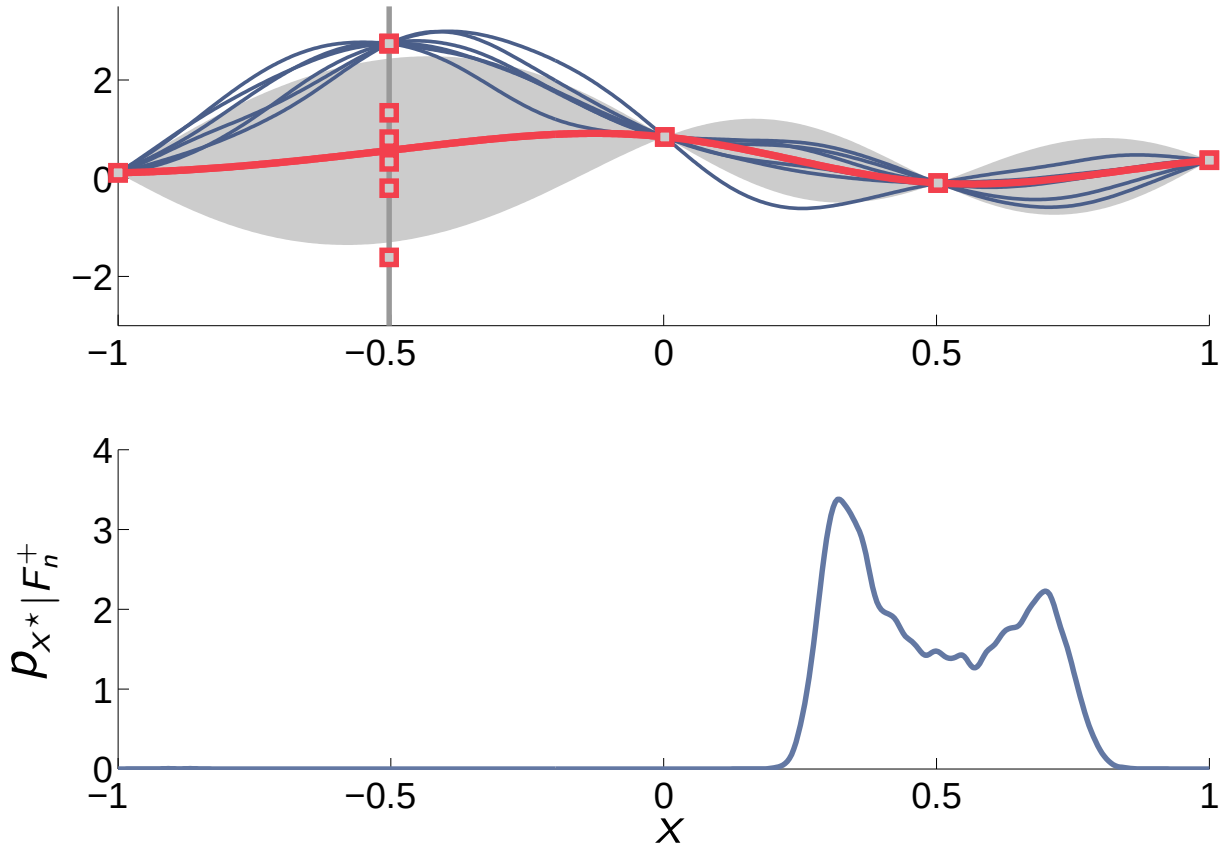
Empirical posterior density of the minimizer



Empirical posterior density of the minimizer



Empirical posterior density of the minimizer



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

$$\lim_{x \to x_0} \mathrm{E}\left[(\xi(x) - \xi(x_0))^2\right] = 0$$

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

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

Prop.

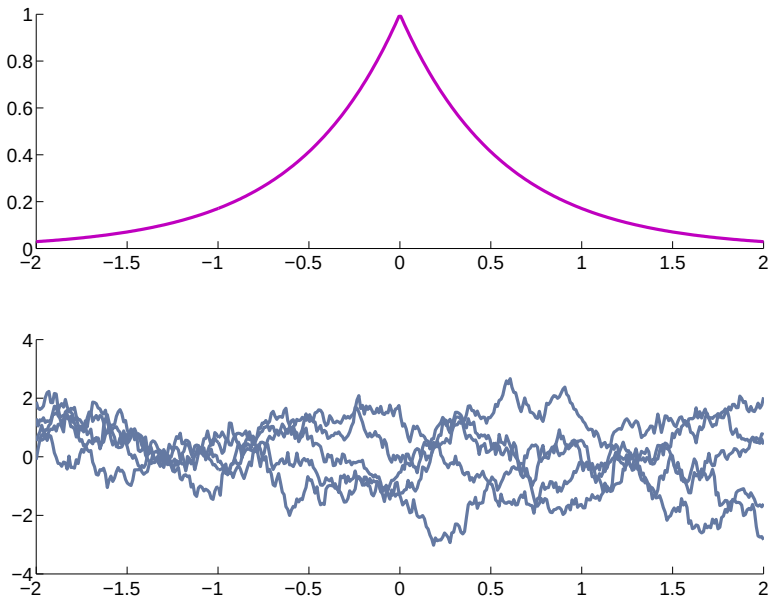
Let ξ be a second-order random process with differentiable mean function and stationary covariance function k. ξ is differentiable in mean-square iff k is two-time differentiable at zero.

Regularity properties of a random process

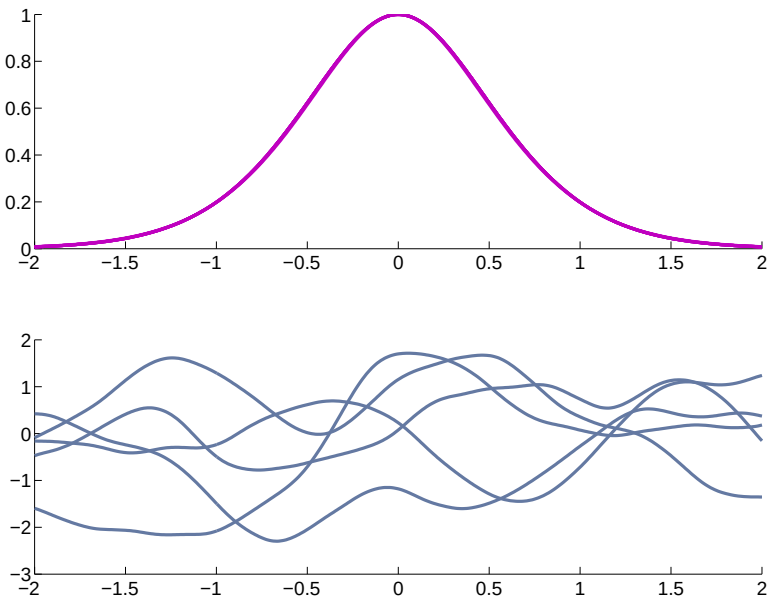
- Differentiability of the covariance function at the origin $\rightarrow$ mean-square differentiability of ξ

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

  $\rightarrow$ 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

  $\rightarrow$ offers the possibility to adjust the regularity of ξ with a single parameter

- The Matérn function:

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

  with

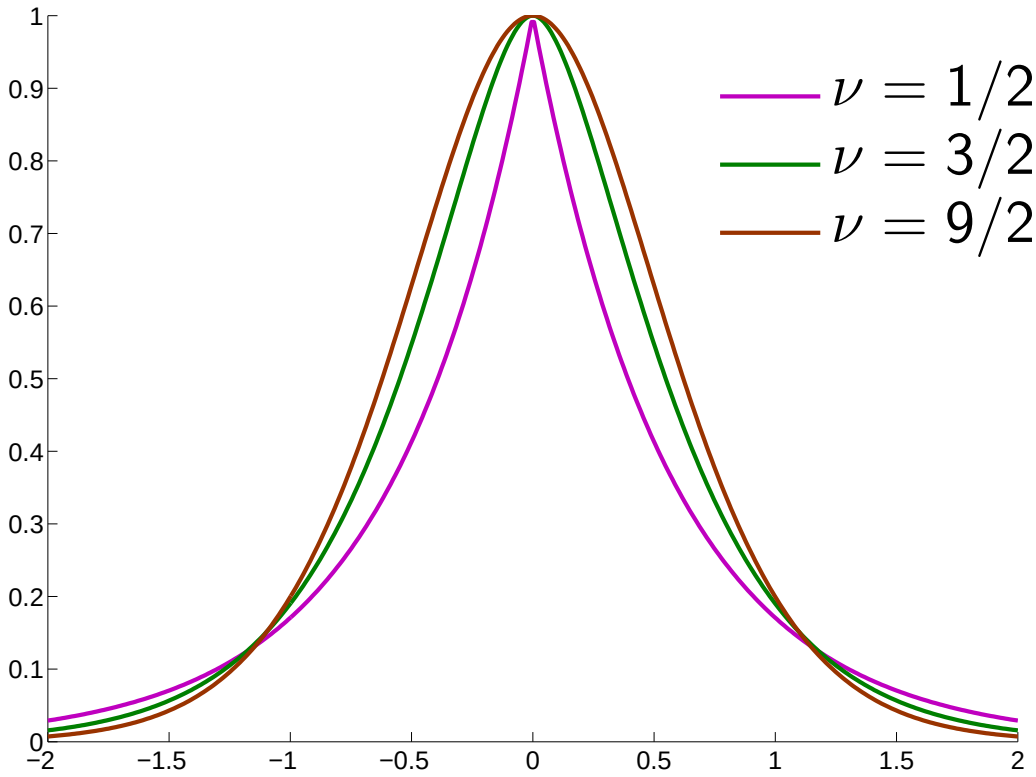
  - Γ the Gamma function
  - $\mathcal{K}_\nu$ the modified Bessel function of the second kind

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

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

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:

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

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

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

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

  $\rightarrow$ makes parameter estimation easier

Parameter estimation by maximum likelihood

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

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

  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

$$m(\cdot) = \beta^{\mathrm{t}} \varphi(\cdot)\,, \tag{5}$$

with

  - β a vector of unknown parameters
  - $\varphi = (\varphi_1, \ldots, \varphi_l)^{\mathrm{t}}$ 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

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

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

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

- 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 $\xi(x_1), \ldots, \xi(x_n)$ is the linear projection

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

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

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

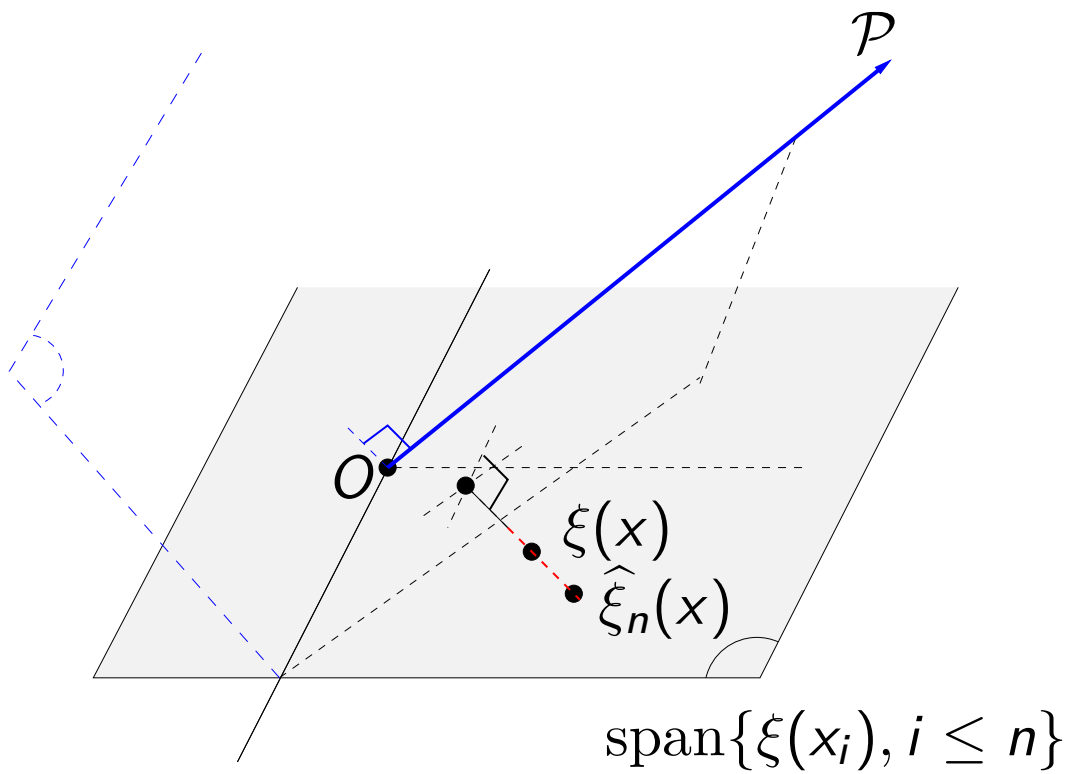
i.e.,

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

- 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

$\widehat{\xi}_n(x)$ is the linear projection of $\xi(x)$ onto $\mathrm{span}\{\xi(x_1), \ldots, \xi(x_n)\}$ 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

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

  with

  - $\underline{\varphi}$ an $l \times n$ matrix with entries $\varphi_i(x_j)$, $i = 1, \ldots, l$, $j = 1, \ldots, n$
  - 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

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

Prop.

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

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

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

$\rightarrow$ 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 $\rightarrow$ 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, $i = 1, \ldots, n$
- 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 $\{x_1, \ldots, x_n\}$.

Parameter estimation with unknown mean function

- Since the dimension of $\mathcal{P}$ is l, the dimension of the space of the measures with support $\{x_1, \ldots, x_n\}$ 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 $Z = W^{\mathsf{T}} \underline{\xi}_n$ is a Gaussian random vector taking its values in $\mathbb{R}^{n-l}$, with zero mean and covariance matrix

$$W^{\mathsf{T}} K(\theta) W$$

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

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

REML

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

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

where $(Q_1 \mid Q_2)$ is an $n \times n$ orthogonal matrix and R is a $I \times I$ 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 $W^{\mathsf{T}} W = I_{n-I}$.

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

What is Bayesian optimization ?

- "wide sense" definition
  - optimization using tools from Bayesian UQ

What is Bayesian optimization ?

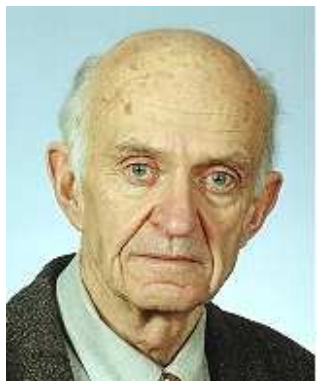
- "wide sense" definition
  - optimization using tools from Bayesian UQ
  - started with Harold Kushner's paper: *A New Method of Locating the Maximum Point of an Arbitrary Multipeak Curve in the Presence of Noise*, J. Basic Engineering, 1964.

What is Bayesian optimization ?

- a slightly more restrictive definition
  - sequential Bayesian decision theory applied to optimization

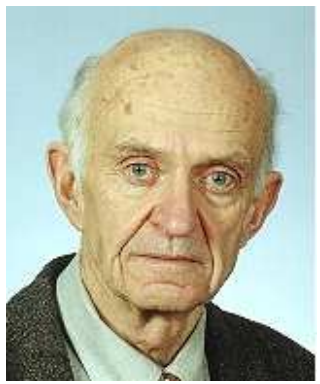
What is Bayesian optimization ?

- a slightly more restrictive definition
  - sequential Bayesian decision theory applied to optimization
  - started with the work of Jonas Mockus and Antanas Žilinskas in the 70's, e.g., *On a Bayes method for seeking an extremum*, Avtomatika i Vychislitel'naya Teknika, 1972 (in Russian)



What is Bayesian optimization ?

- a slightly more restrictive definition
  - sequential Bayesian decision theory applied to optimization
  - started with the work of Jonas Mockus and Antanas Žilinskas in the 70's, e.g., *On a Bayes method for seeking an extremum*, Avtomatika i Vychislitel'naya Teknika, 1972 (in Russian)



- 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

- Bayesian decision theory (BDT) in a nutshell
  - a mathematical framework for decisions under uncertainty
  - uncertainty is captured by probability distributions
  - the "Bayesian agent" aims at minimizing the expected loss

Decision-theoretic framework (cont'd)

- How does this relate to optimization ?

Decision-theoretic framework (cont'd)

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

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"
- a loss function (or utility function)

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"
- a loss function (or utility function)

States of nature

- What are the states of nature in an optimization problem?
- Short answer
  - Everything that "nature" knows but you don't

States of nature

- What are the states of nature in an optimization problem?
- Short answer
  - Everything that "nature" knows but you don't
- More practically: depends on the type of problem
  1. the content of the black box (expensive numerical model)
  2. for stochastic simulators: future responses of the simulator
  3. design under uncertainty: the value of environmental variables
  4. ...

States of nature

- What are the states of nature in an optimization problem?
- Short answer
  - Everything that "nature" knows but you don't
- More practically: depends on the type of problem
  1. the content of the black box (expensive numerical model)
  2. for stochastic simulators: future responses of the simulator
  3. design under uncertainty: the value of environmental variables
  4. ...

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
  - $\Omega = \left\{ f : \mathbb{X} \to \mathbb{R}^p \mid f \text{ such that } \ldots \right\}$

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
  - $\Omega = \left\{ f : \mathbb{X} \to \mathbb{R}^p \mid f \text{ such that } \ldots \right\}$
  - 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 $\omega^\star \in \Omega$ is unknown
- Example (cont'd)
  - a function $f^\star \in \Omega = C(\mathbb{X}; \mathbb{R})$ is inside the black box ($\omega^\star \equiv f^\star$)
  - we don't "know" $f^\star(x)$ until we run the code with input x

Uncertainty quantification (reminder from Lecture #1)

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

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

Uncertainty quantification (reminder from Lecture #1)

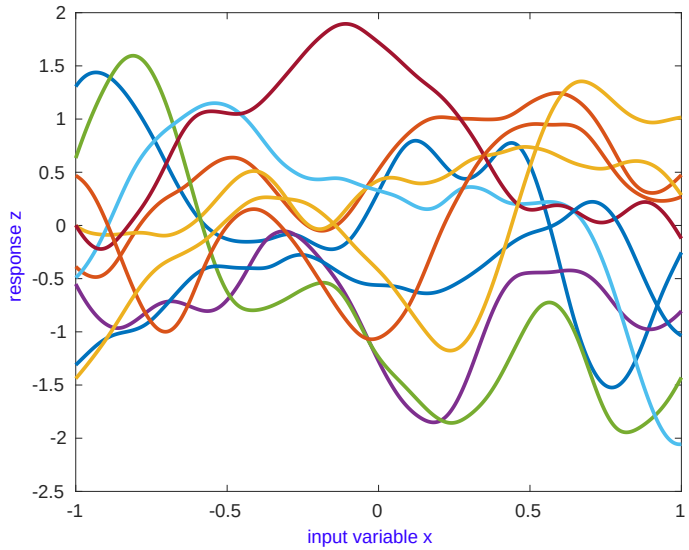
- The true state of nature $\omega^\star \in \Omega$ is unknown
- Example (cont'd)
  - a function $f^\star \in \Omega = C(\mathbb{X}; \mathbb{R})$ is inside the black box ($\omega^\star \equiv f^\star$)
  - we don't "know" $f^\star(x)$ until we run the code with input x

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

- Sequence of decisions $\Rightarrow$ sequence of distributions P_0, P_1, ...
  - P_n corresponds to the agent's beliefs after the n^{th} decision
  - A prior distribution P_0 needs to be specified

Uncertainty quantification: example

- Example (cont'd): if f is known to look more or less like this:

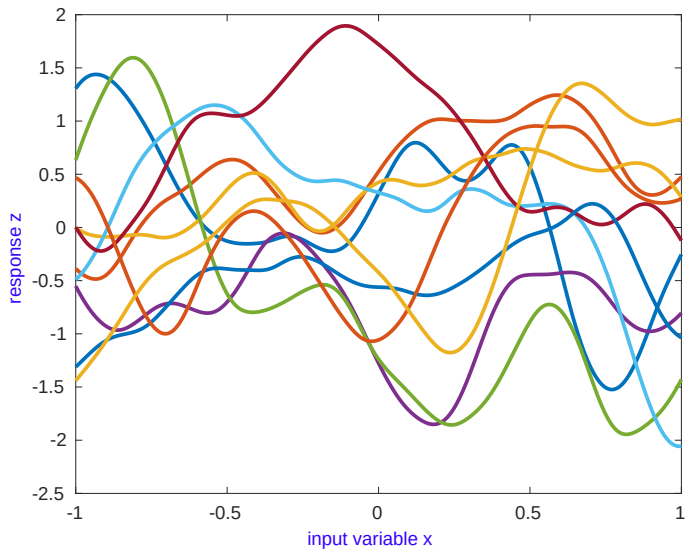


then we can take $\mathsf{P}_0 = \mathcal{GP}(m, k)$

with $m \sim \mathcal{U}(\mathbb{R})$ and k a (stationary) Matérn covariance

Uncertainty quantification: example

- Example (cont'd): if f is known to look more or less like this:



then we can take $\mathrm{P}_0 = \mathcal{GP}(m, k)$
with $m \sim \mathcal{U}(\mathbb{R})$ and k a (stationary) Matérn covariance

- Gaussian process priors are commonly used because
  - they are computationally convenient
  - while allowing a certain modeling flexibility

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

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

Convenient notation

$\xi =$ random function that represents the unknown f

- we will write, e.g., $\mathsf{E}_n\left(\xi(x)\right)$ instead of $\int_\Omega f(x)\,\mathsf{P}_n(\mathrm{d}f)$ ☺

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"
- a loss function (or utility function)

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"
- a loss function (or utility function)

Decisions

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

Decisions: intermediate decisions

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

Decisions: intermediate decisions

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

Decisions: stopping decision

- Several types of decisions in an optimization procedure:
  - intermediate decisions
  - 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
- 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 $x^* = \text{argmin}_{x \in \mathbb{X}} f(x)$
  - and/or an estimate of the minimum $M^* = \min_{x \in \mathbb{X}} f(x)$

  with $\mathbb{X}$ a "known" input space

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 $x^* = \text{argmin}_{x \in \mathbb{X}} f(x)$
  - and/or an estimate of the minimum $M^* = \min_{x \in \mathbb{X}} f(x)$

  with $\mathbb{X}$ a "known" input space

- 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

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

Notations

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

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

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

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 $\mathsf{P}_n \to \mathsf{P}_{n+1}$

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 $\mathrm{P}_n \to \mathrm{P}_{n+1}$

Notations: available information

I_n = the information obtained as a result of the n^{th} decision

F_n = the information available at time n

- Mathematically, $\mathrm{P}_n = \mathrm{P}_0\left(\cdot \mid F_n\right) = \mathrm{P}_{n-1}\left(\cdot \mid I_n\right)$

- Various settings can be addressed
  - depending on what we define as I_n ☺

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

Notations

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

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

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

- 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 $F_n = (X_1, \xi(X_1), \ldots, X_n, \xi(X_n))$
  - $\xi(X_i) = f^\star(X_i)$ is the true, scalar, value of the model at X_i

Transitions: examples

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

- Many other (interesting) settings are possible !
  - stochastic simulators
    - the output is a random draw $Z_n \sim$ some distrib. $\mathrm{P}^{Z_n|X_n}$
    - $I_n = (X_n, Z_n)$ and $F_n = (X_1, Z_1, \ldots, X_n, Z_n)$

Transitions: examples

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

- Many other (interesting) settings are possible !
  - stochastic simulators
    - the output is a random draw $Z_n \sim$ some distrib. $\mathrm{P}^{Z_n|X_n}$
    - $I_n = (X_n, Z_n)$ and $F_n = (X_1, Z_1, \ldots, X_n, Z_n)$
  - availability of gradients (e.g., adjoint code)

Transitions: examples

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

- Many other (interesting) settings are possible !
  - stochastic simulators
    - the output is a random draw $Z_n \sim$ some distrib. $\mathrm{P}^{Z_n|X_n}$
    - $I_n = (X_n, Z_n)$ and $F_n = (X_1, Z_1, \ldots, X_n, Z_n)$
  - availability of gradients (e.g., adjoint code)
  - batch setting and/or multiple outputs

Transitions: examples

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

- Many other (interesting) settings are possible !
  - stochastic simulators
    - the output is a random draw $Z_n \sim$ some distrib. $\mathrm{P}^{Z_n|X_n}$
    - $I_n = (X_n, Z_n)$ and $F_n = (X_1, Z_1, \ldots, X_n, Z_n)$
  - availability of gradients (e.g., adjoint code)
  - batch setting and/or multiple outputs
  - variable run-times, "simulation failures"...

