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Bayesian Optimization

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

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Lecture 1: From meta-models to UQ

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

Lecture 2: Bayesian optimization (BO)

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

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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\textsubscript{x} and CO

- \( f : X \subset \mathbb{R}^d \rightarrow \mathbb{R} \) performance as a function of design parameters (\( d = 20 \sim 100 \))

- Computing \( f(x) \) takes 5 \sim 20 \) hours

- Objective: estimate \( x^* = \arg\max_X f(x) \)

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

For simplification $\rightarrow$ drop $u$
Black-box modeling

Let \( f : \mathbb{X} \rightarrow \mathbb{R} \) be a real function defined on \( \mathbb{X} \subseteq \mathbb{R}^d \), where

- \( \mathbb{X} \) is the input/parameter domain of the computer simulation under study, or the factor (from Latin, “which acts”) space
- \( f \) is a performance or cost function (a function of the outputs of the computer simulation)
Black-box modeling

- Let $x_1, \ldots, x_n \in \mathbb{X}$ 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 $x$?
- The problem is that of constructing an approximation / an estimator $\hat{f}_n$ of $f$ from $\mathcal{D}_n$
- Such a $\hat{f}_n$ also called a model or a meta-model (because the numerical simulator is a model itself) of $f$
A simple curve fitting problem

- Suppose that we are given a data set of \( n \) simulation results, i.e., evaluations results of an unknown function \( f : [0, 1] \rightarrow \mathbb{R} \), at points \( x_1, \ldots, x_n \).

- A data set of size \( n = 8 \):
A simple curve fitting problem

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

- Fundamental example: **linear model**

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

where functions $r_i : \mathbb{X} \to \mathbb{R}$ 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 → minimize the sum of squared errors

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

- Linear fit
A simple curve fitting problem

- Quadratic fit
A simple curve fitting problem

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

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

with

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

(a truncated Fourier series)

- The increase in the number of parameters yields an ill-defined problem \((l \gg n)\)
A simple curve fitting problem

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

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

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

- $n = 8$, $m = 50$, $l = 101$, $C = 10^{-8}$
A simple curve fitting problem

- The regularization principle alone is not enough to obtain a good approximation
- As modeling capacity increases, overfitting may arise
A simple curve fitting problem

To avoid overfitting, we should try a regularization that penalizes high frequencies more.

For instance, take

\[
\|\theta\| = \theta_1^2 + \sum_{k=1}^{m} \frac{\theta_{2k}^2 + \theta_{2k+1}^2}{(1 + (2k\pi)^{\alpha})^2}
\]
A simple curve fitting problem

$n = 8$, $m = 50$, $l = 101$, $C = 10^{-8}$, $\alpha = 1.3$
A simple curve fitting problem

- From this example, we can see that the construction of a regularization scheme should result from a procedure that takes into account the data (using cross-validation, for instance) and/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
    - 1970: ridge regression (Hoerl, Kennard)
    - 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
Lecture 1: From meta-models to UQ

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1.5 Complements on Gaussian processes
Why a Bayesian approach?

- Objective: infer properties about $f : \mathbb{X} \rightarrow \mathbb{R}$ through pointwise evaluations

- Why a Bayesian approach?
  - a principled approach to choose a regularization scheme according to prior information
  - through probability calculus and/or Monte Carlo simulations, the user can infer properties about the unknown function
  - for instance: given prior knowledge and $\mathcal{D}_n$, what is the probability that the global maximum of $f$ is greater than a given threshold $u \in \mathbb{R}$?

- Main idea: use a statistical model of the observations, together with a probability model for the parameter of the statistical model
Some reminders about probabilities

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

Def.

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

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

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

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

- Case of a random variable with a density

  $$P(X \in [a, b]) = P^X([a, b]) = \int_a^b p^X(x)dx$$
A real-valued random variable $Z$ is said to be \textit{Gaussian} $\mathcal{N}(\mu, \sigma^2)$, if it has the continuous \textit{probability density function}

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

- The mean of $Z$ (also called expectation or first-order moment) is
  \[
  E(Z) = \int_{\mathbb{R}} z \, g_{\mu,\sigma^2}(z) \, dz = \mu
  \]
  and its second-order moment is defined as
  \[
  E(Z^2) = \int_{\mathbb{R}} z^2 \, g_{\mu,\sigma^2}(z) \, dz = \sigma^2 + \mu^2
  \]
- The variance of $Z$ is defined as
  \[
  \text{var}(Z) = E[(Z - E(Z))^2] = E[Z^2] - E[Z]^2 = \sigma^2
  \]
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 \( Z \) → 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** \( \Pi \) on \( (\Theta, \Xi) \) → probability model that describes uncertainty about \( \theta \) 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 assume a prior distribution about \(\theta_1\) and \(\theta_2\) 
  (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 \((\theta_1, \theta_2)\) 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