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"
- a loss function (or utility function)

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" ✓
- a loss function (or utility function)

Loss function

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

Notation

$$\begin{aligned} L : \Omega \times \mathbb{D} &\rightarrow \mathbb{R} \\ (\omega, \underline{d}) &\mapsto L(\omega, \underline{d}) \end{aligned}$$

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

Loss function

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

Notation

$$\begin{aligned} L : \Omega \times \mathbb{D} &\to \mathbb{R} \\ (\omega, \underline{d}) &\mapsto L(\omega, \underline{d}) \end{aligned}$$

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

- The Bayes-optimal strategy is, by definition:

$$\begin{aligned} \underline{D} &= \operatorname{argmin} \mathrm{E}_0 \left(L(\underline{D}) \right) \\ &= \operatorname{argmin} \int_\Omega L(\omega, \underline{D}(\omega)) \, \mathrm{P}_0(\mathrm{d}\omega) \end{aligned}$$

where $\underline{D}$ ranges over all strategies

Loss function: example

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

Loss function: example

- Example (cont'd)
  - Assume that we want to find the minimizer of f
    - $\underline{d} = (x_1, \ldots, x_n, \widehat{x})$
    - with $\widehat{x}$ our estimate of argmin f
  - A standard loss function for this situation is the linear loss:

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

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

Loss function: example

- Example (cont'd)
  - Assume that we want to find the minimizer of f
    - $\underline{d} = (x_1, \ldots, x_n, \widehat{x})$
    - with $\widehat{x}$ our estimate of argmin f
  - A standard loss function for this situation is the linear loss:

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

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

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

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

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

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" ✓
- a loss function (or utility function)

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" ✓
- a loss function (or utility function) ✓

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

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" ✓
- a loss function (or utility function) ✓

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

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)
    - $F_n = (X_1, Z_1, \ldots, X_n, Z_n)$

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)
    - $F_n = (X_1, Z_1, \ldots, X_n, Z_n)$

- Recall the Bayes-optimal strategy (algorithm):

$$\begin{aligned} \underline{D}^{\text{Bayes}} &= \operatorname{argmin}_{\underline{D}} \, \mathrm{E}_0 \left(L(D_{N+1}) \right) \\ &= \operatorname{argmin}_{\underline{D}} \int_\Omega L(\omega, D_{N+1}(\omega)) \, \mathrm{P}_0(\mathrm{d}\omega) \end{aligned}$$

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

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

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

Notations

$$X_{n+1} = \varphi_n(X_1, Z_1, \ldots, X_n, Z_n) = \varphi_n(F_n)$$
$$D_{N+1} = \varphi_N(X_1, Z_1, \ldots, X_N, Z_N) = \varphi_N(F_N)$$

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

Notations

$$X_{n+1} = \varphi_n(X_1, Z_1, \ldots, X_n, Z_n) = \varphi_n(F_n)$$
$$D_{N+1} = \varphi_N(X_1, Z_1, \ldots, X_N, Z_N) = \varphi_N(F_N)$$

- Goal: find the functions $\varphi_0, \ldots, \varphi_N$

Optimal terminal decision

Notation

$$\begin{aligned} \mathsf{E}_n = \mathsf{E}(\cdot \mid F_n) &= \text{conditional expectation with respect to } F_n \\ &= \text{expectation with respect to the probability } \mathsf{P}_n \end{aligned}$$

Optimal terminal decision

Notation

$$\mathsf{E}_n = \mathsf{E}(\cdot \mid F_n) = \text{conditional expectation with respect to } F_n$$
$$= \text{expectation with respect to the probability } \mathsf{P}_n$$

- Consider any incomplete strategy $X_1, \ldots X_N$
- Claim: the optimal terminal decision is

$$D_{N+1} = \varphi_N^{\text{Bayes}}(X_1, Z_1, \ldots, X_N, Z_N) = \operatorname{argmin}_d \mathsf{E}_N(L(d))$$

where d runs over all possible values for the terminal decision

Optimal terminal decision: proof

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

Optimal terminal decision: proof

- Take any strategy $\underline{D} = (X_1, \ldots, X_N, D_{N+1})$
- Consider the modified strategy $\underline{D}' = \left(X_1, \ldots, X_N, D'_{N+1}\right)$ where $D'_{N+1} = \varphi_N^{\text{Bayes}}(X_1, Z_1, \ldots, X_N, Z_N)$
- Then, by definition of φ_N^{Bayes},

$$\begin{aligned} \mathrm{E}_N\left(L(D_{N+1})\right) &= \mathrm{E}_N\left(L(d)\right)_{|d=D_{N+1}} \\ &\geq \min_d \mathrm{E}_N\left(L(d)\right) = \mathrm{E}_N\left(L(D'_{N+1})\right) \end{aligned}$$

Optimal terminal decision: proof

- Take any strategy $\underline{D} = (X_1, \ldots, X_N, D_{N+1})$
- Consider the modified strategy $\underline{D}' = \left(X_1, \ldots, X_N, D'_{N+1}\right)$ where $D'_{N+1} = \varphi_N^{\text{Bayes}}(X_1, Z_1, \ldots, X_N, Z_N)$
- Then, by definition of φ_N^{Bayes},

$$\begin{aligned} \mathrm{E}_N\left(L(D_{N+1})\right) &= \mathrm{E}_N\left(L(d)\right)_{|d=D_{N+1}} \\ &\geq \min_d \mathrm{E}_N\left(L(d)\right) = \mathrm{E}_N\left(L(D'_{N+1})\right) \end{aligned}$$

- and thus

$$\begin{aligned} \mathrm{E}_0(L(D_{N+1})) &= \mathrm{E}_0\left(\mathrm{E}_N\left(L(D_{N+1})\right)\right) \\ &\geq \mathrm{E}_0\left(\mathrm{E}_N\left(L(D'_{N+1})\right)\right) = \mathrm{E}_0(L(D'_{N+1})) \quad \blacksquare \end{aligned}$$

Vocabulary: posterior (Bayes) risk at time N

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

$$R_N(d) = \mathrm{E}_N\left(L(d)\right)$$

("risk" is a synonym for "expected loss")

Vocabulary: posterior (Bayes) risk at time N

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

$$R_N(d) = \mathrm{E}_N\left(L(d)\right)$$

("risk" is a synonym for "expected loss")

- Define the posterior Bayes risk at time N:

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

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

Example (cont'd): linear loss

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

Example (cont'd): linear loss

- Recall the setting
  - goal: minimize f
  - $d_{N+1} = \widehat{x}$ is an estimate of $X^*(f) = \operatorname{argmin} f$
  - $L(f, \widehat{x}) = f(\widehat{x}) - \min f$
- Compute the posterior risk at time N for a given $\widehat{x} \in \mathbb{X}$:

$$\begin{aligned} R_N(\widehat{x}) = \mathsf{E}_N\left(L(\xi, \widehat{x})\right) &= \mathsf{E}_N\left(\xi(\widehat{x}) - \min \xi\right) \\ &= \widehat{\xi}_N(\widehat{x}) - \mathsf{E}_N\left(\min \xi\right) \end{aligned}$$

Example (cont'd): linear loss

- Recall the setting
  - goal: minimize f
  - $d_{N+1} = \widehat{x}$ is an estimate of $X^*(f) = \operatorname{argmin} f$
  - $L(f, \widehat{x}) = f(\widehat{x}) - \min f$
- Compute the posterior risk at time N for a given $\widehat{x} \in \mathbb{X}$:

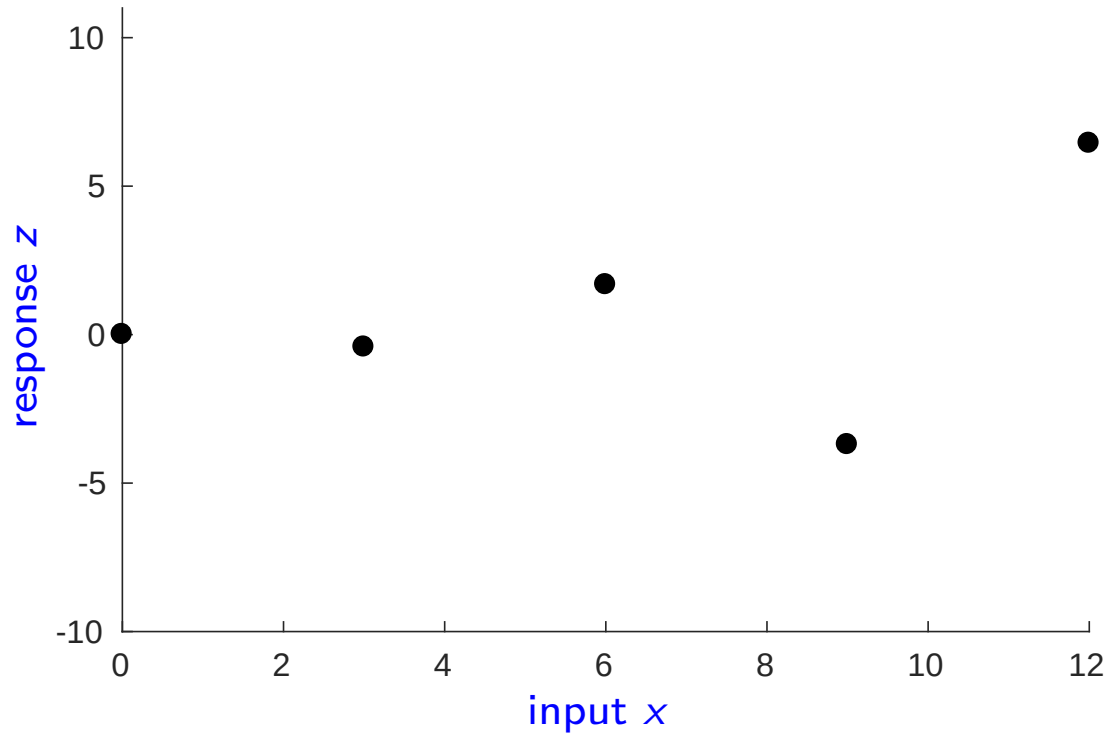
$$\begin{aligned} R_N(\widehat{x}) = \mathsf{E}_N\left(L(\xi, \widehat{x})\right) &= \mathsf{E}_N\left(\xi(\widehat{x}) - \min \xi\right) \\ &= \widehat{\xi}_N(\widehat{x}) - \mathsf{E}_N\left(\min \xi\right) \end{aligned}$$

- Thus the optimal terminal decision is

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

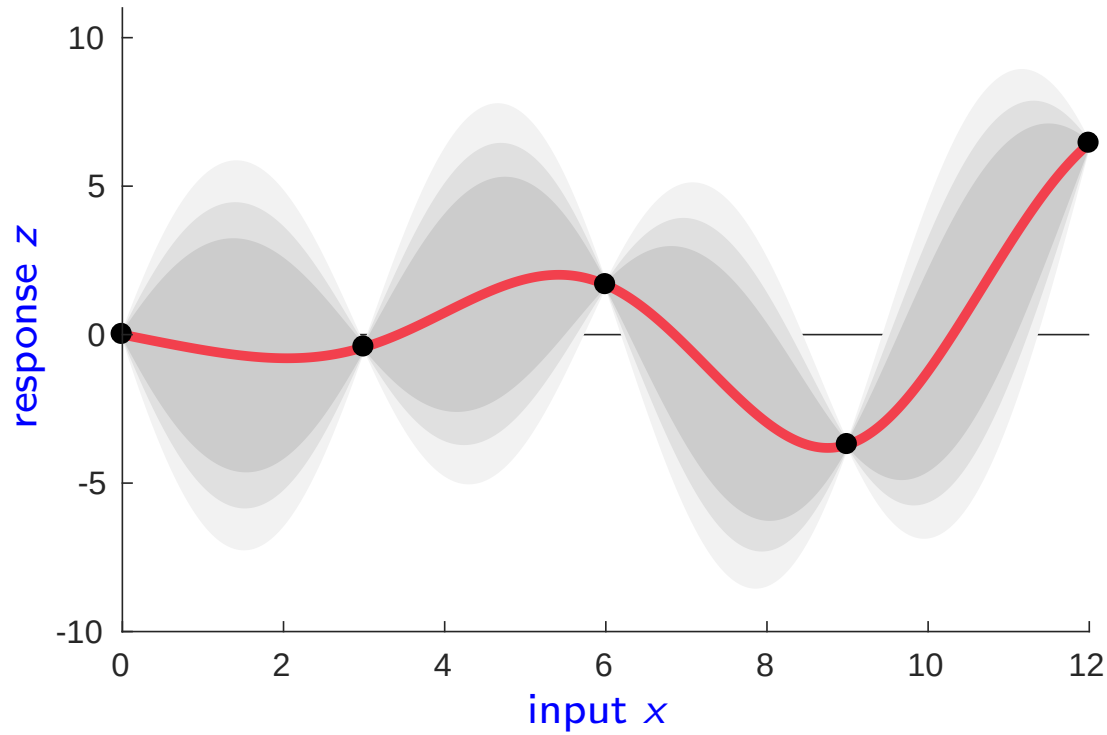
Example (cont'd): linear loss

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



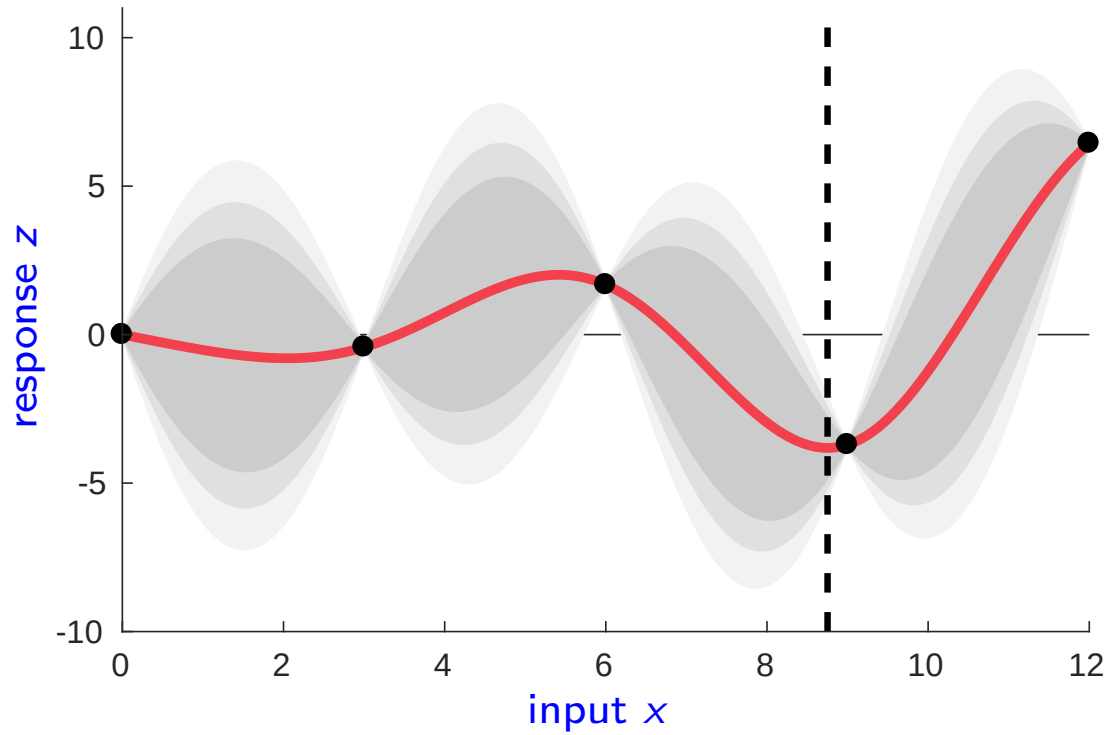
Example (cont'd): linear loss

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



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

$$\widehat{X}^{\text{Bayes}} = \operatorname{argmin} \widehat{\xi}_N$$
$$R_N^{\text{Bayes}} = \min \widehat{\xi}_N - \mathrm{E}_N(\min \xi)$$

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

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

- To summarize, we have for this example

$$\widehat{X}^{\text{Bayes}} = \operatorname{argmin} \widehat{\xi}_N$$
$$R_N^{\text{Bayes}} = \min \widehat{\xi}_N - \mathrm{E}_N(\min \xi)$$

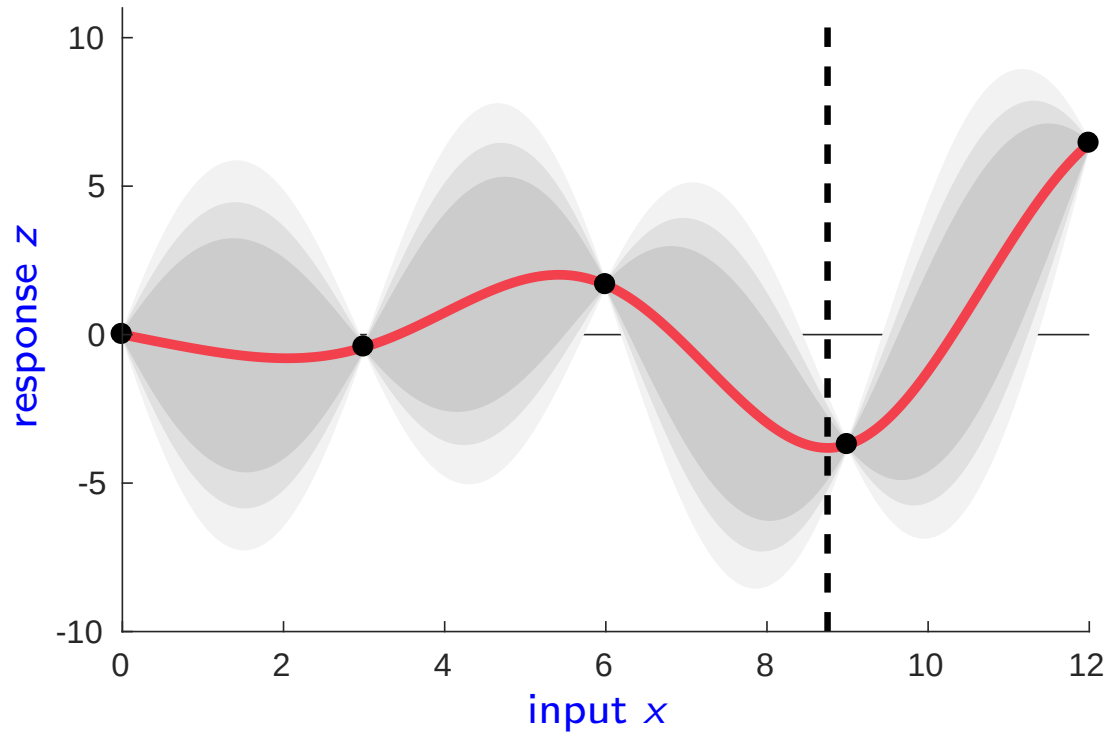
- Remark: in general, $\widehat{X}^{\text{Bayes}} \notin \{X_1, \ldots, X_N\}$
  - the value of the function at $\widehat{X}^{\text{Bayes}}$ is not known

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

$$\widehat{X}^{\text{Bayes},1} = \operatorname{argmin}_{x \in \{X_1, \ldots, X_N\}} \xi(x)$$
$$R_N^{\text{Bayes},1} = \min_{i \leq N} \xi(X_i) - \mathrm{E}_N(\min \xi)$$

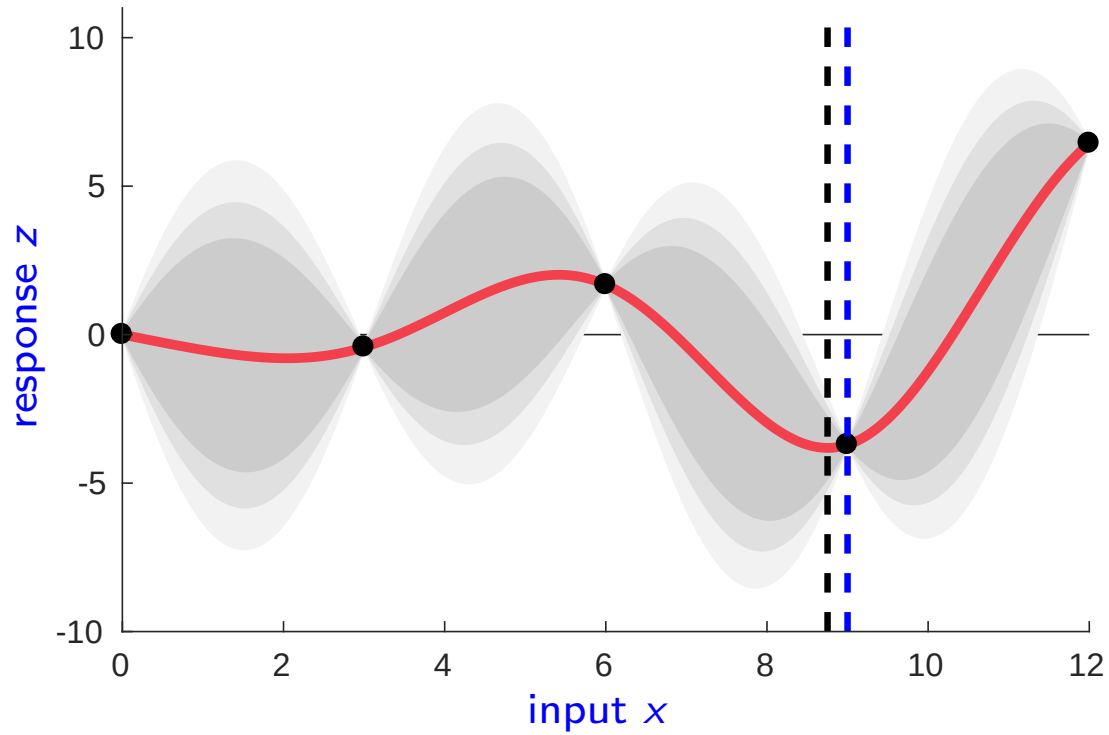
Example (cont'd): linear loss

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 $\widehat{\xi}$ does not "overshoot"

(e.g., for a Brownian motion prior)

Finding X_N^{Bayes} (last evaluation point)

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

Finding X_N^{Bayes} (last evaluation point)

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

Notation

$\mathsf{E}_{n,x}(Y)$ will mean: "compute $\mathsf{E}_n(Y)$, assuming that $X_{n+1} = x$"

Finding X_N^{Bayes} (last evaluation point)

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

Notation

$\mathsf{E}_{n,x}(Y)$ will mean: "compute $\mathsf{E}_n(Y)$, assuming that $X_{n+1} = x$"

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

$$\mathsf{E}_{n,x}(Y) = \mathsf{E}_n\left(g\left(X_1, Z_1, \ldots, X_n, Z_n, x, Z_x\right)\right)$$

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

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

Finding X_N^{Bayes} (last evaluation point)

- Given $x_N \in \mathbb{X}$, consider the following strategy at time $N-1$:
  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

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

- 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)

- 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

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

- Claim: the optimal decision rule for the last evaluation is

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

- 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 $\underline{D} = (X_1, \ldots, X_{N-1}, X_N, D_{N+1})$,

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

Finding X_N^{Bayes}: proof

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

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

- Let $\underline{D}' = \left(X_1, \ldots, X_{N-1}, X_N', D_{N+1}'\right)$,
  where $X_N' = \varphi_{N-1}^{\text{Bayes}}(F_{N-1})$ and $D_{N+1}' = \varphi_N^{\text{Bayes}}(F_{N-1}, X_N', Z_N')$

Finding X_N^{Bayes}: proof

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

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

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

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

Finding X_N^{Bayes}: proof

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

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

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

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

- Thus $\mathsf{E}_0\left(L(D_{N+1})\right) \geq \mathsf{E}_0\left(L(D'_{N+1})\right)$ ∎

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

- Recall our linear loss example

$$\widehat{X}^{\text{Bayes}} = \operatorname{argmin} \widehat{\xi}_N$$
$$R_N^{\text{Bayes}} = \min \widehat{\xi}_N - \mathsf{E}_N (\min \xi)$$

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

- Recall our linear loss example

$$\widehat{X}^{\text{Bayes}} = \operatorname{argmin} \widehat{\xi}_N$$
$$R_N^{\text{Bayes}} = \min \widehat{\xi}_N - \mathsf{E}_N (\min \xi)$$

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

$$R_{N-1}(F_{N-1}, x_N) = E_{N-1,x_N} \left(R_N^{\text{Bayes}}(F_N) \right)$$
$$= \mathsf{E}_{N-1,x_N} \left(\min \widehat{\xi}_N \right) - \mathsf{E}_{N-1} (\min \xi)$$

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

- Recall our linear loss example

$$\widehat{X}^{\text{Bayes}} = \operatorname{argmin} \widehat{\xi}_N$$
$$R_N^{\text{Bayes}} = \min \widehat{\xi}_N - \mathsf{E}_N (\min \xi)$$

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

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

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

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

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

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

- Equivalently,

$$X_N = \text{argmax}_{x_N} \underbrace{\min \widehat{\xi}_{N-1} - \mathsf{E}_{N-1,x_N}\left(\min \widehat{\xi}_N\right)}_{\rho^{\text{KG}}_{N-1}(x_N) \geq 0}$$

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

- Equivalently,

$$X_N = \text{argmax}_{x_N} \underbrace{\min \widehat{\xi}_{N-1} - \mathsf{E}_{N-1,x_N}\left(\min \widehat{\xi}_N\right)}_{\rho_{N-1}^{\text{KG}}(x_N) \geq 0}$$

- Nowadays called the Knowledge Gradient (KG) criterion

(Frazier, Powell & co-authors, 2008, 2009, 2011)

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

- Equivalently,

$$X_N = \text{argmax}_{x_N} \underbrace{\min \widehat{\xi}_{N-1} - \mathsf{E}_{N-1,x_N}\left(\min \widehat{\xi}_N\right)}_{\rho^{\text{KG}}_{N-1}(x_N) \geq 0}$$

- Nowadays called the Knowledge Gradient (KG) criterion

(Frazier, Powell & co-authors, 2008, 2009, 2011)

- Remarks
  - applicable to "noisy" observations as well
    - a.k.a. simulation-based optimization

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

- Equivalently,

$$X_N = \text{argmax}_{x_N} \underbrace{\min \widehat{\xi}_{N-1} - \mathsf{E}_{N-1,x_N}\left(\min \widehat{\xi}_N\right)}_{\rho^{\text{KG}}_{N-1}(x_N) \geq 0}$$

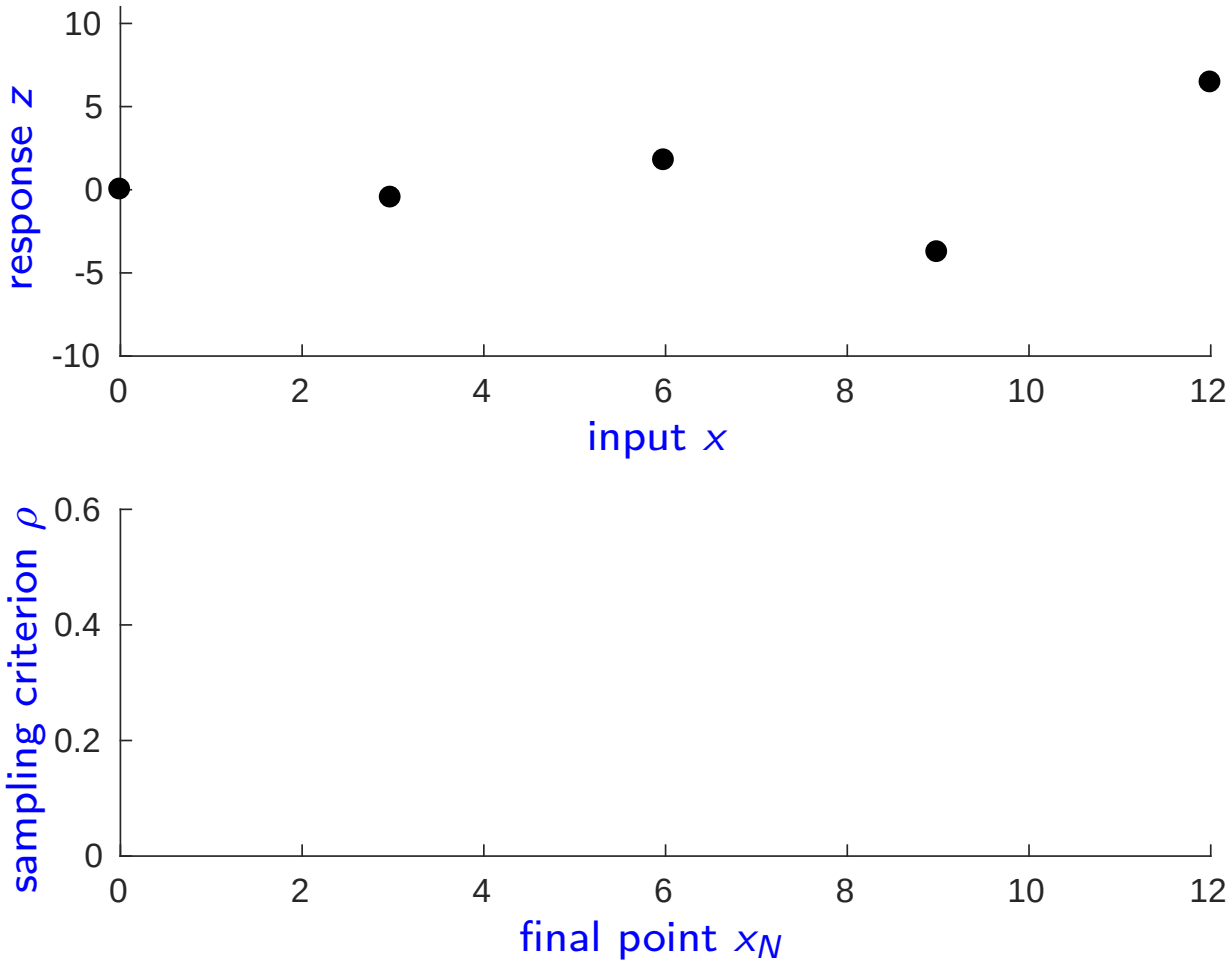
- Nowadays called the Knowledge Gradient (KG) criterion

(Frazier, Powell & co-authors, 2008, 2009, 2011)

- Remarks
  - applicable to "noisy" observations as well
    - a.k.a. simulation-based optimization
  - even with a GP prior, ρ^{KG} is not exactly computable in general
    - idea: approx. max over a finite grid (more about that later)

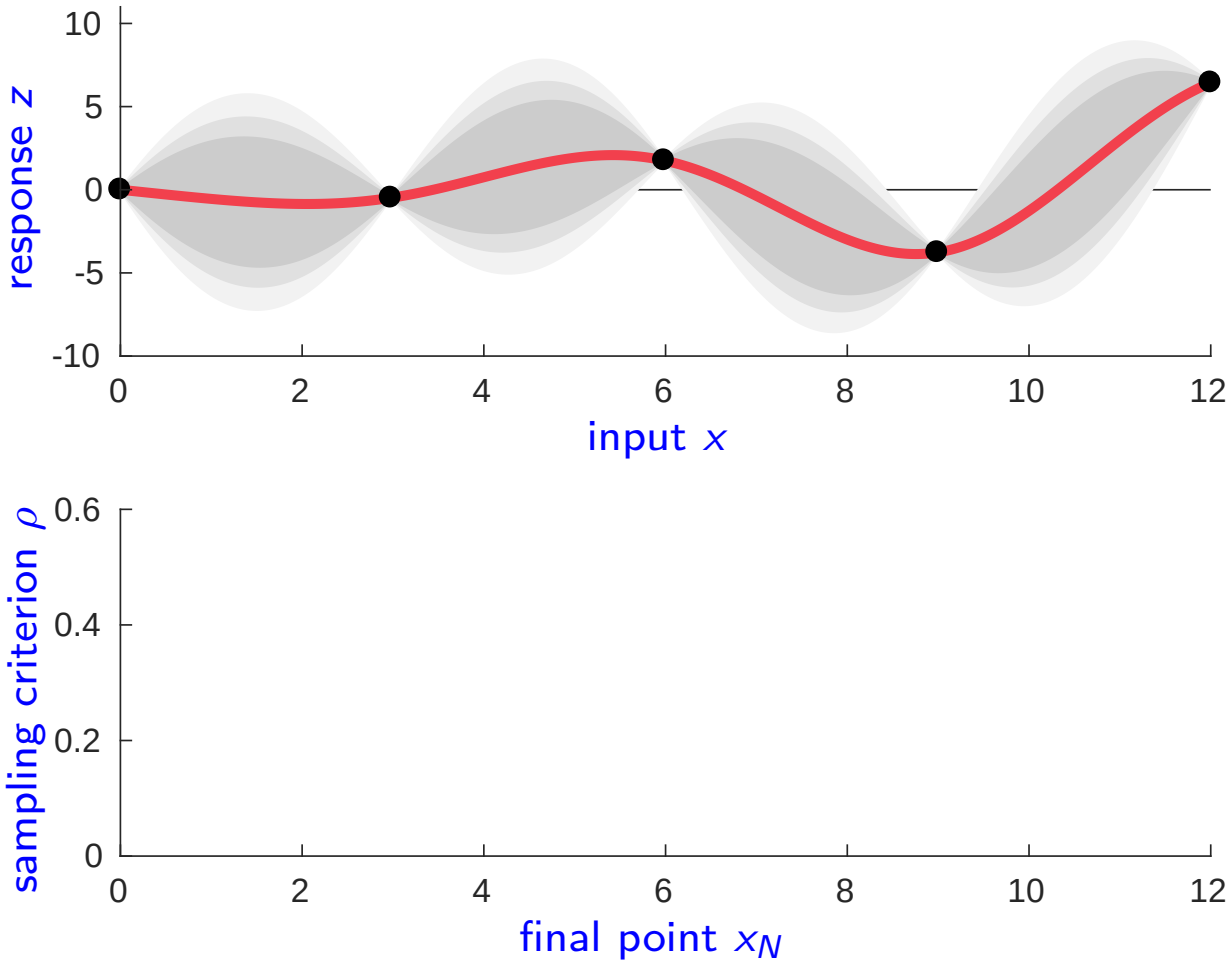
Finding X_N^{Bayes}: example (cont'd)

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



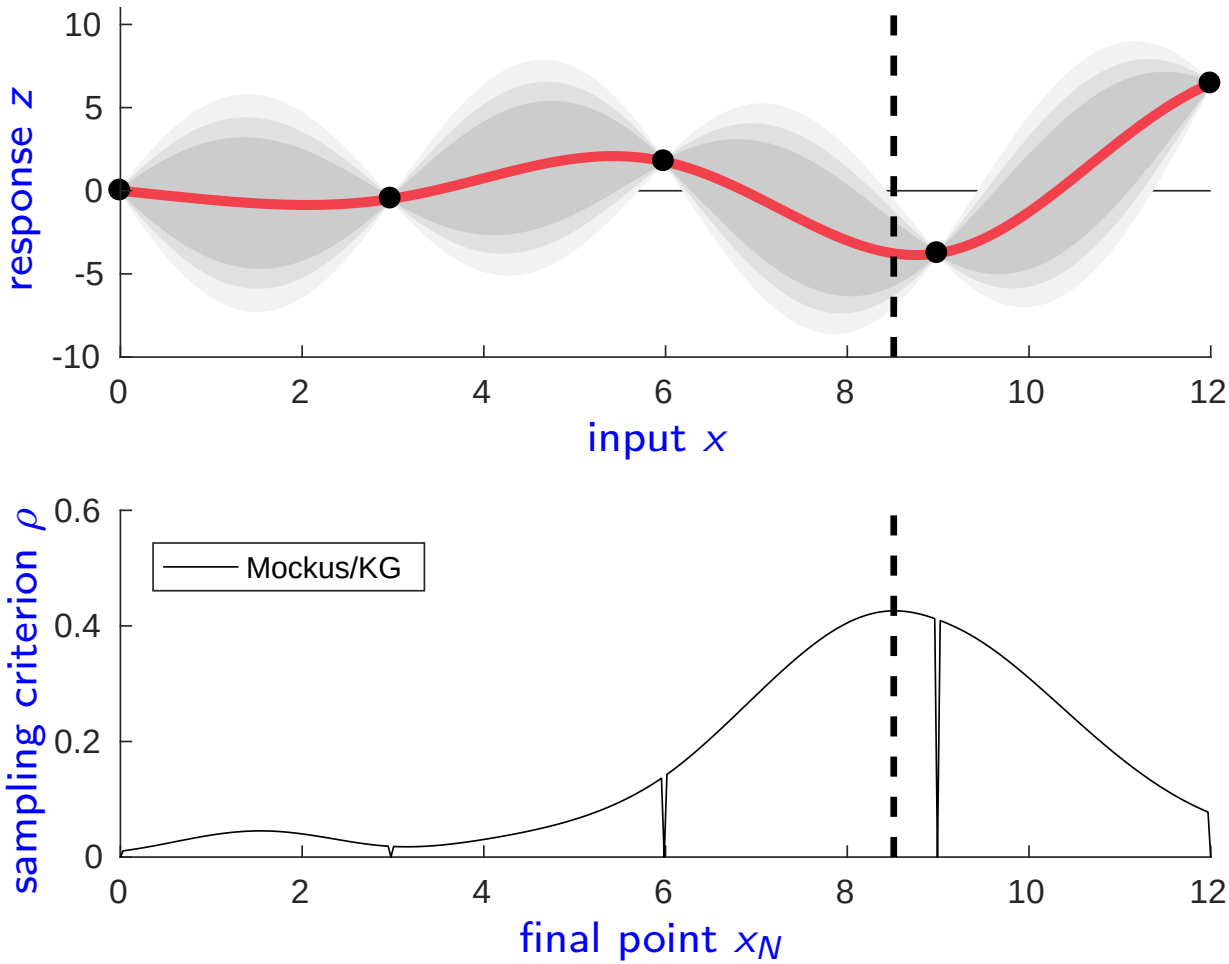
Finding X_N^{Bayes}: example (cont'd)

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



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

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



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

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

- Recall the following variant

$$\widehat{X}^{\text{Bayes},1} = \text{argmin}_{x \in \{X_1,\ldots,X_N\}} \xi(x)$$
$$R_N^{\text{Bayes},1} = \min_{i \le N} \xi(X_i) - \mathsf{E}_N(\min \xi)$$

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

- Recall the following variant

$$\widehat{X}^{\text{Bayes},1} = \text{argmin}_{x \in \{x_1,\ldots,x_N\}} \xi(x)$$
$$R_N^{\text{Bayes},1} = \min_{i \le N} \xi(X_i) - \mathsf{E}_N(\min \xi)$$

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

$$X_N = \text{argmax}_{x_N} \; M_{N-1} - \mathsf{E}_{N-1,x_N}(M_N)$$

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

- Recall the following variant

$$\begin{aligned}\widehat{X}^{\text{Bayes},1} &= \text{argmin}_{x\in\{X_1,\ldots,X_N\}}\,\xi(x)\\ R_N^{\text{Bayes},1} &= \min_{i\le N}\xi(X_i) - \mathsf{E}_N\left(\min\xi\right)\end{aligned}$$

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

$$\begin{aligned}X_N &= \text{argmax}_{x_N}\; M_{N-1} - \mathsf{E}_{N-1,x_N}\left(M_N\right)\\ &= \text{argmax}_{x_N}\; \underbrace{\mathsf{E}_{N-1}\left(\left(M_{N-1}-\xi(x_N)\right)_+\right)}_{\rho_n^{\text{EI}}(x_N)\,\ge\,0}\end{aligned}$$

- This is the Expected Improvement (EI) criterion

(Mockus et al 1978; Jones, Schonlau & Wlech, 1998)

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

- Recall the following variant

$$\begin{aligned}\widehat{X}^{\text{Bayes},1} &= \text{argmin}_{x\in\{X_1,\ldots,X_N\}}\,\xi(x)\\ R_N^{\text{Bayes},1} &= \min_{i\leq N}\xi(X_i) - \text{E}_N\left(\min\xi\right)\end{aligned}$$

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

$$\begin{aligned}X_N &= \text{argmax}_{x_N}\; M_{N-1} - \text{E}_{N-1,x_N}\left(M_N\right)\\ &= \text{argmax}_{x_N}\; \underbrace{\text{E}_{N-1}\left(\left(M_{N-1}-\xi(x_N)\right)_+\right)}_{\rho_n^{\text{EI}}(x_N)\geq 0}\end{aligned}$$

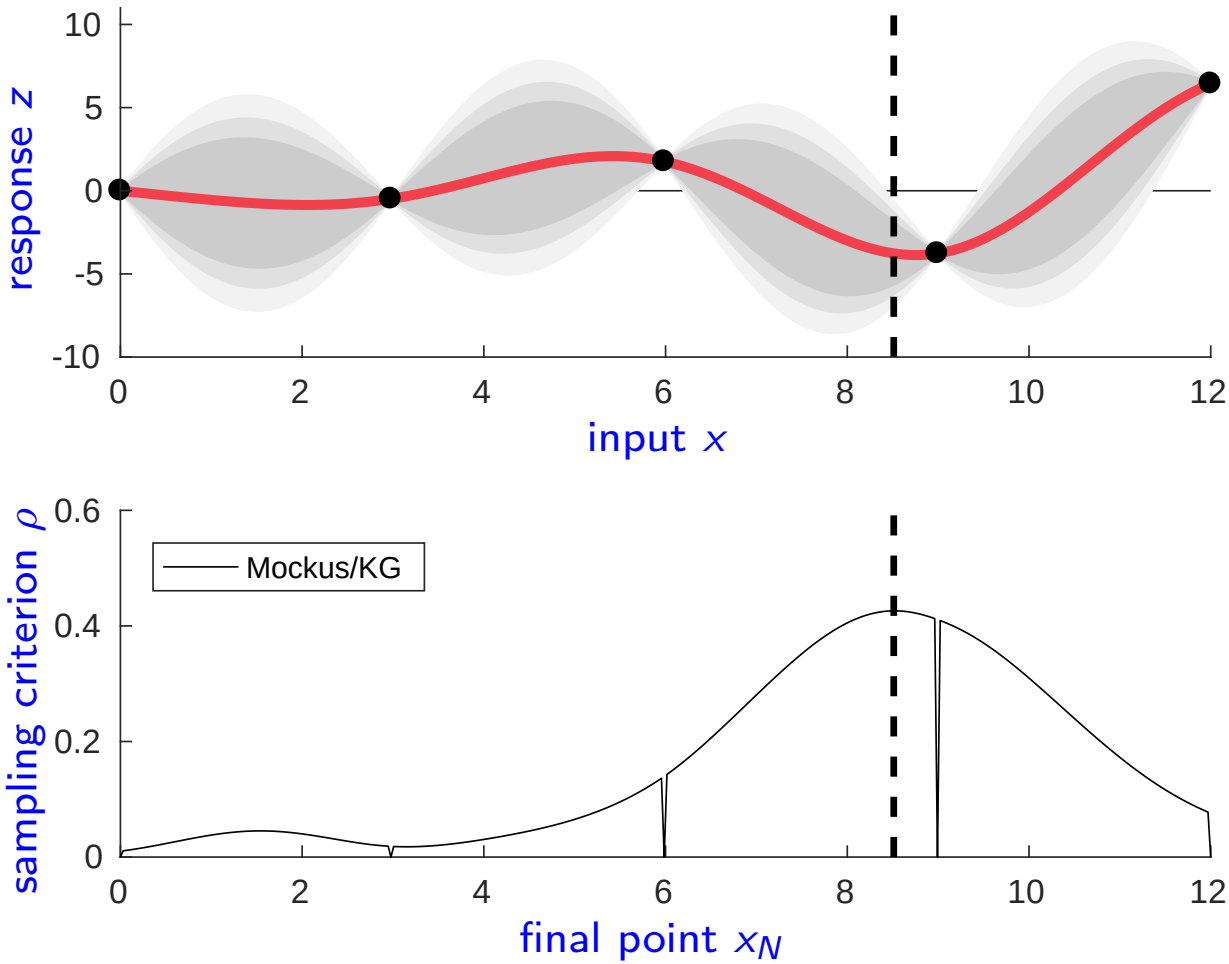
- This is the Expected Improvement (EI) criterion

(Mockus et al 1978; Jones, Schonlau & Wlech, 1998)

- Computable analytically for GP priors $\Rightarrow$ most commonly used (for *deterministic* numerical models)

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

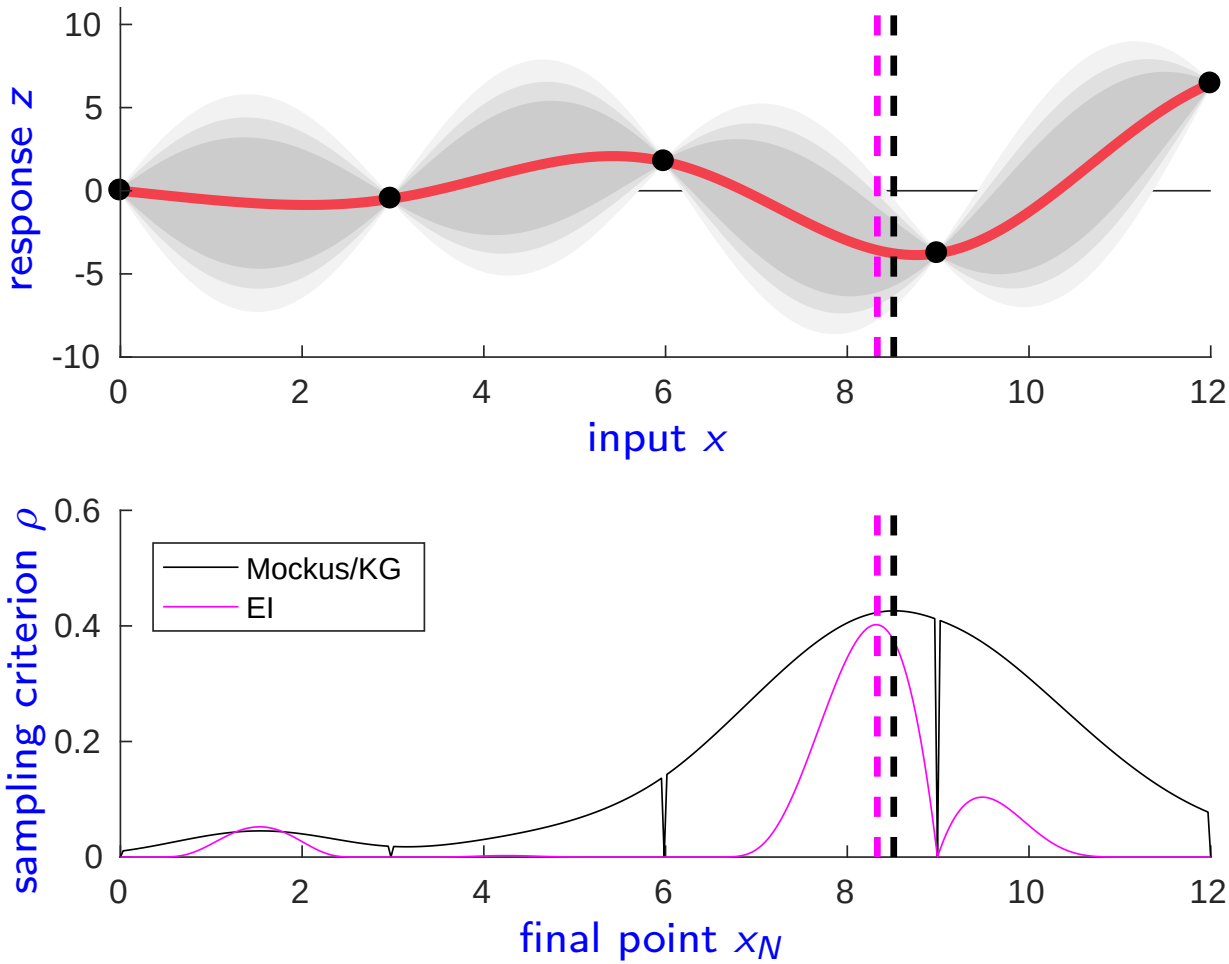
Same example as before, $n = 5$, but assume now that $N = 6$.