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

with

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

Bayesian model?
Assume the following statistical model for the observations:

\[
\begin{align*}
    Z_i &= \xi(x_i) + \varepsilon_i, \quad i = 1, \ldots, n \\
    \xi(x) &= \theta^t r(x), \quad x \in X \\
    \varepsilon_i &\sim \mathcal{N}(0, \sigma^2_\varepsilon)
\end{align*}
\]

or equivalently,

\[
Z_i \sim \mathcal{N}(\theta^t r(x_i), \sigma^2_\varepsilon), \quad i = 1, \ldots, n
\]

Moreover, choose a prior distribution for \( \theta \):

\[
\theta_j \overset{\text{indep}}{\sim} \mathcal{N}(0, \sigma^2_\theta), \quad j = 1, \ldots, 2m + 1
\]

The rvs \( Z_i \) constitute a Bayesian model of the observations.

\( \xi \) is a random function / random process \( \rightarrow \) prior about \( f \).
Random process

Def.

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

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

- we use a random process $\xi$ as a stochastic model of the unknown function $f$
- $f$ is viewed as as sample paths of $\xi$
- $\xi$ represents our knowledge about $f$ before any evaluation has been made
- the distribution $\Pi = P^\xi$ is a prior about $f$
Here, $\xi(\omega, \cdot) = \theta(\omega)^t r(\cdot)$

Fixing $\omega$ (a sample path) amounts to “choosing” a value for the random vector $\theta$
Example of sample paths with

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

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 $\omega_0 = \frac{2\pi}{10}$, $\alpha = 1.5$
The choice of a prior in a Bayesian approach reflects the user’s knowledge about uncertain parameters.

In the case of function approximation → regularity of the function.
Bayesian approach

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

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- Objective: compute posterior distributions from data
A “simplification” of the Bayesian model for the simple curve fitting problem

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

Def.
A real-valued random vector \( Z = (Z_1, \ldots, Z_d) \in \mathbb{R}^d \) 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, \( \mu = (E[Z_1], \ldots, E[Z_d]) \in \mathbb{R}^d \), and the **covariance** of the pairs of components \( (Z_i, Z_j) \), \( i, j \in \{1, \ldots, d\} \),
  \[
  \text{cov}(Z_i, Z_j) = E[(Z_i - E(Z_i))(Z_j - E(Z_j))]
  \]

- If \( Z \in \mathbb{R}^d \) is a Gaussian vector with mean \( \mu \in \mathbb{R}^d \) and covariance matrix \( \Sigma \in \mathbb{R}^{d \times d} \), we shall write \( Z \sim \mathcal{N}(\mu, \Sigma) \)
Exercise: Let $Z \sim \mathcal{N}(\mu, \Sigma)$. Determine $E\left(\sum_{i=1}^{d} a_i Z_i\right)$ and $\text{var}\left(\sum_{i=1}^{d} a_i Z_i\right)$

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

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

→ measures the similarity between $Z_i$ and $Z_j$
Gaussian random vectors: correlation

$\rho = 0$

$\rho = 0.8$
Gaussian random processes

► Recall that a random process is a set $\xi = \{\xi(x), x \in X\}$ of random variables indexed by the elements of $X$

► Gaussian random process

→ generalization of a Gaussian random vector

Def.

$\xi$ is a Gaussian random process iff, $\forall n \in \mathbb{N}, \forall x_1, \ldots, x_n \in X$, 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
  \[
  \begin{cases}
  \xi(x) = \theta^t r(x), & x \in \mathbb{X} \\
  \theta_j \overset{\text{indep}}{\sim} \mathcal{N}(0, \sigma^2_{\theta_j}), & j = 1, \ldots, 2m + 1
  \end{cases}
  \]
  then, \(\forall x_1, \ldots, x_n \in \mathbb{X}\), and \(\forall a_1, \ldots, a_n \in \mathbb{R}\),

  \[
  \sum_{i=1}^{n} a_i \xi(x_i) = \sum_{i} a_i \left( \sum_{j} \theta_j r_j(x_i) \right)
  \]

  \[
  = \sum_{j} \left( \sum_{i} a_i r_j(x_i) \right) \theta_j \sim \mathcal{N}(0, \sum_{j} \left( \sum_{i} a_i r_j(x_i) \right)^2 \sigma^2_{\theta_j})
  \]