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

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

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



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

The Bayes-optimal strategy

- Recall the optimal terminal decision rule

$$\varphi_N^{\text{Bayes}}(F_N) = \operatorname{argmin}_d \mathrm{E}_N\left(L(d)\right)$$
$$R_N^{\text{Bayes}}(F_N) = \min_d \mathrm{E}_N\left(L(d)\right)$$

The Bayes-optimal strategy

- Recall the optimal terminal decision rule

$$\varphi_N^{\text{Bayes}}(F_N) = \operatorname{argmin}_d \mathrm{E}_N\left(L(d)\right)$$
$$R_N^{\text{Bayes}}(F_N) = \min_d \mathrm{E}_N\left(L(d)\right)$$

- Recall the optimal rule for the last evaluation

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

The Bayes-optimal strategy

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

$$\varphi_{n-1}^{\text{Bayes}}(F_{n-1}) = \operatorname{argmin}_{x_n} \mathrm{E}_{n-1,x_n}\left(R_n^{\text{Bayes}}(F_n)\right)$$
$$R_{n-1}^{\text{Bayes}}(F_{n-1}) = \min_{x_n} \mathrm{E}_{n-1,x_n}\left(R_n^{\text{Bayes}}(F_n)\right)$$

- This is called backward induction (or dynamic programming)

The Bayes-optimal strategy

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

$$\varphi_{n-1}^{\text{Bayes}}(F_{n-1}) = \operatorname{argmin}_{x_n} \mathrm{E}_{n-1,x_n}\left(R_n^{\text{Bayes}}(F_n)\right)$$
$$R_{n-1}^{\text{Bayes}}(F_{n-1}) = \min_{x_n} \mathrm{E}_{n-1,x_n}\left(R_n^{\text{Bayes}}(F_n)\right)$$

- This is called backward induction (or dynamic programming)

- So what ? Can we use this ?

The Bayes-optimal strategy

- More explicitely, the optimal decision for the first evaluation is

$$X_1 = \text{argmin}_{x_1} \mathrm{E}_{0,x_1} \Big(\min_{x_2} \mathrm{E}_{1,x_2} \Big(\ldots \min_{x_N} \mathrm{E}_{N-1,x_N} \Big(\min_d \mathrm{E}_N \left(L(d) \right) \Big) \Big) \Big)$$

The Bayes-optimal strategy

- More explicitely, the optimal decision for the first evaluation is

$$X_1 = \text{argmin}_{x_1} \mathrm{E}_{0,x_1}\left(\min_{x_2} \mathrm{E}_{1,x_2}\left(\ldots \min_{x_N} \mathrm{E}_{N-1,x_N}\left(\min_d \mathrm{E}_N\left(L(d)\right)\right)\right)\right)$$

- Very difficult to use in practice beyond $N = 1$ or 2
  - each "min" is an optim. problem that needs to be solved...
  - each "$\mathrm{E}_{n,x}$" 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

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
- For any $n \leq N$, let $\overline{L}_n = \min_d \mathrm{E}_n\left(L(d)\right)$

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
- For any $n \leq N$, let $\overline{L}_n = \min_d \mathrm{E}_n\left(L(d)\right)$

Generic myopic BO algorithm

- For n from 0 to $N-1$
  - Compute $X_{n+1} = \operatorname{argmin}_x \mathrm{E}_{n,x_{n+1}}\left(\overline{L}_{n+1}\right)$
  - Make an evaluation at X_{n+1}
- Output $D_{N+1} = \operatorname{argmin} \mathrm{E}_N\left(L(d)\right)$

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
    2. use MCMC/SMC to sample from the posterior

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
    2. use MCMC/SMC to sample from the posterior
  - plug-in approach
    - use $\mathrm{P}_n^{\theta} \approx \delta_{\widehat{\theta}_n}$, with $\widehat{\theta}_n$ an estimator of θ (MML, LOO-CV...)
    - enough initial data is needed for this approach

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
    2. use MCMC/SMC to sample from the posterior
  - plug-in approach
    - use $\mathrm{P}_n^{\theta} \approx \delta_{\widehat{\theta}_n}$, with $\widehat{\theta}_n$ an estimator of θ (MML, LOO-CV...)
    - enough initial data is needed for this approach

Generic myopic BO algorithm with hyper-parameter estimation

- Init: (space-filling) DoE of size $n0$ (rule of thumb: $n_0 = 10\,d$)
- For n from n_0 to $N-1$
  - once in a while, Estimate hyper-parameters (plug-in/fully Bayes)
  - Compute $X_{n+1} = \operatorname{argmin}_x \mathrm{E}_{n,x_{n+1}}\left(\overline{L}_{n+1}\right)$
  - Make an evaluation at X_{n+1}
- Output $D_{N+1} = \operatorname{argmin} \mathrm{E}_N\left(L(d)\right)$

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
    - if accurate convergence is not needed

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

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

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

Multi-objective problems

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

Multi-objective problems

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

Pareto domination relation

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

Multi-objective problems

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

Pareto domination relation

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

- 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)

Multi-objective problems

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

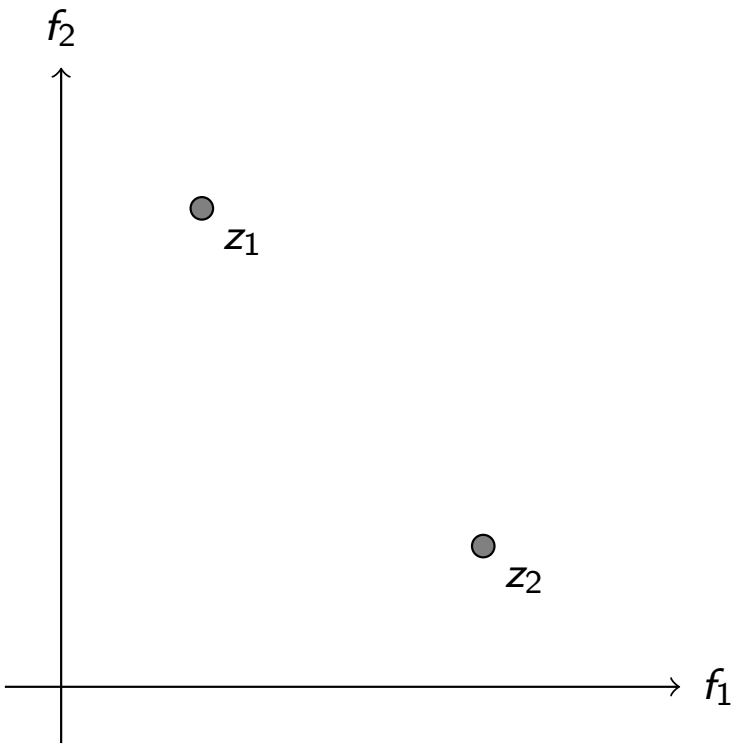
Pareto domination relation

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

- 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)
  - 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

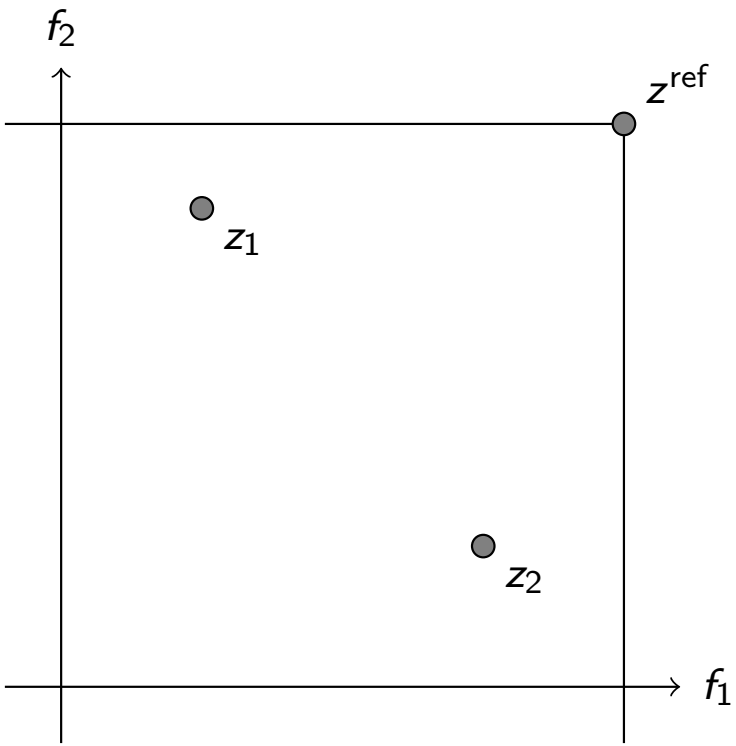
- EHVI: a natural extension of EI (Emmerich et al, 2006)



Noiseless evaluations

Multi-objective problems

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

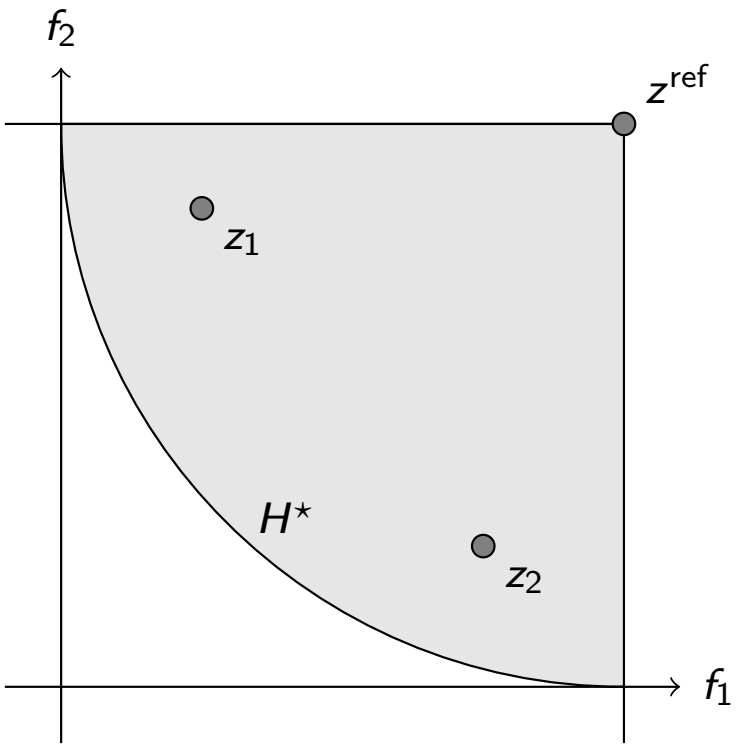


Noiseless evaluations

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

Multi-objective problems

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



Noiseless evaluations

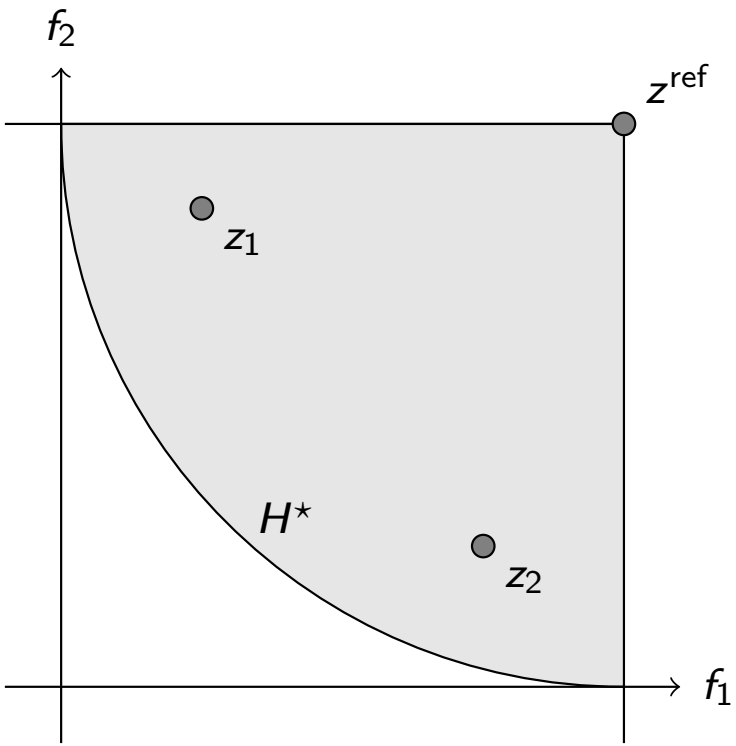
$\mathbb{B} = \Pi_{j=1}^{p} \left]-\infty; z_j^{\text{ref}}\right]$: bounding box

True dominated region:

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

Multi-objective problems

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



Noiseless evaluations

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

True dominated region:

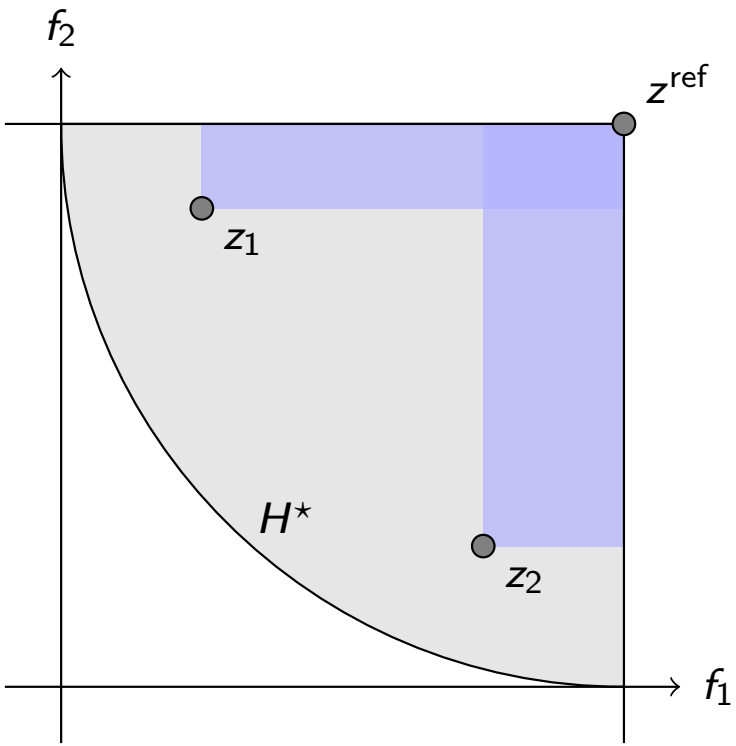
$$H^\star(f) = \{z \in \mathbb{B},\ \exists x \in \mathbb{X}, f(x) \preceq z\}$$

Loss function:

$$L(f, \widehat{H}) = |H^\star(f) \triangle \widehat{H}|$$

Multi-objective problems

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



Noiseless evaluations

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

True dominated region:

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

Loss function:

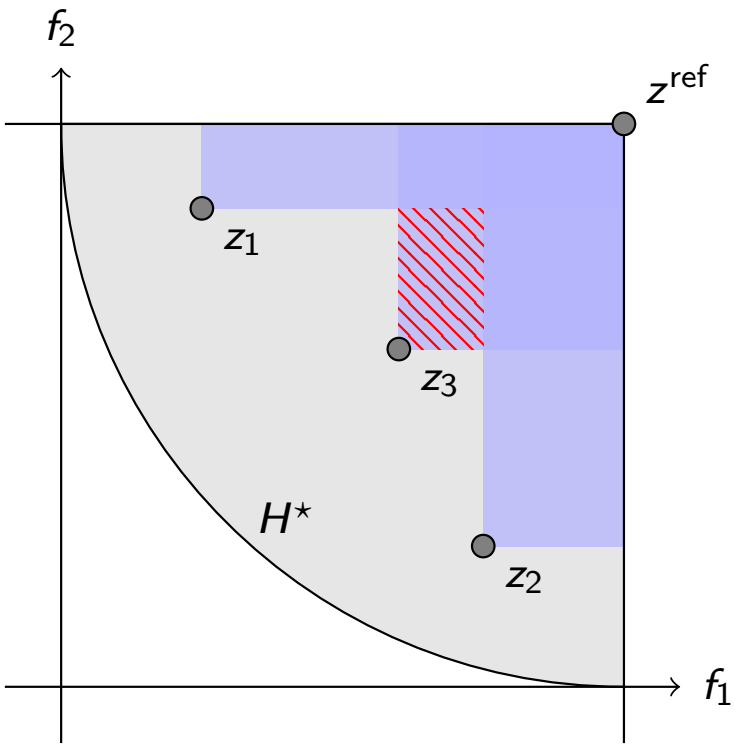
$$L(f, \widehat{H}) = |H^\star(f) \triangle \widehat{H}|$$

Best "safe" estimator:

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

Multi-objective problems

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



Noiseless evaluations

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

True dominated region:

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

Loss function:

$$L(f, \widehat{H}) = |H^\star(f) \triangle \widehat{H}|$$

Best "safe" estimator:

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

$$\rho_n^{\text{EHVI}}(x_{n+1}) = \mathbb{E}_{n,x_{n+1}}\left(|H_{n+1} \setminus H_n|\right)$$

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.

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.
- Many other sampling criteria have been proposed
  - See Feliot et al (2017, section 2.2) and references therein

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.
- Many other sampling criteria have been proposed
  - See Feliot et al (2017, section 2.2) and references therein

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-contrained problem:
  - $f = (f_{\mathrm{o}}, f_{\mathrm{c},1}, \ldots, f_{\mathrm{c},q})$, with
  - $f_{\mathrm{o}} : \mathbb{X} \to \mathbb{R}$, to be minimized,
  - $f_{\mathrm{c},j} : \mathbb{X} \to \mathbb{R}$, $1 \leq j \leq q$, must be ≤ 0.

Inequality-constrained problems

- Single-objective, inequality-contrained problem:
  - $f = (f_{\mathrm{o}}, f_{\mathrm{c},1}, \ldots, f_{\mathrm{c},q})$, with
  - $f_{\mathrm{o}} : \mathbb{X} \to \mathbb{R}$, to be minimized,
  - $f_{\mathrm{c},j} : \mathbb{X} \to \mathbb{R}$, $1 \leq j \leq q$, must be ≤ 0.
- Consider the following loss function

$$L(f, \widehat{x}) = \begin{cases} f_{\mathrm{o}}(\widehat{x}) - f_{\mathrm{o}}^{\star} & \text{if } f_{\mathrm{c}}(\widehat{x}) \leq 0, \\ +\infty & \text{otherwise.} \end{cases}$$

where $f_{\mathrm{o}}^{\star} = \min_{x : f_{\mathrm{c}}(x) \leq 0} f_{\mathrm{o}}(x)$

Inequality-constrained problems

- Assuming
  - noiseless evaluations,
  - independent priors on objective and constraint functions,
  - $\exists i \leq n,\ \xi_{\mathrm{c}}(X_i) = f_{\mathrm{c}}(X_i) \leq 0$,

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

$$\rho_n^{\mathsf{EIC}}(x_{n+1}) = \rho_{\mathrm{o},n}^{\mathsf{EI}}(x_{n+1}) \cdot \underbrace{\Pi_{j=1}^{q} \mathrm{P}_n\left(\xi_{\mathrm{c},j}(x_{n+1}) \leq 0\right)}_{\text{Proba of Feasibility (PF)}}.$$

Inequality-constrained problems

- Assuming
  - noiseless evaluations,
  - independent priors on objective and constraint functions,
  - $\exists i \leq n,\ \xi_{\mathrm{c}}(X_i) = f_{\mathrm{c}}(X_i) \leq 0$,

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

$$\rho_n^{\mathsf{EIC}}(x_{n+1}) = \rho_{\mathrm{o},n}^{\mathsf{EI}}(x_{n+1}) \cdot \underbrace{\Pi_{j=1}^{q} \mathrm{P}_n\left(\xi_{\mathrm{c},j}(x_{n+1}) \leq 0\right)}_{\text{Proba of Feasibility (PF)}}.$$

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

Inequality-constrained problems

- Assuming
  - noiseless evaluations,
  - independent priors on objective and constraint functions,
  - $\exists i \leq n,\ \xi_{\mathrm{c}}(X_i) = f_{\mathrm{c}}(X_i) \leq 0$,

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

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

- 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)

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)

Announcement

Paul Feliot's PhD defense will take place

on Wednesday, July 12, 2017, 2 PM,

at CentraleSupelec (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...)

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...)
- Aggregation-based approaches
  - Multi-objective: ParEGO (Knowles, 2006)
  - Constrained: Augmented Lagrangian methods (Gramacy et al, 2016; Picheny et al, 2016)

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...)
- Aggregation-based approaches
  - Multi-objective: ParEGO (Knowles, 2006)
  - Constrained: Augmented Lagrangian methods (Gramacy et al, 2016; Picheny et al, 2016)
- Batch of evaluations: multi-point criteria
  - Ginsbourger et al (2010), Chevalier & Ginsbourger (2013), Chevalier et al (2014), Marmin et al (2015)

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...)
- Aggregation-based approaches
  - Multi-objective: ParEGO (Knowles, 2006)
  - Constrained: Augmented Lagrangian methods (Gramacy et al, 2016; Picheny et al, 2016)
- Batch of evaluations: multi-point criteria
  - 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 ☺

Design under uncertainty

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

Design under uncertainty

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

"Design under uncertainty" framework

- objective functions: $f_{\mathrm{o},j}(x, u)$, $1 \leq j \leq p$
- constraint functions: $f_{\mathrm{c},j}(x, u)$, $1 \leq j \leq q$
- 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

- Principle of the worst-case (minimax) approach
  - Define an uncertainty set $\mathbb{U}$
  - Optimize by considering the worst $u \in \mathbb{U}$
- For instance, assuming a single-objective problem:

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

(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 $u \in \mathbb{U}$
- For instance, assuming a single-objective problem:

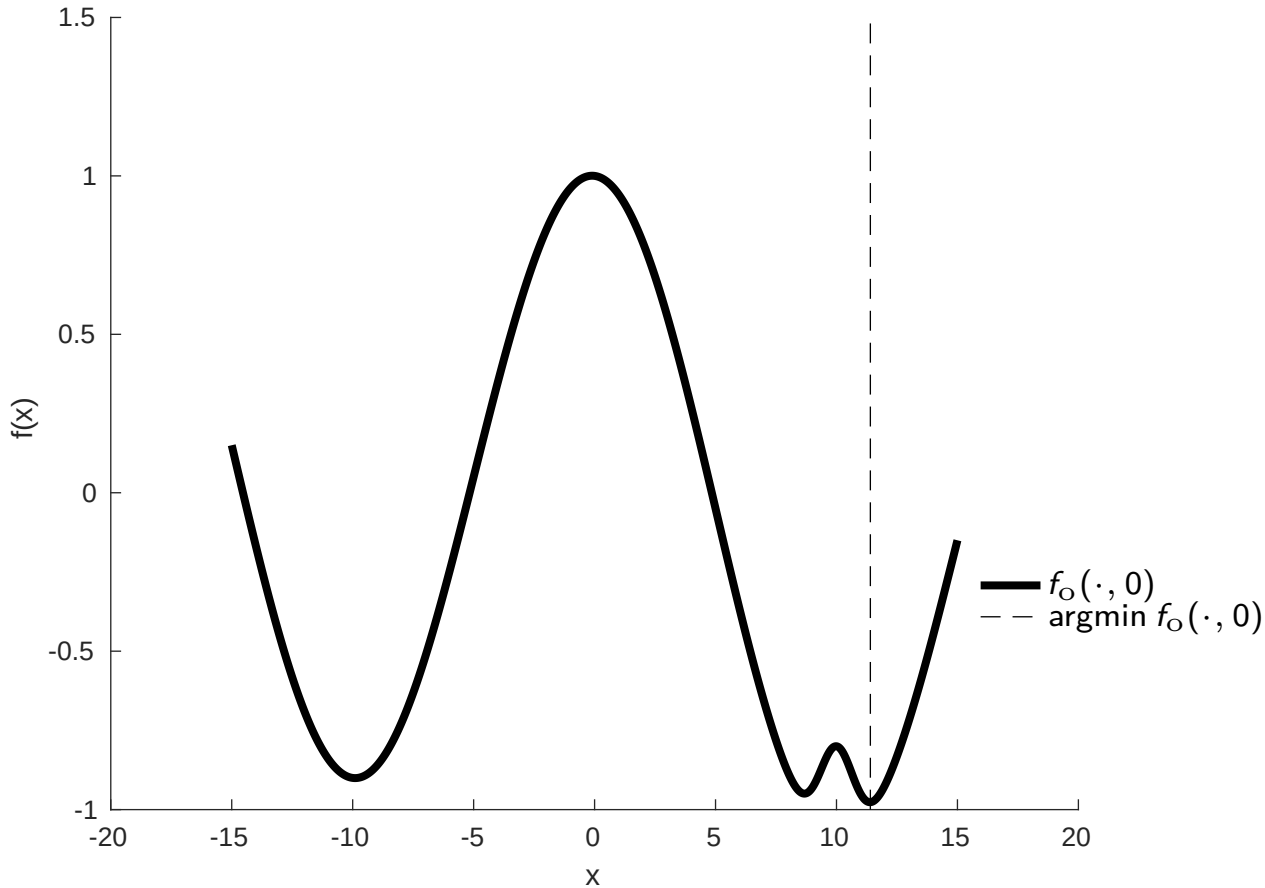
$$\text{minimize} \max_{u \in \mathbb{U}} f_{\text{o}}(x, u)$$

- If the problem has constraints, they become:

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

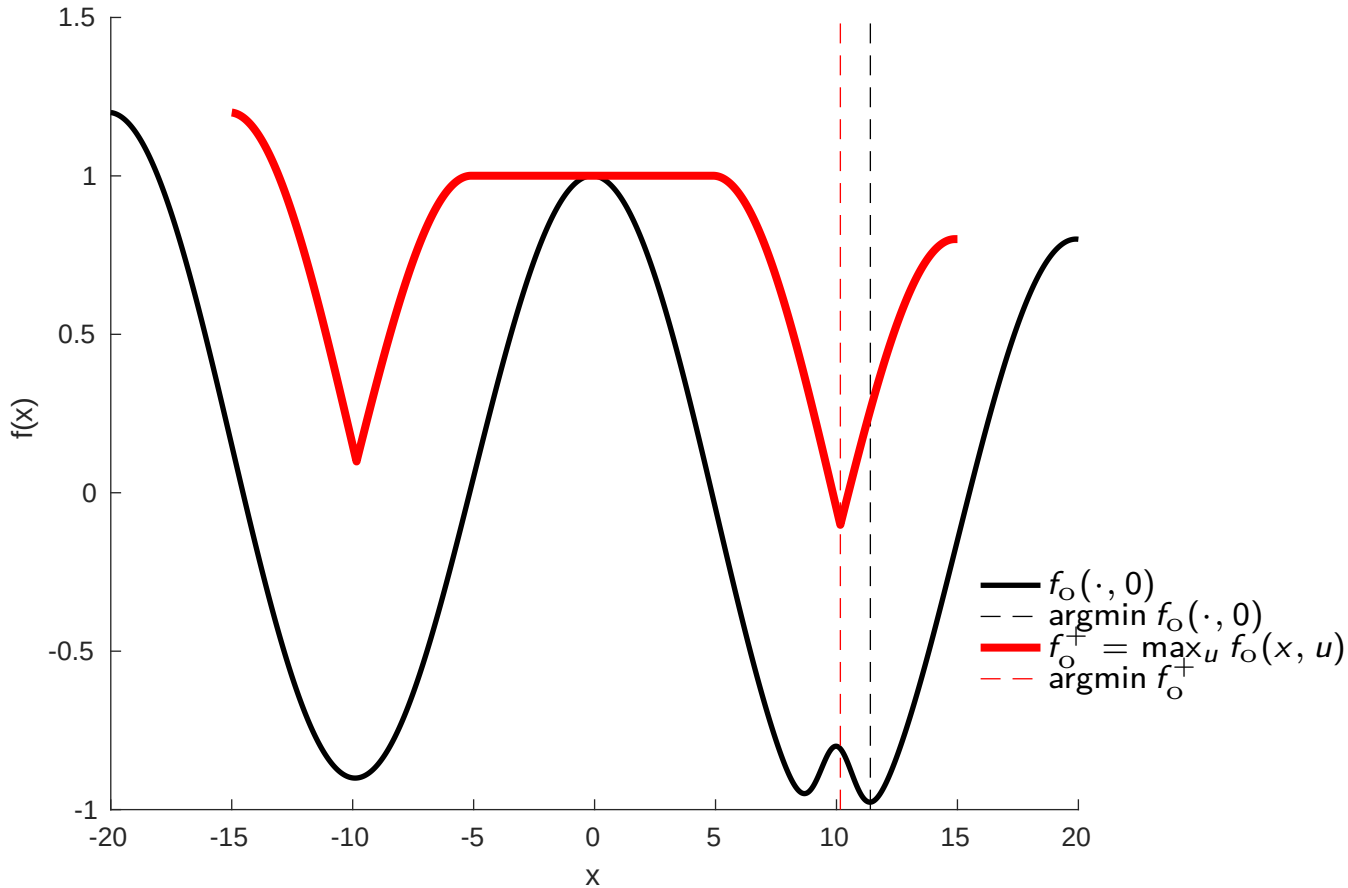
Example 1: Illustration of the worst-case approach

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



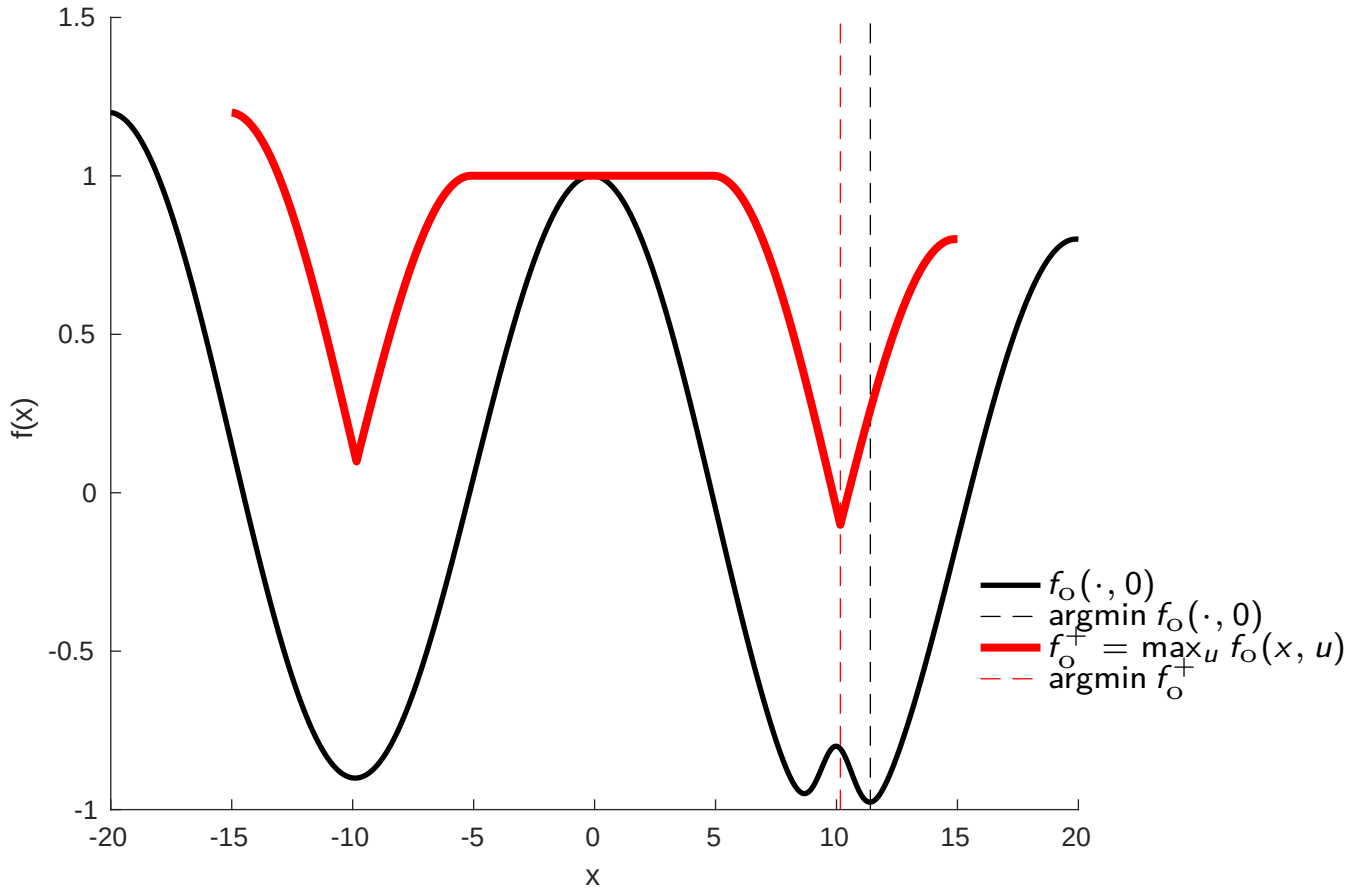
Example 1: Illustration of the worst-case approach

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



Example 1: Illustration of the worst-case approach

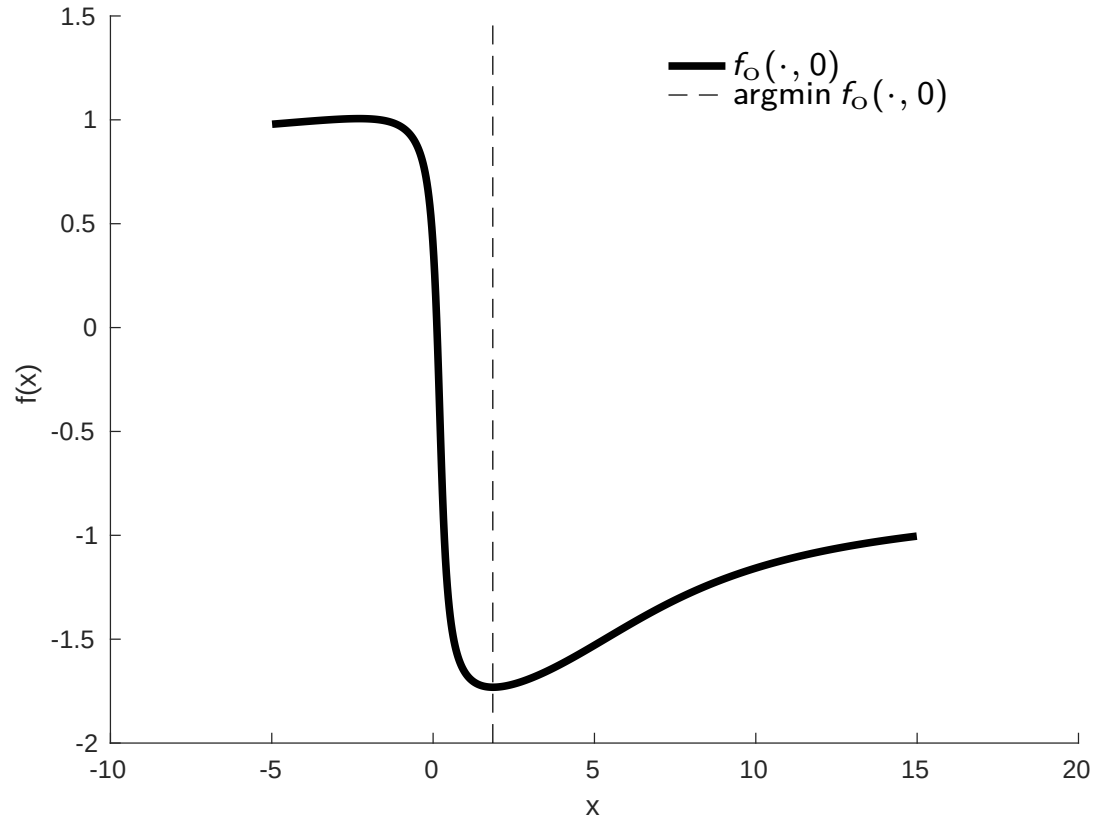
Example: $f_{\mathrm{o}}(x,u) = \widetilde{f}(x+u)$, with $u \in \mathbb{U} = [-\delta;\delta]$, $\delta = 5$



Remark: very conservative, the nominal performance is ignored

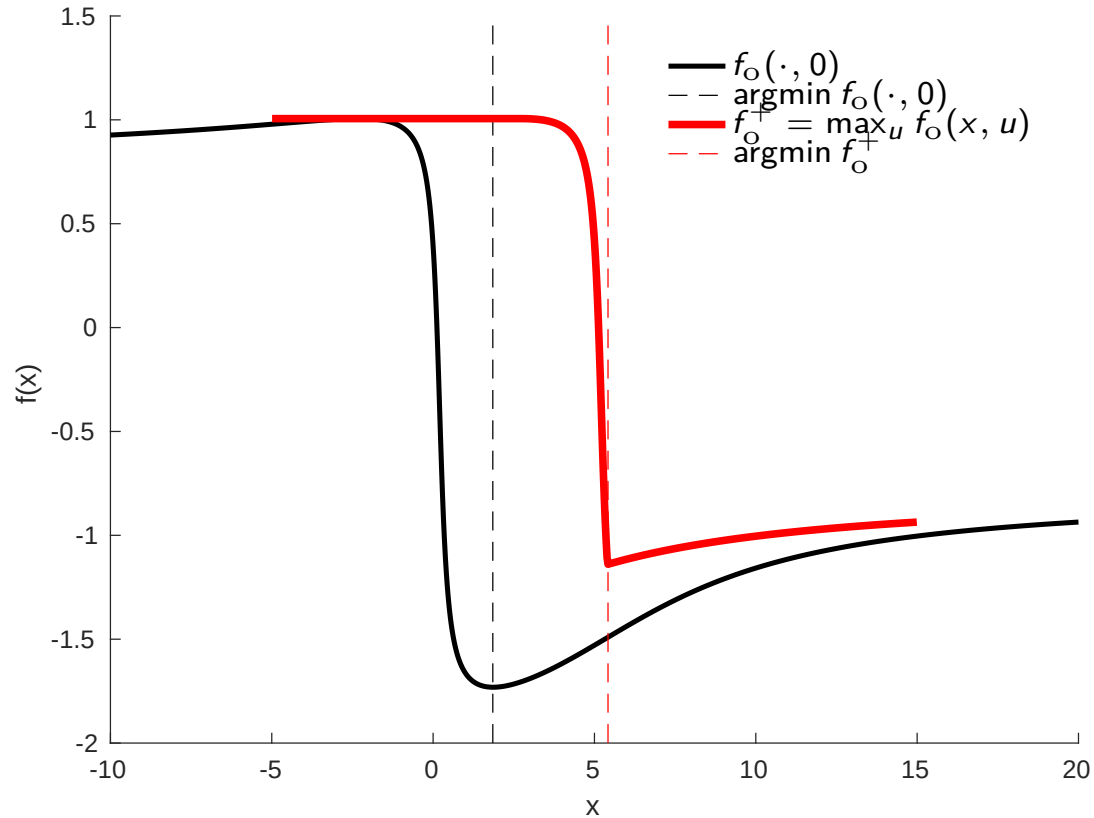
Example 2: Illustration of the worst-case approach

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



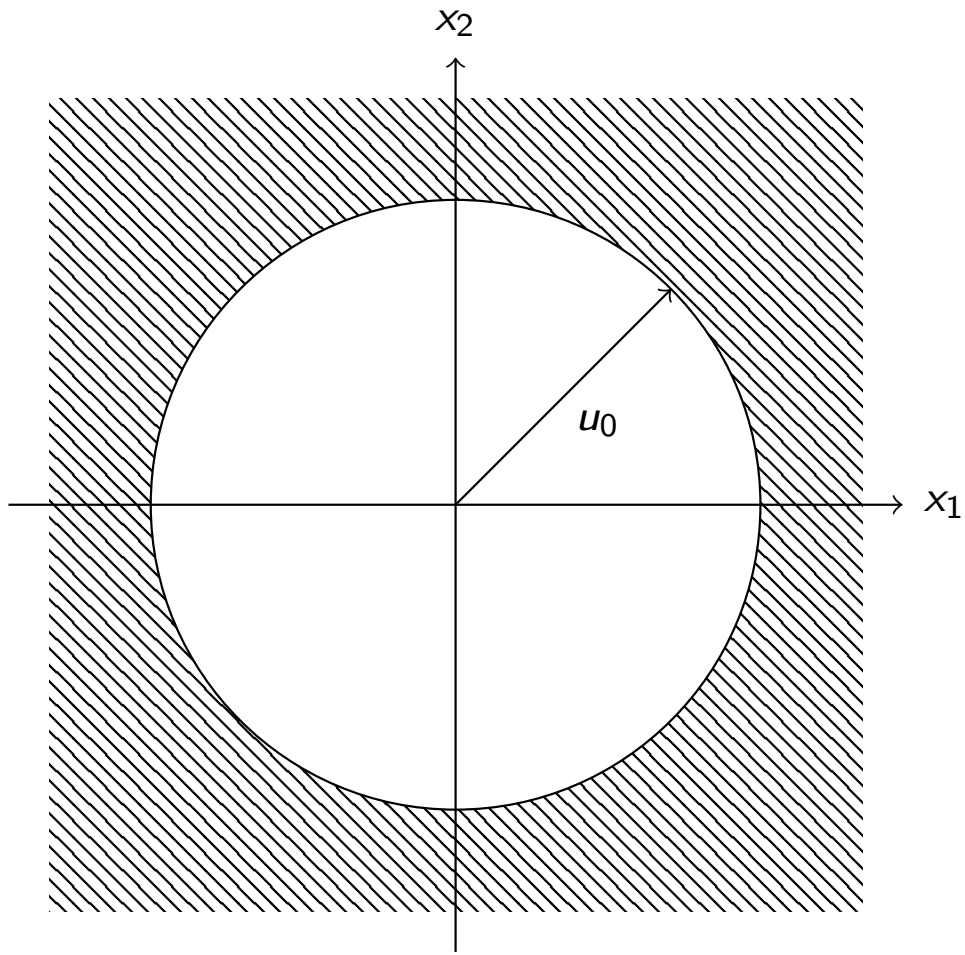
Example 2: Illustration of the worst-case approach

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



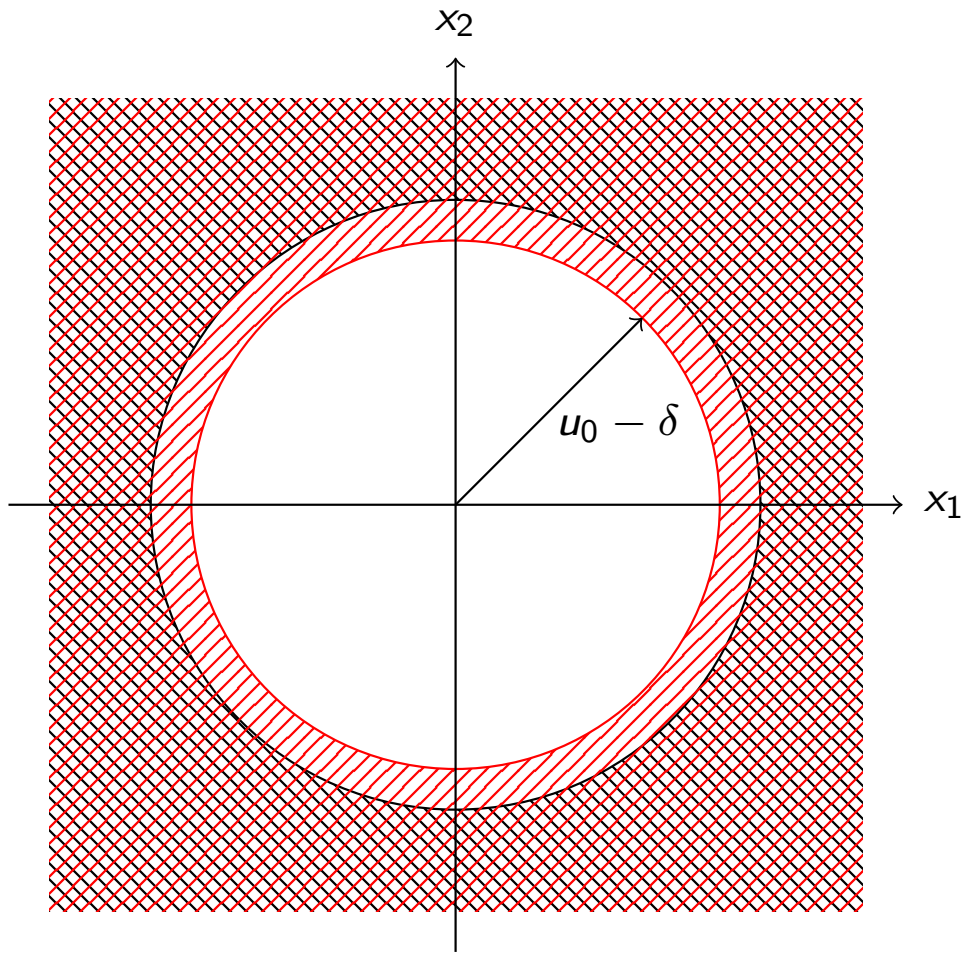
Another example: worst-case approach for a constraint

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 $u \in \mathbb{U} = [u_0 - \delta; u_0 + \delta]$



(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 ☺

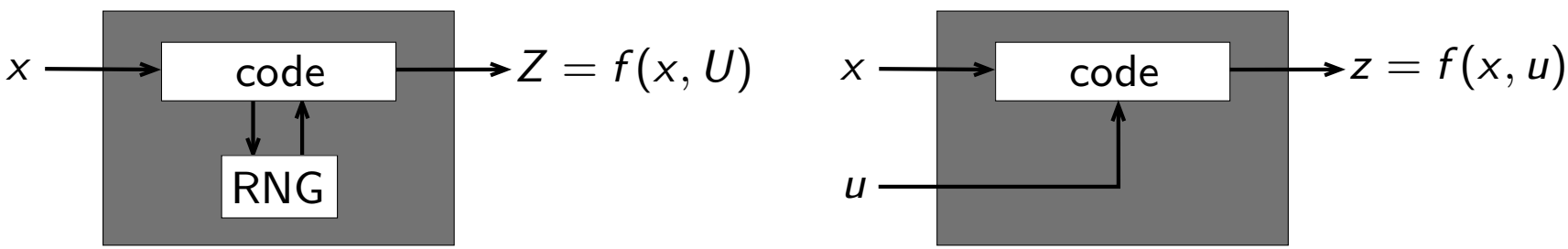
The probabilistic approach

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

The probabilistic approach

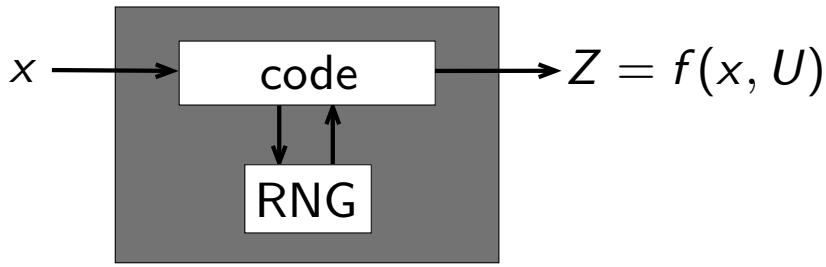
- From now, we focus on the probabilistic approach
  - u is considered as random $\rightarrow$ $U \sim \mathrm{P}^U$
  - can be a random vector ($\in \mathbb{R}^m$), or a more complicated object

- Numerical models: two important settings
  - stochastic simulators
  - environmental variables



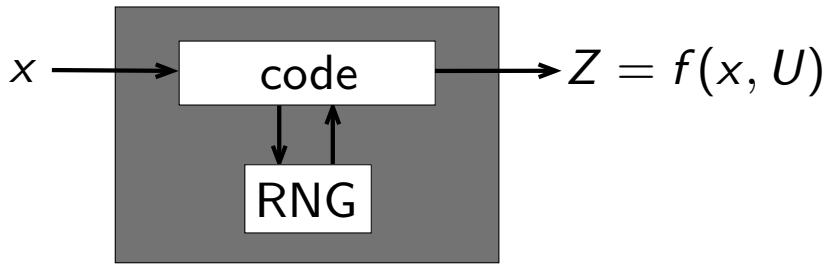
where $f = (f_{\mathrm{o},1}, \ldots, f_{\mathrm{o},p}, f_{\mathrm{c},1}, \ldots, f_{\mathrm{c},q})$

The "stochastic simulator" setting



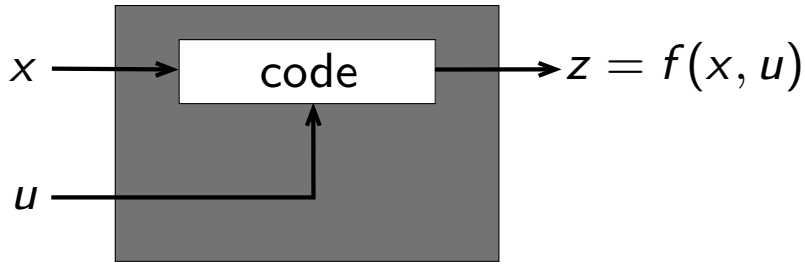
- Features of the black box
  - U is not directly accessible
  - only x can be chosen by the algorithm; $Z = f(x, U)$ is observed
  - P^U is not known explicitely

The "stochastic simulator" setting



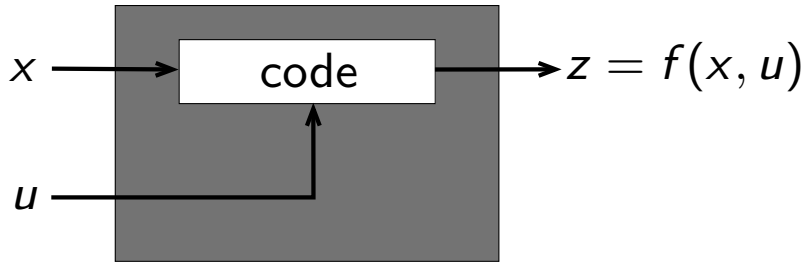
- Features of the black box
  - U is not directly accessible
  - only x can be chosen by the algorithm; $Z = f(x, U)$ is observed
  - P^U is not known explicitely
- "State of nature" (the things that we don't know)
  - the family $\left(\mathrm{P}_x^Z\right)$ of conditional distributions
  - the RV U_1, $U_2 \ldots$ that will be generated when running the computer model with inputs x_1, $x_2 \ldots$
  - the RV U_{real} that defines the $f(x, U_{\mathrm{real}})$ ultimately realized

The "environmental variables" setting



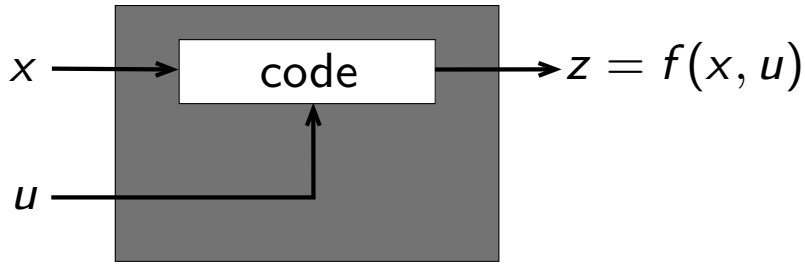
- Features of the black box
  - the simulator remains deterministic
  - P^U is specified separately, usually explicitely
  - the algorithm can choose (x, u) pairs to be evaluated

The "environmental variables" setting



- Features of the black box
  - the simulator remains deterministic
  - P^U is specified separately, usually explicitely
  - the algorithm can choose (x, u) pairs to be evaluated
- "State of nature" (the things that we don't know)
  - the deterministic function $f : (x, u) \mapsto f(x, u)$
  - the RV U_{real} that defines the $f(x, U_{\mathrm{real}})$ ultimately realized

The "environmental variables" setting



- Features of the black box
  - the simulator remains deterministic
  - P^U is specified separately, usually explicitely
  - the algorithm can choose (x, u) pairs to be evaluated
- "State of nature" (the things that we don't know)
  - the deterministic function $f : (x, u) \mapsto f(x, u)$
  - the RV U_{real} that defines the $f(x, U_{\mathrm{real}})$ ultimately realized
- The two settings can be mixed ☺

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

- 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}.

- 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

Optimization of a mean response

- Assume
  - single objective $f = f_{\mathrm{o}}$, 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 $f = f_{\mathrm{o}}$, 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

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

Optimization of a mean response

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

$$\mathsf{E}_N\left(L\left((\xi, U_{\text{real}}), \widehat{x}\right)\right) = \mathsf{E}_N\left(\xi(\widehat{x}, U_{\text{real}})\right) - \mathsf{E}_N\left(\min \xi(\cdot, U_{\text{real}})\right)$$

Optimization of a mean response

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

$$\begin{aligned}\mathsf{E}_N\left(L\left((\xi, U_{\text{real}}), \widehat{x}\right)\right) &= \mathsf{E}_N\left(\xi(\widehat{x}, U_{\text{real}})\right) - \mathsf{E}_N\left(\min \xi(\cdot, U_{\text{real}})\right) \\ &= \mathsf{E}_N\left(\overline{\xi}(\widehat{x})\right) - \mathsf{E}_N\left(\min \xi(\cdot, U_{\text{real}})\right)\end{aligned}$$

where $\overline{\xi}(x) = \int \xi(x, u)\, \mathsf{P}^U(\mathrm{d}u)$

Optimization of a mean response

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

$$\begin{aligned}\mathsf{E}_N\left(L\left((\xi, U_{\text{real}}), \widehat{x}\right)\right) &= \mathsf{E}_N\left(\xi(\widehat{x}, U_{\text{real}})\right) - \mathsf{E}_N\left(\min \xi(\cdot, U_{\text{real}})\right) \\ &= \mathsf{E}_N\left(\overline{\xi}(\widehat{x})\right) - \mathsf{E}_N\left(\min \xi(\cdot, U_{\text{real}})\right)\end{aligned}$$

where $\overline{\xi}(x) = \int \xi(x, u)\, \mathsf{P}^U(\mathrm{d}u)$

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

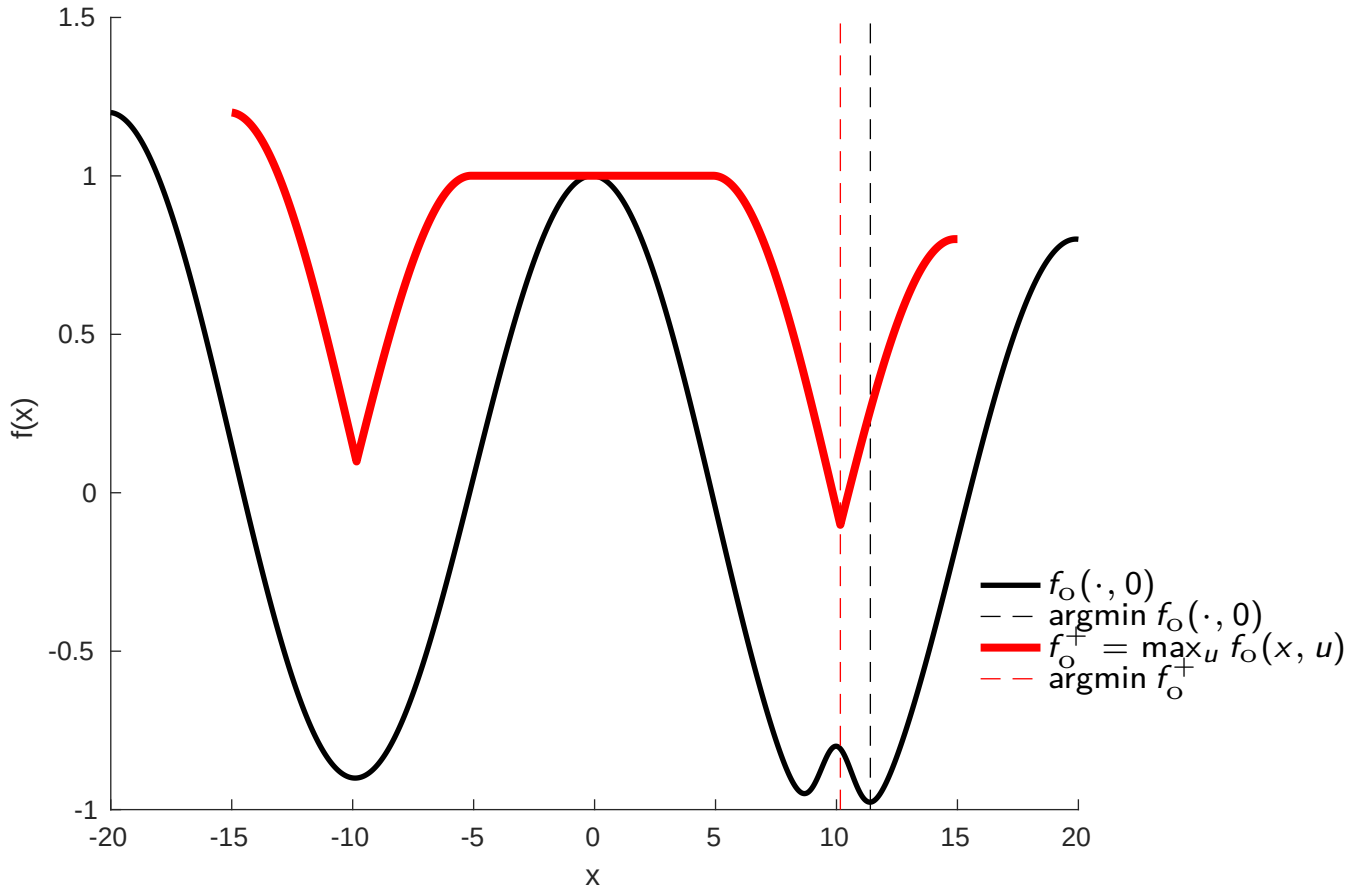
Equivalent "deterministic" problem

$$\min_x \overline{f}(x), \quad \text{with } \overline{f}(x) = \int f(x, u)\, \mathsf{P}^U(\mathrm{d}u)$$

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

Example 1: Illustration of the worst-case approach

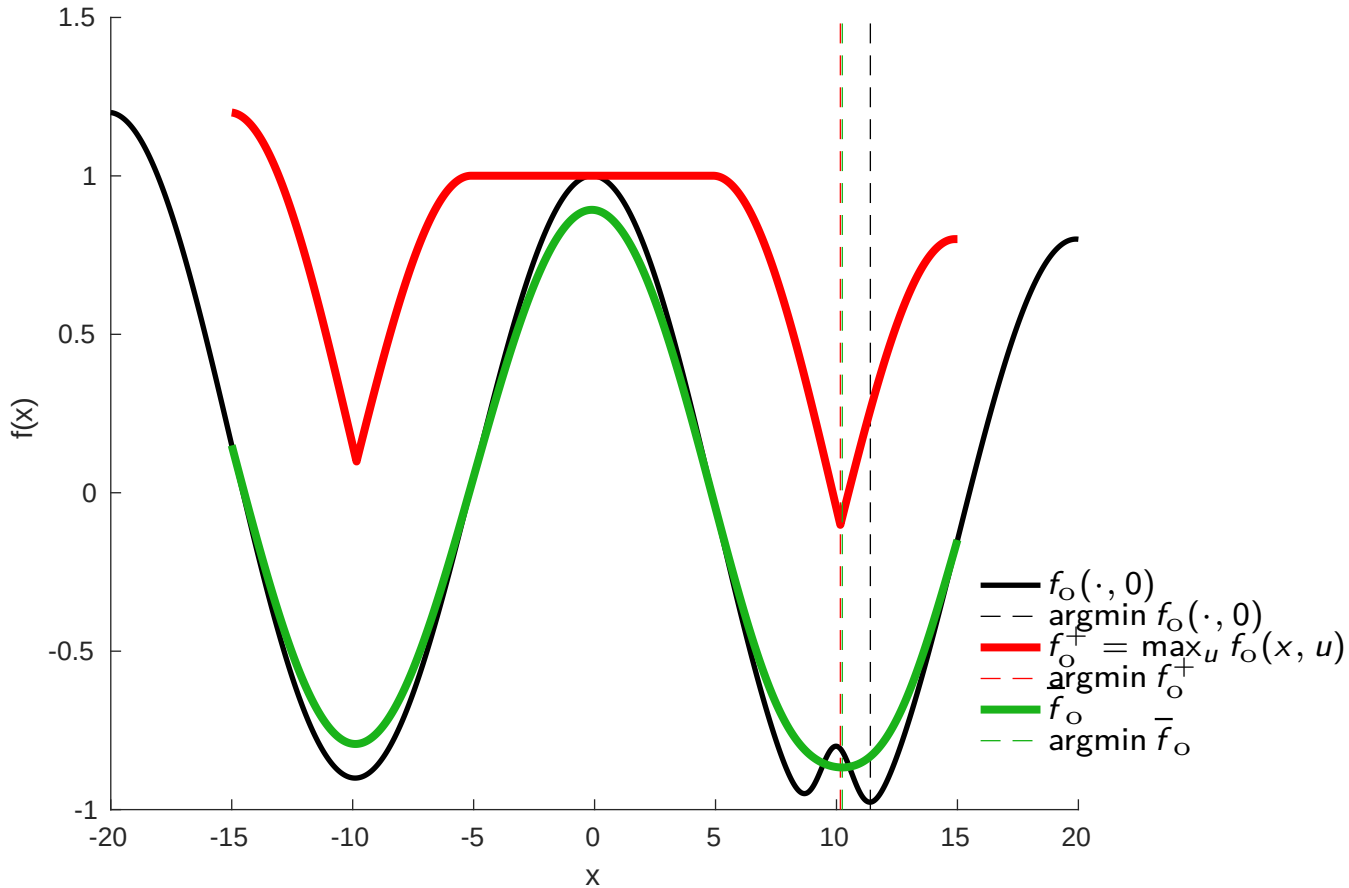
Example: $f_o(x,u) = \widetilde{f}(x+u)$, with $u \in \mathbb{U} = [-\delta;\delta]$, $\delta = 5$



Remark: very conservative, the nominal performance is ignored

Example 1: Worst-case versus probabilistic approach

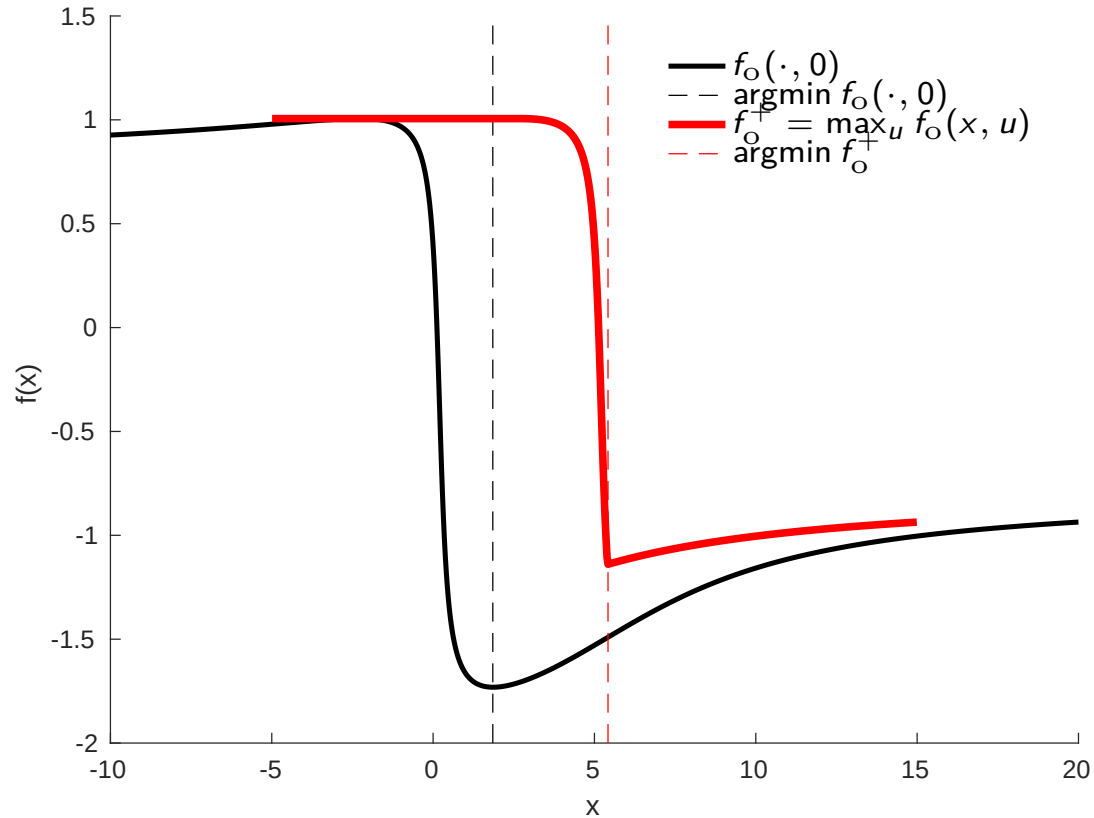
Example: $f_{\mathrm{o}}(x,u) = \widetilde{f}(x+u)$, with $u \in \mathbb{U} = [-\delta;\delta]$, $\delta = 5$



$\overline{f}_{\mathrm{o}} = \mathrm{E}\left(f_{\mathrm{o}}(\cdot,U)\right)$, with $U \sim \mathcal{N}(0,s^2)$, s.t. $\mathrm{P}\left(|U| \leq \delta\right) = 99.9\%$

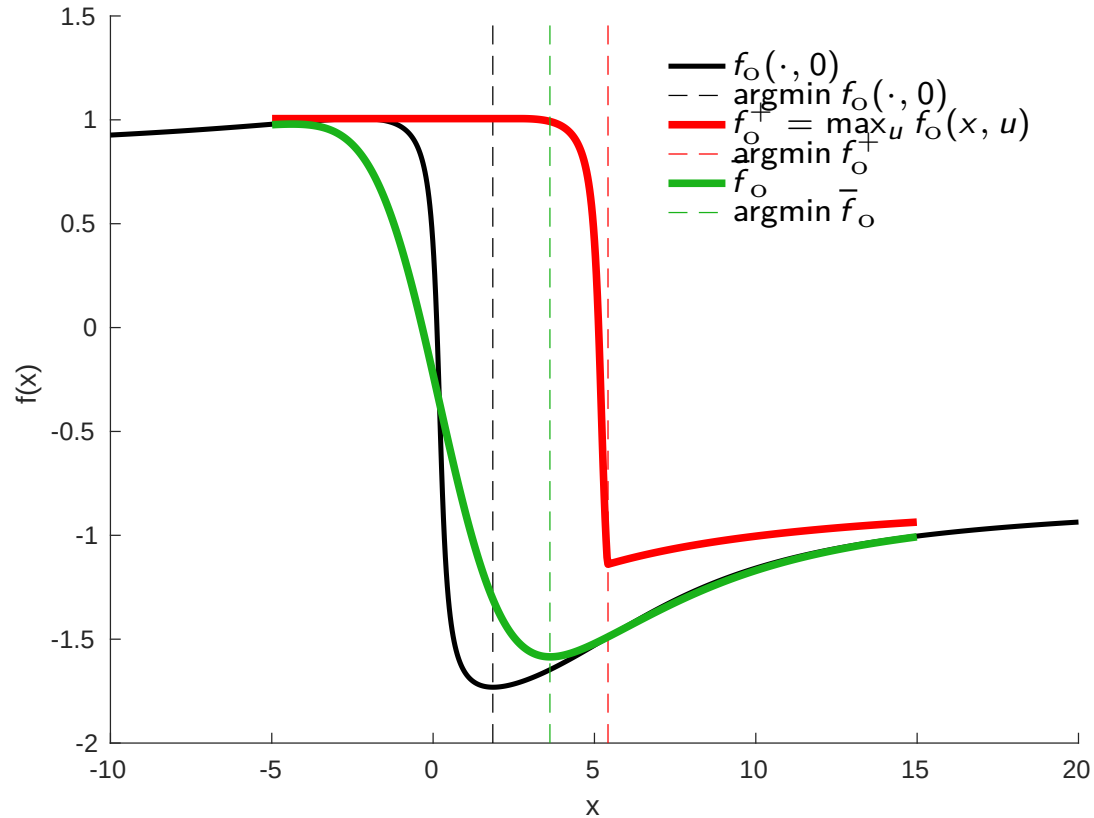
Example 2: Illustration of the worst-case approach

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



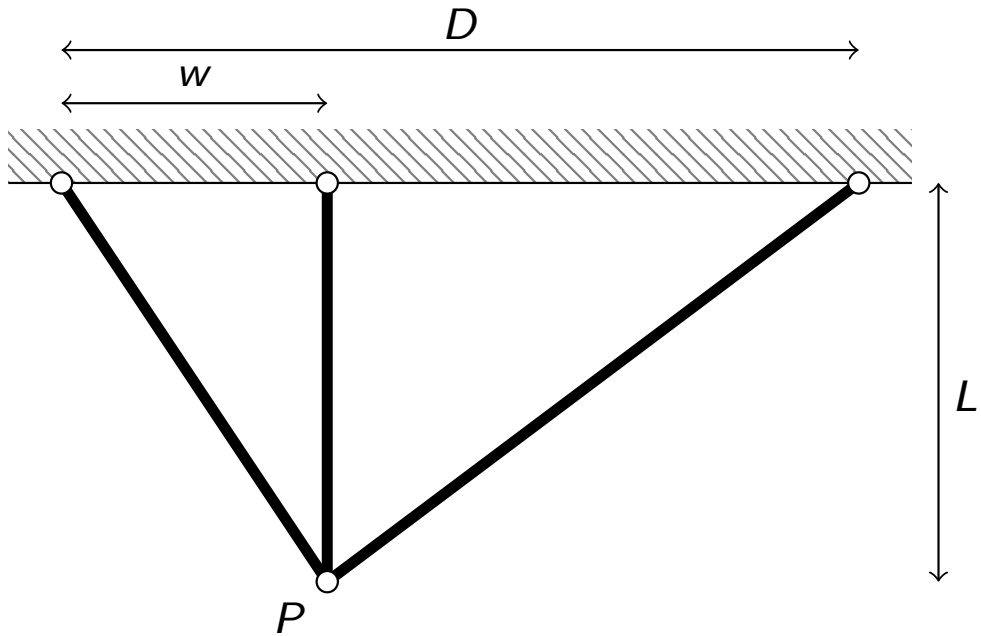
Example 2: Worst-case versus probabilistic approach

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

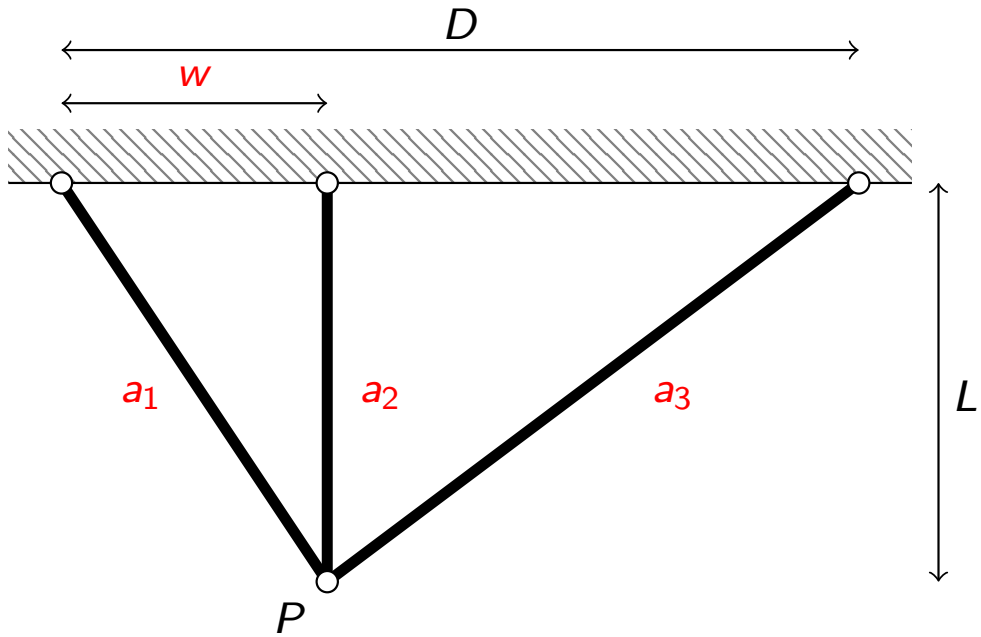


$\overline{f}_o = \mathrm{E}\,(f_o(\cdot,U))$, with $U \sim \mathcal{N}(0,s^2)$, s.t. $\mathrm{P}\,(|U| \leq \delta) = 99.9\%$

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

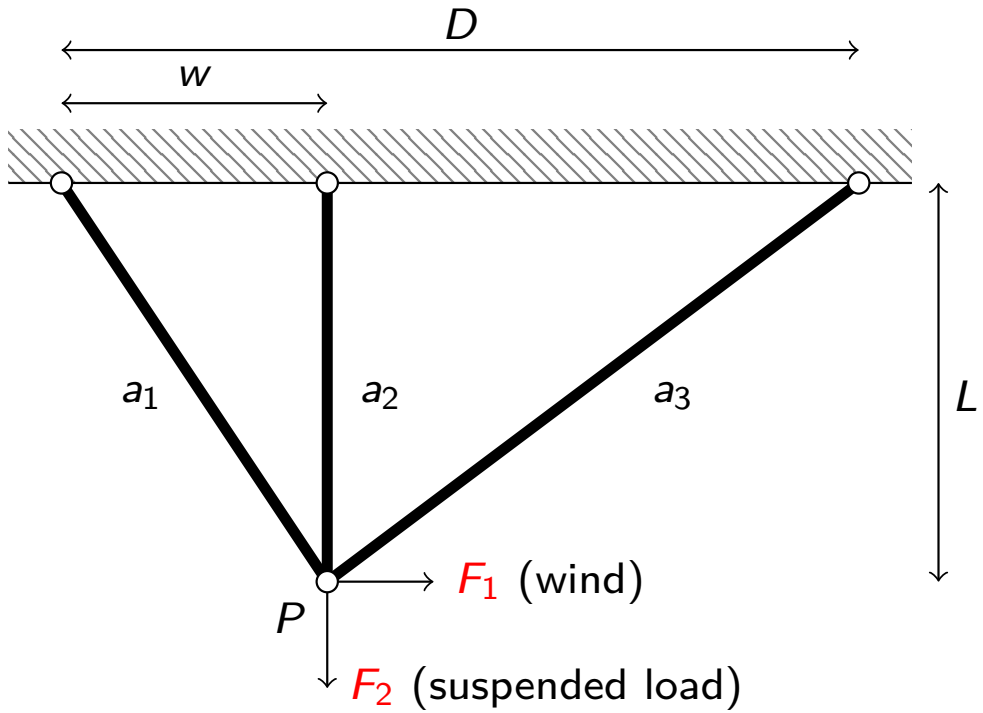


Example 3: Three-bar truss (Koski, 1985; Das, 1997)



- Design variables: $x = (a_1, a_2, a_3, w)$
  - a_j: cross-section of bar j

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



- Design variables: $x = (a_1, a_2, a_3, w)$
  - a_j: cross-section of bar j
- Environmental variables: $U = (F_1, F_2)$

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

- Our (supposedly expensive) numerical model computes
  - the displacement $y = (y_1, y_2)$ of point P,
  - the stress σ_j in each bar ($1 \leq j \leq 3$).

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

- Our (supposedly expensive) numerical model computes
  - the displacement $y = (y_1, y_2)$ of point P,
  - the stress σ_j in each bar ($1 \leq j \leq 3$).
- We will consider the following problem:
  - minimize $\mathrm{E}_U(\|y\|)$
  - under the constraints: $x_{\min} \leq x \leq x_{\max}$, $V \leq V_{\max}$

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

- Our (supposedly expensive) numerical model computes
  - the displacement $y = (y_1, y_2)$ of point P,
  - the stress σ_j in each bar ($1 \leq j \leq 3$).
- We will consider the following problem:
  - minimize $\mathrm{E}_U(\|y\|)$
  - 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 $\overline{f}$
  - inner loop: integration (MC, quadrature...) to compute $\overline{f}$

Breaking the "double loop"

- Natural "double loop" approach
  - outer loop: ordinary optimization algorithm applied to $\overline{f}$
  - inner loop: integration (MC, quadrature...) to compute $\overline{f}$
- Drawback: typically require large number of evaluations

Breaking the "double loop"

- Natural "double loop" approach
  - outer loop: ordinary optimization algorithm applied to $\overline{f}$
  - inner loop: integration (MC, quadrature...) to compute $\overline{f}$
- Drawback: typically require large number of evaluations
- Bayesian optimization breaks the double loop ☺
  - Construct a Bayesian model for f, not $\overline{f}$
  - Remark: can be achieved using other surrogate-model based approaches (see Janusevkis & 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: $\overline{f} = \int f(\cdot, u) \, \mathrm{P}^U(\mathrm{d}u)$
- $\overline{f}$ is a function of f
  - priors cannot be specified independently

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: $\overline{f} = \int f(\cdot, u)\, \mathrm{P}^U(\mathrm{d}u)$
- $\overline{f}$ is a function of f
  - priors cannot be specified independently

Gaussian process priors are, again, very convenient

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

with

$$m_{\overline{\xi}}(x) = \int m(x, u)\, \mathrm{P}^U(\mathrm{d}u)$$

$$k_{\overline{\xi}}(x, y) = \iint k((x, u), (y, v))\, \mathrm{P}^U(\mathrm{d}u)\mathrm{P}^U(\mathrm{d}v)$$

Proof

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

$$m_{\overline{\xi}}(x) = \mathrm{E}\left(\overline{\xi}(x)\right) = \mathrm{E}\left(\int \xi(x,u)\,\mathrm{P}^U(du)\right)$$
$$= \int m(x,u)\,\mathrm{P}^U(du)$$

- Computation of the covariance function: idem with bilinearity

$$k_{\overline{\xi}}(x,y) = \mathrm{cov}\left(\overline{\xi}(x), \overline{\xi}(y)\right)$$
$$= \mathrm{cov}\left(\int \xi(x,u)\,\mathrm{P}^U(du), \int \xi(x,v)\,\mathrm{P}^U(dv)\right)$$
$$= \iint k((x,u),(y,v))\,\mathrm{P}^U(du)\mathrm{P}^U(\mathrm{d}v) \qquad \blacksquare$$

Prior model (cont'd)

- Actually, we can say much better:

Jointly Gaussian processes

If $\xi \sim \mathcal{GP}(m, k)$, then ξ and $\overline{\xi}$ are jointly Gaussian, and
$k_{\xi,\overline{\xi}}((x,u),y) = \mathrm{cov}(\xi(x,u), \overline{\xi}(y)) = \int k((x,u),(y,v))\,\mathrm{P}^U(\mathrm{d}v)$

Prior model (cont'd)

- Actually, we can say much better:

Jointly Gaussian processes

If $\xi \sim \mathcal{GP}(m, k)$, then ξ and $\overline{\xi}$ are jointly Gaussian, and
$k_{\xi,\overline{\xi}}((x,u),y) = \mathrm{cov}(\xi(x,u), \overline{\xi}(y)) = \int k((x,u),(y,v))\,\mathrm{P}^U(\mathrm{d}v)$

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

Prior model (cont'd)

- Actually, we can say much better:

Jointly Gaussian processes

If $\xi \sim \mathcal{GP}(m, k)$, then ξ and $\overline{\xi}$ are jointly Gaussian, and
$k_{\xi,\overline{\xi}}((x,u),y) = \mathrm{cov}(\xi(x,u), \overline{\xi}(y)) = \int k((x,u),(y,v))\,\mathrm{P}^U(\mathrm{d}v)$

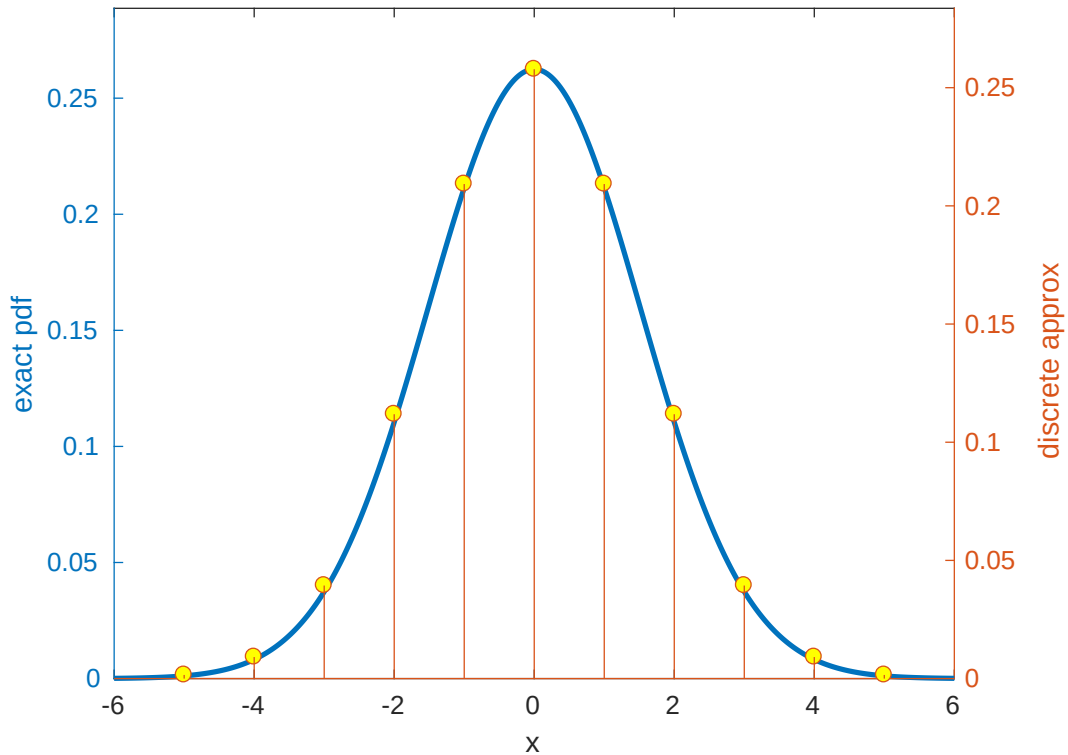
- Remark: $m_{\overline{\xi}}$, $k_{\overline{\xi}}$ and $k_{\xi,\overline{\xi}}$ can be computed exactly
  - if P^U is discrete ($\mathrm{P}^U = \sum_{j=1}^{n_U} w_j \delta_{u_j}$)
  - if P^U is (a mixture of) Gaussian(s), for some particular k
  - see Girard (2004) for exact formulas & approximations
- Important special case: $\xi(x,u) = \widetilde{\xi}(x+u)$
  - If ξ is a GP iff $\widetilde{\xi}$ is a GP
  - $m_\xi(x,u) = m_{\widetilde{\xi}}(x+u)$ and $k_\xi((x,u),(u,v)) = k_{\widetilde{\xi}}(x+u, y+v)$

Examples 1 and 2: discretization of P^U

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

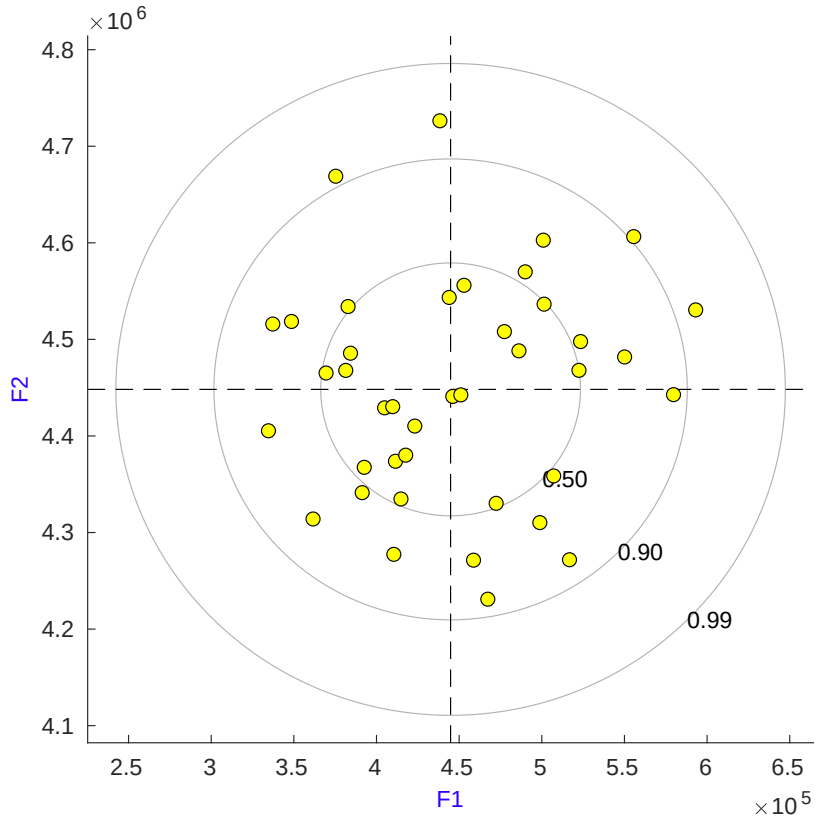
Examples 1 and 2: discretization of P^U

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

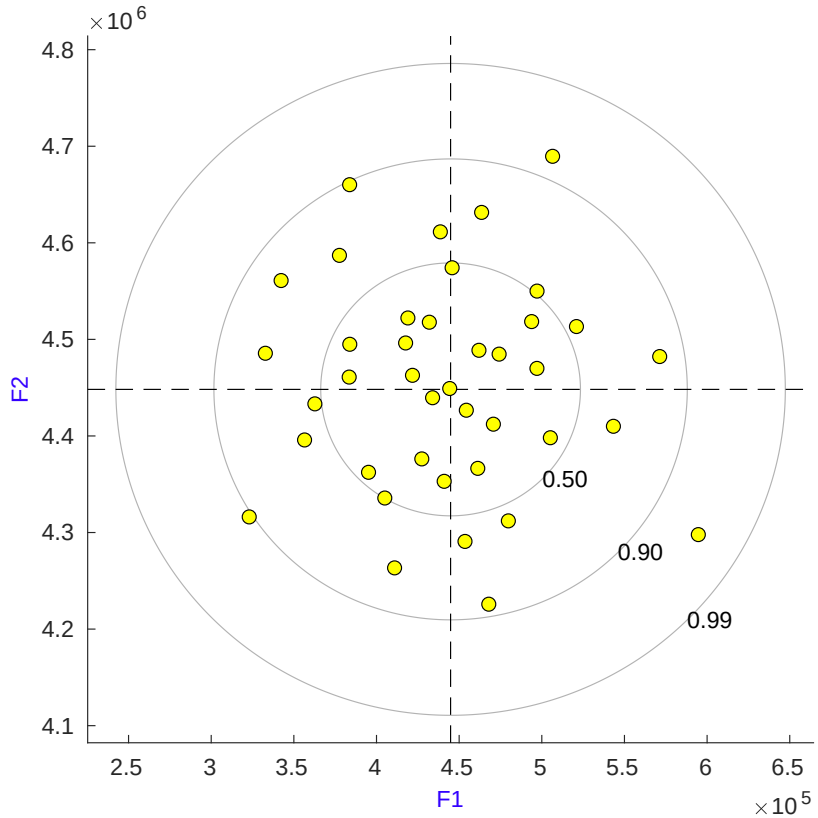
- Here, $U = \begin{pmatrix} F_1 \\ F_2 \end{pmatrix}$ and $\mathrm{P}^U = \mathcal{N}\left(\begin{pmatrix} \mu_{F_1} \\ \mu_{F_2} \end{pmatrix}, \begin{pmatrix} \sigma^2_{F_1} & 0 \\ 0 & \sigma^2_{F_2} \end{pmatrix} \right)$



Monte Carlo sample of size $n_U = 50$

Example 3: discretization of P^U

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



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

Sampling strategy: what ?

- What decision(s) do we have to make at each step ?
  - i.e, what do we need to provide to run the numerical model ?

Sampling strategy: what ?

- What decision(s) do we have to make at each step ?
  - i.e, what do we need to provide to run the numerical model ?
- General case
  - numerical model $f : (x, u) \mapsto f(x, u)$, defined on $\mathbb{X} \times \mathbb{U}$
  - at each step, we must select a pair $(X_{n+1}, U_{n+1}) \in \mathbb{X} \times \mathbb{U}$

Sampling strategy: what ?

- What decision(s) do we have to make at each step ?
  - i.e, what do we need to provide to run the numerical model ?
- General case
  - numerical model $f : (x, u) \mapsto f(x, u)$, defined on $\mathbb{X} \times \mathbb{U}$
  - at each step, we must select a pair $(X_{n+1}, U_{n+1}) \in \mathbb{X} \times \mathbb{U}$
- Important special case
  - $f(x, u) = \widetilde{f}(x + u)$
  - 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

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

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
  - other strategies are proposed in the literature
    - Williams et al 2000; Janusevkis 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 $\widehat{x} \in \mathbb{X}$:

$$\mathrm{E}_N\left(L\left((\xi, U_{\mathrm{real}}), \widehat{x}\right)\right) = \mathrm{E}_N\left(\overline{\xi}(\widehat{x})\right) - \mathrm{E}_N\left(\min_{\mathbb{X}} \xi(\cdot, U_{\mathrm{real}})\right)$$

Sampling strategy: one step look-ahead

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

$$\begin{aligned}\overline{L}_n &= \min_{\mathbb{X}} \mathsf{E}_n\left(\overline{\xi}(x)\right) - \mathsf{E}_n\left(\min_{\mathbb{X}} \xi(\cdot, U_{\text{real}})\right) \\ &= \min_{\mathbb{X}} m_{\overline{\xi},n} - \mathsf{E}_n\left(\min_{\mathbb{X}} \xi(\cdot, U_{\text{real}})\right)\end{aligned}$$

Sampling strategy: one step look-ahead

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

$$\begin{aligned}\overline{L}_n &= \min_{\mathbb{X}} \mathsf{E}_n\left(\overline{\xi}(x)\right) - \mathsf{E}_n\left(\min_{\mathbb{X}} \xi(\cdot, U_{\text{real}})\right) \\ &= \min_{\mathbb{X}} m_{\overline{\xi},n} - \mathsf{E}_n\left(\min_{\mathbb{X}} \xi(\cdot, U_{\text{real}})\right)\end{aligned}$$

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

$$(X_{n+1}, U_{n+1}) = \operatorname{argmin}_{x_{n+1}, u_{n+1}} \mathsf{E}_{n,(x_{n+1},u_{n+1})}\left(\overline{L}_{n+1}\right)$$

Sampling strategy: one step look-ahead

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

$$\begin{aligned}\overline{L}_n &= \min_{\mathbb{X}} \mathsf{E}_n\left(\overline{\xi}(x)\right) - \mathsf{E}_n\left(\min_{\mathbb{X}} \xi(\cdot, U_{\text{real}})\right) \\ &= \min_{\mathbb{X}} m_{\overline{\xi},n} - \mathsf{E}_n\left(\min_{\mathbb{X}} \xi(\cdot, U_{\text{real}})\right)\end{aligned}$$

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

$$\begin{aligned}(X_{n+1}, U_{n+1}) &= \operatorname{argmin}_{x_{n+1},u_{n+1}} \mathsf{E}_{n,(x_{n+1},u_{n+1})}\left(\overline{L}_{n+1}\right) \\ &= \operatorname{argmin}_{x_{n+1},u_{n+1}} \mathsf{E}_{n,(x_{n+1},u_{n+1})}\left(\min_{\mathbb{X}} m_{\overline{\xi},n+1}\right)\end{aligned}$$

Sampling strategy: one step look-ahead

- Equivalently,

$$(X_{n+1}, U_{n+1}) = \text{argmax}_{x_{n+1}, u_{n+1}} \ \rho_n(x_{n+1}, u_{n+1})$$

where ρ_n denotes the corresponding "expected improvement"

$$\begin{aligned}\rho_n(x_{n+1}, u_{n+1}) &= \overline{L}_n - \mathsf{E}_{n,(x_{n+1},u_{n+1})}\left(\overline{L}_{n+1}\right) \\ &= \min \mathbb{X}\, m_{\overline{\xi},n} - \mathsf{E}_{n,(x_{n+1},u_{n+1})}\left(\min \mathbb{X}\, m_{\overline{\xi},n+1}\right)\end{aligned}$$

Sampling strategy: one step look-ahead

- Equivalently,

$$(X_{n+1}, U_{n+1}) = \text{argmax}_{x_{n+1}, u_{n+1}} \ \rho_n(x_{n+1}, u_{n+1})$$

where ρ_n denotes the corresponding "expected improvement"

$$\begin{aligned}\rho_n(x_{n+1}, u_{n+1}) &= \overline{L}_n - \mathsf{E}_{n,\,(x_{n+1}, u_{n+1})}\left(\overline{L}_{n+1}\right) \\ &= \min \mathbb{X}\, m_{\overline{\xi},n} - \mathsf{E}_{n,\,(x_{n+1}, u_{n+1})}\left(\min \mathbb{X}\, m_{\overline{\xi},n+1}\right)\end{aligned}$$

- 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	$\xi(x) + \mathcal{N}$noise	$\min \xi$
here	$\xi(x, u)$	$\min \overline{\xi}$

Sampling strategy: one step look-ahead

- Comparison with KG as presented in the literature

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

- There is no real difference mathematically: in both cases
  1. the function to be optimized is not observable directly,
  2. the evaluation results and the function to be optimized are jointly Gaussian.

Sampling strategy: one step look-ahead

- Comparison with KG as presented in the literature

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

- There is no real difference mathematically: in both cases
  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:

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

where the min runs over $\mathbb{X}_n^{\text{ref}} \cup \{\tilde{x}_{n+1}\}$.

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:

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

where the min runs over $\mathbb{X}_n^{\text{ref}} \cup \{\tilde{x}_{n+1}\}$.

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:

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

  where the min runs over $\mathbb{X}_n^{\text{ref}} \cup \{\tilde{x}_{n+1}\}$.

- Initially proposed by Scott et al (2011)
  - under the name KGCP ("KG for continuous parameters")
  - with $\mathbb{X}_n^{\text{ref}} = \{X_1, \ldots, X_n\}$

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:

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

  where the min runs over $\mathbb{X}_n^{\text{ref}} \cup \{\tilde{x}_{n+1}\}$.

- Initially proposed by Scott et al (2011)
  - under the name KGCP ("KG for continuous parameters")
  - with $\mathbb{X}_n^{\text{ref}} = \{X_1, \ldots, X_n\}$
- 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

- 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.
- Review/benchmark of existing criteria: Picheny et al (2013)
  - AKG emerges has one of the most efficient criteria
  - Huang et al (2006)'s "augmented EI" also performs well
  - (Entropy-based criteria not benchmarked)

(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.
- Review/benchmark of existing criteria: Picheny et al (2013)
  - AKG emerges has one of the most efficient criteria
  - Huang et al (2006)'s "augmented EI" also performs well
  - (Entropy-based criteria not benchmarked)
- What about simulators with truly non-Gaussian output ?
  - "batch trick" (CLT)
  - see also Browne et al (2016)...

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

- Assume
  - a single objective $f = f_{\mathrm{o}}$, often cheap to evaluate
  - one or several expensive-to-evaluate constraints $f_{\mathrm{c},1}, \ldots, f_{\mathrm{c},q}$
  - "environmental variables" setting

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

- Assume
  - a single objective $f = f_{\mathrm{o}}$, often cheap to evaluate
  - one or several expensive-to-evaluate constraints $f_{\mathrm{c},1}, \ldots, f_{\mathrm{c},q}$
  - "environmental variables" setting

- The so-called RB(D)O formulation reads:

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

Minimize

$$\overline{f_{\mathrm{o}}}(x), \quad \text{where } f_{\mathrm{o}}(x) = \mathrm{E}_U\left(f_{\mathrm{o}}(x, U)\right)$$

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

$$\forall j \leq q, \quad \mathrm{P}_U\left(f_{\mathrm{c},j}(x, U) > 0\right) \leq p_j^{\mathrm{tol}}$$

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

- See Valdebenito & Schuëller (2010) for a survey

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

- See Valdebenito & Schuëller (2010) for a survey
- $\overline{f_{\mathrm{o}}}$ is often cheap to evaluate
  - e.g. volume / mass / manufacturing cost / ...
  - Expectation often computed (or approximated) analytically

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

- See Valdebenito & Schuëller (2010) for a survey
- $\overline{f_{\mathrm{o}}}$ is often cheap to evaluate
  - e.g. volume / mass / manufacturing cost / ...
  - Expectation often computed (or approximated) analytically
- Again, algorithms with a "double loop" structure can be used
  - outer loop: ordinary optimization algorithm with constraints
  - inner loop: reliability analysis method to compute the constraints

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

- See Valdebenito & Schuëller (2010) for a survey
- $\overline{f_{\mathrm{o}}}$ is often cheap to evaluate
  - e.g. volume / mass / manufacturing cost / ...
  - Expectation often computed (or approximated) analytically
- Again, algorithms with a "double loop" structure can be used
  - 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. $\mathrm{P}^U \approx \frac{1}{m}\sum_j \delta_{u_j}$ becomes very expensive or infeasible
  - Dedicated techniques (e.g., FORM/SORM, IS, subset simulation) needed for an efficient evaluation of the constraints

Why RBDO is harder than mean-response optimization

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

- BO: the distribution of $\mathrm{P}_U\left(\xi_{\mathrm{c},j}(x,U) > 0\right)$ 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

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

$\theta^{(0)}, \theta^L, \theta^U, j := 0$
for $i = 1$ **to** n **do**
  $q_{\bar{V}_i} := \min_{\theta^L \leq \theta \leq \theta^U} F^{-1}_{X_i}(x_i, \theta)$
  $q^+_{V_i} := \max_{\theta^L \leq \theta \leq \theta^U} F^{-1}_{X_i}(x_i, \theta)$
end for
$w := v \mapsto \mathbb{1}_{\mathscr{D}_V, \beta_0}(v)$
$k := \Phi^{-1}(97.5\%), \varepsilon_\beta := 10^{-1}$
Refine := **true**, Optimize := **true**
while Refine **and** Optimize **do**
  while Refine **do**
    $\widehat{G} :=$ RefineKrigingModel$(w, k, \varepsilon_\beta) \hookrightarrow$ *Use Algorithm 1*
  end while
  $\widehat{F}^{\,0} := \{x \,:\, \mu_{\widehat{G}}(x) \leq 0\}$
  $\widehat{\beta}^{(j)}, \nabla_\theta \widehat{\beta}^{(j)} :=$ ReliabilityAnalysis$(\widehat{F}^{\,0}, \theta^{(j)})$
  $c^{(j)} := c(\theta^{(j)}), \nabla_\theta c^{(j)} := \nabla_\theta c(\theta^{(j)})$
  $f^{(j)} := f(\theta^{(j)}), \nabla_\theta f^{(j)} := \nabla_\theta f(\theta^{(j)})$
  $d^{(j)} :=$ SolveQuasiSQP$(c^{(j)}, f^{(j)}, \widehat{\beta}^{(j)}, \nabla_\theta c^{(j)}, \nabla_\theta f^{(j)}, \nabla_\theta \widehat{\beta}^{(j)})$
  $s^{(j)} :=$ GoldsteinArmijoStepSizeRule$(c, f, \widehat{\beta}, d^{(j)})$
  $\theta^{(j+1)} := \theta^{(j)} + s^{(j)} d^{(j)}$
  for $i := -1, 0, +1$ **do**
    $\widehat{F}^{\,i} := \{x \,:\, \mu_{\widehat{G}}(x) + ik\sigma_{\widehat{G}}(x) \leq 0\}$
    $\widehat{\beta}^{\,i} :=$ ReliabilityAnalysis$(\widehat{F}^{\,i}, \theta^{(j+1)})$
  end for
  Refine := $\max\left(\widehat{\beta}^{+1} - \widehat{\beta}^{\,0}, \widehat{\beta}^{\,0} - \widehat{\beta}^{-1}\right) > \varepsilon_\beta$
  Optimize := $\left\|\theta^{(j+1)} - \theta^{(j)}\right\| > \varepsilon_\theta$ **or** $\left\|c^{(j+1)} - c^{(j)}\right\| > \varepsilon_c$
    or $\exists\, i \mid f_i > 0$ **or** $\widehat{\beta} < \beta_0$
end while

Algorithm 1 Population-based adaptive refinement strategy

$\mathscr{X} = \emptyset, \mathscr{G} = \emptyset$
$w := x \mapsto w(x)$
$k := \Phi^{-1}(97.5\%), \varepsilon_\beta := 10^{-1}$
Refine := **true**
$\mathbb{P}(x \in \mathbb{M}) := x \mapsto 1$
while Refine **do**
  $\mathscr{P} :=$ MCMCAlgorithm$(\mathscr{C})$
  $\mathscr{X}_{\text{new}} :=$ KMeansAlgorithm$(\mathscr{P}, K)$
  $\mathscr{G}_{\text{new}} := g(\mathscr{X}_{\text{new}})$
  $\mathscr{X} := \{\mathscr{X}, \mathscr{X}_{\text{new}}\}, \mathscr{G} := \{\mathscr{G}, \mathscr{G}_{\text{new}}\}$
  $\widehat{G} :=$ MaximumLikelihoodKrigingModel
    $(\mathscr{X}, \mathscr{G}, f(\bullet), R(\bullet, \ell), \ell_L, \ell_U)$
  $\mathbb{P}(x \in \mathbb{M}) := x \mapsto \Phi\left(\frac{k\sigma_{\widehat{G}}(x) - \mu_{\widehat{G}}(x)}{\sigma_{\widehat{G}}(x)}\right) - \Phi\left(\frac{-k\sigma_{\widehat{G}}(x) - \mu_{\widehat{G}}(x)}{\sigma_{\widehat{G}}(x)}\right)$
  $\mathscr{C} := x \mapsto \mathbb{P}(x \in \mathbb{M})\, w(x)$
  for $i := -1, 0, +1$ **do**
    $\widehat{F}^{\,i} := \{x \,:\, \mu_{\widehat{G}}(x) + ik\sigma_{\widehat{G}}(x) \leq 0\}$
    $\widehat{\beta}^{\,i} :=$ ReliabilityAnalysis$(\widehat{F}^{\,i})$
  end for
  Refine := $\max\left(\widehat{\beta}^{+1} - \widehat{\beta}^{\,0}, \widehat{\beta}^{\,0} - \widehat{\beta}^{-1}\right) > \varepsilon_\beta$
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

$\theta^{(0)}, \theta^L, \theta^U, j := 0$
for $i = 1$ **to** n **do**
  $q_{\bar{V}_i} := \min_{\theta^L \leq \theta \leq \theta^U} F^{-1}_{X_i}(x_i, \theta)$
  $q^+_{V_i} := \max_{\theta^L \leq \theta \leq \theta^U} F^{-1}_{X_i}(x_i, \theta)$
end for
$w := v \mapsto \mathbb{1}_{\mathscr{D}_V, \beta_0}(v)$
$k := \Phi^{-1}(97.5\%), \varepsilon_\beta := 10^{-1}$
Refine := **true**, Optimize := **true**
while Refine **and** Optimize **do**
  while Refine **do**
    $\widehat{G} :=$ RefineKrigingModel$(w, k, \varepsilon_\beta)$ ↪ *Use Algorithm 1*
  end while
  $\widehat{F}^{\,0} := \{x \,:\, \mu_{\widehat{G}}(x) \leq 0\}$
  $\widehat{\beta}^{(j)}, \nabla_\theta \widehat{\beta}^{(j)} :=$ ReliabilityAnalysis$(\widehat{F}^{\,0}, \theta^{(j)})$
  $c^{(j)} := c(\theta^{(j)}), \nabla_\theta c^{(j)} := \nabla_\theta c(\theta^{(j)})$
  $f^{(j)} := f(\theta^{(j)}), \nabla_\theta f^{(j)} := \nabla_\theta f(\theta^{(j)})$
  $d^{(j)} :=$ SolveQuasiSQP$(c^{(j)}, f^{(j)}, \widehat{\beta}^{(j)}, \nabla_\theta c^{(j)}, \nabla_\theta f^{(j)}, \nabla_\theta \widehat{\beta}^{(j)})$
  $s^{(j)} :=$ GoldsteinArmijoStepSizeRule$(c, f, \widehat{\beta}, d^{(j)})$
  $\theta^{(j+1)} := \theta^{(j)} + s^{(j)} d^{(j)}$
  for $i := -1, 0, +1$ **do**
    $\widehat{F}^{\,i} := \{x \,:\, \mu_{\widehat{G}}(x) + ik\sigma_{\widehat{G}}(x) \leq 0\}$
    $\widehat{\beta}^{\,i} :=$ ReliabilityAnalysis$(\widehat{F}^{\,i}, \theta^{(j+1)})$
  end for
  Refine := $\max\left(\widehat{\beta}^{+1} - \widehat{\beta}^{\,0}, \widehat{\beta}^{\,0} - \widehat{\beta}^{-1}\right) > \varepsilon_\beta$
  Optimize := $\left\|\theta^{(j+1)} - \theta^{(j)}\right\| > \varepsilon_\theta$ **or** $\left\|c^{(j+1)} - c^{(j)}\right\| > \varepsilon_c$ **or** $\exists\, i \mid f_i > 0$ **or** $\widehat{\beta} < \beta_0$
end while

Algorithm 1 Population-based adaptive refinement strategy

$\mathscr{X} = \emptyset, \mathscr{G} = \emptyset$
$w := x \mapsto w(x)$
$k := \Phi^{-1}(97.5\%), \varepsilon_\beta := 10^{-1}$
Refine := **true**
$\mathbb{P}(x \in \mathbb{M}) := x \mapsto 1$
while Refine **do**
  $\mathscr{P} :=$ MCMCAlgorithm$(\mathscr{C})$
  $\mathscr{X}_{\text{new}} :=$ KMeansAlgorithm$(\mathscr{P}, K)$
  $\mathscr{G}_{\text{new}} := g(\mathscr{X}_{\text{new}})$
  $\mathscr{X} := \{\mathscr{X}, \mathscr{X}_{\text{new}}\}, \mathscr{G} := \{\mathscr{G}, \mathscr{G}_{\text{new}}\}$
  $\widehat{G} :=$ MaximumLikelihoodKrigingModel $(\mathscr{X}, \mathscr{G}, f(\bullet), R(\bullet, \ell), \ell_L, \ell_U)$
  $\mathbb{P}(x \in \mathbb{M}) := x \mapsto \Phi\left(\frac{k\sigma_{\widehat{G}}(x) - \mu_{\widehat{G}}(x)}{\sigma_{\widehat{G}}(x)}\right) - \Phi\left(\frac{-k\sigma_{\widehat{G}}(x) - \mu_{\widehat{G}}(x)}{\sigma_{\widehat{G}}(x)}\right)$
  $\mathscr{C} := x \mapsto \mathbb{P}(x \in \mathbb{M})\, w(x)$
  for $i := -1, 0, +1$ **do**
    $\widehat{F}^{\,i} := \{x \,:\, \mu_{\widehat{G}}(x) + ik\sigma_{\widehat{G}}(x) \leq 0\}$
    $\widehat{\beta}^{\,i} :=$ ReliabilityAnalysis$(\widehat{F}^{\,i})$
  end for
  Refine := $\max\left(\widehat{\beta}^{+1} - \widehat{\beta}^{\,0}, \widehat{\beta}^{\,0} - \widehat{\beta}^{-1}\right) > \varepsilon_\beta$
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,

RBDO and other formulations: alternative approach

- A general alternative approach in two (or three) 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,
  3. optionally Reduce the uncertainty on the most promising designs.

RBDO and other formulations: alternative approach

- A general alternative approach in two (or three) 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,
  3. optionally Reduce the uncertainty on the most promising designs.

- In step 1. constraints can be taken into account as objectives
  - i.e., the contraint $\mathrm{P}_U\left(f_{\mathrm{c},j}(x,U) > 0\right) \leq p_j^{\mathrm{tol}}$
  - becomes: $\min_x f_{\mathrm{c},j}(x,u_0)$ u.c. $f_{\mathrm{c},j}(x,u_0) \leq 0$

RBDO and other formulations: alternative approach

- A general alternative approach in two (or three) 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,
  3. optionally Reduce the uncertainty on the most promising designs.

- In step 1. constraints can be taken into account as objectives
  - i.e., the contraint $\mathrm{P}_U\left(f_{\mathrm{c},j}(x,U) > 0\right) \leq p_j^{\mathrm{tol}}$
  - becomes: $\min_x f_{\mathrm{c},j}(x,u_0)$ u.c. $f_{\mathrm{c},j}(x,u_0) \leq 0$

- 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 . . .

References I

Julien Bect, Emmanuel Vazquez, et al.
STK: a Small (Matlab/Octave) Toolbox for Kriging. Release 2.4.2, 2017.
URL `http://kriging.sourceforge.net`.

Aharon Ben-Tal, Laurent El Ghaoui, and Arkadi Nemirovski.
Robust optimization.
Princeton University Press, 2009.

Romain Benassi.
Nouvel algorithme d'optimisation bayésien utilisant une approche Monte-Carlo séquentielle.
PhD thesis, Supélec, 2013.

Romain Benassi, Julien Bect, and Emmanuel Vazquez.
Bayesian optimization using sequential Monte Carlo.
In *Learning and Intelligent Optimization. 6th International Conference, LION 6, Paris, France, January 16-20, 2012, Revised Selected Papers*, volume 7219 of *Lecture Notes in Computer Science*, pages 339–342. Springer, 2012.

Dimitris Bertsimas, David B Brown, and Constantine Caramanis.
Theory and applications of robust optimization.
SIAM review, 53(3):464–501, 2011.

References II

Barron Bichon, Sankaran Mahadevan, and Michael Eldred.
Reliability-based design optimization using efficient global reliability analysis.
In *50th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference 17th AIAA/ASME/AHS Adaptive Structures Conference 11th AIAA No*, page 2261, 2009.

Mickael Binois and Victor Picheny.
GPareto: Gaussian Processes for Pareto Front Estimation and Optimization.
R package version 1.0.3, 2016.

Jean-Marc Bourinet, Cécile Mattrand, and Vincent Dubourg.
A review of recent features and improvements added to FERUM software.
In H. Furuta, D. M. Frangopol, and M. Shinozuka, editors, *Proc. 10th International Conference on Structural Safety and Reliability (ICOSSAR 2009), Osaka, Japan, September 13–17, 2009*. CRC Press, 2009.

Thomas Browne, Bertrand Iooss, Loïc Le Gratiet, Jérôme Lonchampt, and Emmanuel Remy.
Stochastic simulators based optimization by gaussian process metamodels–application to maintenance investments planning issues.
Quality and Reliability Engineering International, 32(6):2067–2080, 2016.

References III

Clément Chevalier and David Ginsbourger.
Fast computation of the multi-points expected improvement with applications in batch selection.
In *International Conference on Learning and Intelligent Optimization*, pages 59–69. Springer, 2013.

Clément Chevalier, Julien Bect, David Ginsbourger, Emmanuel Vazquez, Victor Picheny, and Yann Richet.
Fast parallel kriging-based stepwise uncertainty reduction with application to the identification of an excursion set.
Technometrics, 56(4):455–465, 2014.

Indraneel Das.
Nonlinear multicriteria optimization and robust optimality.
PhD thesis, Rice University, 1997.

Vincent Dubourg.
Adaptive surrogate models for reliability analysis and reliability-based design optimization.
PhD thesis, Université Blaise Pascal-Clermont-Ferrand II, 2011.

References IV

Vincent Dubourg, Bruno Sudret, and Jean Marc Bourinet.
Reliability-based design optimization using kriging surrogates and subset simulation.
Structural and Multidisciplinary Optimization, 44(5):673–690, 2011.

Michael Emmerich, Kyriakos C. Giannakoglou, and Boris Naujoks.
Single- and multi-objective evolutionary optimization assisted by Gaussian random field metamodels.
IEEE Transactions on Evolutionary Computation, 10(4):421–439, 2006.

Paul Feliot, Julien Bect, and Emmanuel Vazquez.
A Bayesian approach to constrained single-and multi-objective optimization.
Journal of Global Optimization, 67(1-2):97–133, 2017.

Alexander Forrester, András Sóbester, and Andy Keane.
Engineering design via surrogate modelling: a practical guide.
John Wiley & Sons, 2008.

Peter Frazier, Warren Powell, and Savas Dayanik.
The knowledge-gradient policy for correlated normal beliefs.
INFORMS journal on Computing, 21(4):599–613, 2009.

References V

Peter I Frazier, Warren B Powell, and Savas Dayanik.
A knowledge-gradient policy for sequential information collection.
SIAM Journal on Control and Optimization, 47(5):2410–2439, 2008.

David Ginsbourger, Rodolphe Le Riche, and Laurent Carraro.
Kriging is well-suited to parallelize optimization.
In *Computational Intelligence in Expensive Optimization Problems*, pages 131–162. Springer Science & Business Media, 2010.

Agathe Girard.
Approximate methods for propagation of uncertainty with gaussian process models.
PhD thesis, University of Glasgow, 2004.

Robert B. Gramacy, Genetha A. Gray, Sebastien Le Digabel, Herbert K. H. Lee, Pritam Ranjan, Garth Wells, and Stefan M. Wild.
Modeling an augmented lagrangian for blackbox constrained optimization.
Technometrics, 58(1):1–11, 2016.

Philipp Hennig and Christian J. Schuler.
Entropy search for information-efficient global optimization.
Journal of Machine Learning Research, 13(Jun):1809–1837, 2012.

References VI


José Miguel Hernández-Lobato, Matthew W. Hoffman, and Zoubin Ghahramani.
Predictive entropy search for efficient global optimization of black-box functions.
In *Advances in Neural Information Processing Systems*, pages 918–926, 2014.


José Miguel Hernández-Lobato, Michael A. Gelbart, Matthew W. Hoffman, Ryan P. Adams, and Zoubin Ghahramani.
Predictive entropy search for Bayesian optimization with unknown constraints.
In *ICML*, pages 1699–1707, 2015.


Deng Huang, Theodore T. Allen, William I. Notz, and R. Allen Miller.
Sequential kriging optimization using multiple-fidelity evaluations.
Structural and Multidisciplinary Optimization, 32(5):369–382, 2006.


Janis Janusevskis and Rodolphe Le Riche.
Simultaneous kriging-based estimation and optimization of mean response.
Journal of Global Optimization, 55(2):313–336, 2013.


Donald R. Jones, Matthias Schonlau, and William J. Welch.
Efficient global optimization of expensive black-box functions.
Journal of Global Optimization, 13(4):455–492, 1998.

References VII

Joshua Knowles.
ParEGO: A hybrid algorithm with on-line landscape approximation for expensive multiobjective optimization problems.
IEEE Transactions on Evolutionary Computation, 10(1):50–66, 2006.

Juhani Koski.
Defectiveness of weighting method in multicriterion optimization of structures.
Communications in Applied Numerical Methods, 1(6):333–337, 1985.

Sébastien Marmin, Clément Chevalier, and David Ginsbourger.
Differentiating the multipoint expected improvement for optimal batch design.
In *International Workshop on Machine Learning, Optimization and Big Data*, pages 37–48. Springer, 2015.

Julien Marzat, Eric Walter, and Hélène Piet-Lahanier.
Worst-case global optimization of black-box functions through kriging and relaxation.
Journal of Global Optimization, 55(4):707, 2013.

Julien Marzat, Eric Walter, and Hélène Piet-Lahanier.
A new expected-improvement algorithm for continuous minimax optimization.
Journal of Global Optimization, 64(4):785–802, 2016.

References VIII


Jonas Mockus, Vytautas Tiesis, and Antanas Žilinskas.
The application of Bayesian methods for seeking the extremum.
In L. C. W. Dixon and G. P. Szegö, editors, *Towards Global Optimization*, volume 2, pages 117–129, North Holland, New York, 1978.


Victor Picheny, Tobias Wagner, and David Ginsbourger.
A benchmark of kriging-based infill criteria for noisy optimization.
Structural and Multidisciplinary Optimization, 48(3):607–626, 2013.


Victor Picheny, David Ginsbourger, and Roustant Olivier et al.
DiceOptim: Kriging-Based Optimization for Computer Experiments, 2016a.
R package version 2.0, 2016.


Victor Picheny, Robert B. Gramacy, Stefan Wild, and Sebastien Le Digabel.
Bayesian optimization under mixed constraints with a slack-variable augmented lagrangian.
In *Advances in Neural Information Processing Systems*, pages 1435–1443, 2016b.


Carl R. Rasmussen and Christopher K. I. Williams.
Gaussian Processes for Machine Learning.
MIT Press, 2006.

References IX


Samee Ur Rehman and Matthijs Langelaar.
Efficient infill sampling for unconstrained robust optimization problems.
Engineering Optimization, 48(8):1313–1332, 2016.


Samee Ur Rehman, Matthijs Langelaar, and Fred van Keulen.
Efficient kriging-based robust optimization of unconstrained problems.
Journal of Computational Science, 5(6):872–881, 2014.


Olivier Roustant, David Ginsbourger, and Yves Deville.
DiceKriging, DiceOptim: Two R packages for the analysis of computer experiments by kriging-based metamodeling and optimization.
Journal of Statistical Software, 51(1), 2012.


Thomas J. Santner, Brian J. Williams, and William Notz.
The Design and Analysis of Computer Experiments.
Springer Verlag, 2003.


Matthias Schonlau, William J. Welch, and Donald R. Jones.
Global versus local search in constrained optimization of computer models.
In *New Developments and Applications in Experimental Design: Selected Proceedings of a 1997 Joint AMS-IMS-SIAM Summer Conference*, volume 34 of *IMS Lecture Notes-Monographs Series*, pages 11–25, 1998.

References X

Warren Scott, Peter Frazier, and Warren Powell.
The correlated knowledge gradient for simulation optimization of continuous parameters using gaussian process regression.
SIAM Journal on Optimization, 21(3):996–1026, 2011.

Michael L. Stein.
Interpolation of Spatial Data: Some Theory for Kriging.
Springer, New York, 1999.

Marcos A. Valdebenito and Gerhart I. Schuëller.
A survey on approaches for reliability-based optimization.
Structural and Multidisciplinary Optimization, 42(5):645–663, 2010.

Emmanuel Vazquez.
Modélisation comportementale de systèmes non-linéaires multivariables par méthodes à noyaux et applications.
PhD thesis, Univ Paris XI, Orsay, France, 2005.

Julien Villemonteix.
Optimisation de fonctions coûteuses Modèles gaussiens pour une utilisation efficace du budget d'évaluations: théorie et pratique industrielle.
PhD thesis, Université Paris Sud-Paris XI, 2008.

References XI


Julien Villemonteix, Emmanuel Vazquez, and Éric Walter.
An informational approach to the global optimization of expensive-to-evaluate functions.
Journal of Global Optimization, 44(4):509–534, 2009.


Brian J. Williams, Thomas J. Santner, and William I. Notz.
Sequential design of computer experiments to minimize integrated response functions.
Statistica Sinica, pages 1133–1152, 2000.


Brian J. Williams, Thomas J. Santner, William I. Notz, and J. S. Lehman.
Sequential design of computer experiments for constrained optimization.
In *Statistical Modelling and Regression Structures*, pages 449–472.
Physica-Verlag HD, 2010.