- Thus, \(\xi = \theta^t r\) is a Gaussian process
Gaussian random processes

- A Gaussian process is characterized by
  - its mean function
    
    \[ m : x \in X \mapsto \mathbb{E}[\xi(x)] \]
  - and its covariance function
    
    \[ k : (x, y) \in X^2 \mapsto \text{cov}(\xi(x), \xi(y)) \]
- Notation: \( \xi \sim \mathcal{GP}(m, k) \)
Exercise: determine $\mathbb{E} \left( \sum_{i=1}^{d} a_i \xi(x_i) \right)$ and $\text{var} \left( \sum_{i=1}^{d} a_i \xi(x_i) \right)$

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

The distribution of a linear combination of a Gaussian process $\mathcal{GP}(m, k)$ can be simply obtained as a function of $m$ and $k$. 
If
\[
\begin{aligned}
\xi(x) &= \theta^t r(x), \quad x \in \mathbb{X} \\
\theta_j &\overset{\text{indep}}{\sim} \mathcal{N}(0, \sigma_{\theta_j}^2), \quad j = 1, \ldots, 2m + 1
\end{aligned}
\]
then,
\[
\xi \sim \mathcal{GP}(0, k)
\]
with
\[
k : (x, y) \mapsto \sum_j \sigma_{\theta_j}^2 r_j(x) r_j(y)
\]
Covariance function corresponding to

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

with $\omega_0 = \frac{2\pi}{10}$, $\alpha = 4$
Covariance function corresponding to

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

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**:

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

- **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 $\rho$ is the correlation function of $\xi$. 
Stationary covariances

- The graph of the correlation function is a symmetric "bell curve" shape.
We have, by C-S,

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

Recall, Bochner’s spectral representation theorem

**Theorem**

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

\[ k(h) = \int_{\mathbb{R}^d} e^{i(u, h)} d\mu(u) , \]

where \( \mu \) 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 $\xi$. 

![Graphs of Gaussian process simulations]
Gaussian process simulation

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

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

$$K = CC^t,$$

with $C$ a lower triangular matrix (such a factorization exists since $K$ is a sdp matrix)
- Let $\varepsilon = (\varepsilon_1, \ldots, \varepsilon_n)^t$ a Gaussian vector with $\varepsilon_i \overset{i.i.d.}{\sim} \mathcal{N}(0, 1)$
- Then $C\varepsilon \sim \mathcal{N}(0, K)$
“Simplification” of the Bayesian model for the simple curve fitting problem

- Instead of choosing the model

\[
\begin{align*}
\xi(x) &= \theta^t r(x), \quad x \in X \\
\theta_j &\overset{\text{indep}}{\sim} \mathcal{N}(0, \sigma_{\theta_j}^2), \quad j = 1, \ldots, 2m + 1
\end{align*}
\]

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
How to compute a posterior distribution, given the Gaussian-process prior $\xi$ 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 \((\Omega, \mathcal{A}, P)\) be a probability space. Given two events \(A, B \in \mathcal{A}\) such that \(P(B) \neq 0\), define the *probability of \(A\) given \(B\) (or conditional on \(B\))* by

\[
P(A \mid B) = \frac{P(A \cap B)}{P(B)}
\]
The notion of conditional density

Def.

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

Define the conditional density of \(X\) given the event \(T = t\) by

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

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

- Define

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

$\rightarrow$ 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
A fundamental notion: conditional expectation

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

\[
E(X \mid T = t) \overset{\Delta}{=} \int_{\mathbb{R}} x p^{X\mid T}(x \mid t) dx = h(t)
\]

Def.
The random variable \(E(X \mid T) = h(T)\) is called the conditional expectation of \(X\) given \(T\)
Conditional expectation

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

Theorem

Under the previous assumptions, the solution of the problem

$$\hat{X} = \arg\min_Y E[(X - Y)^2]$$

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

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

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

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

(2) The operator $\pi_H : X \mapsto E(X \mid T)$ 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) $\forall \alpha \in \mathbb{R}, E(\alpha X + Y \mid T) = \alpha E(X \mid T) + E(Y \mid T)$ a.s.
   ii) $E(E[X \mid T]) = E(X)$
   iii) If $X \perp \perp T$, $E(X \mid T) = E(X)$
Conditional expectation: Gaussian random variables

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

- Gaussian linear space

**Def.**

A linear subspace $G$ of $L^2(\Omega, \mathcal{A}, P)$ is Gaussian iff $\forall X_1, \ldots, X_n \in G$ 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 $E(X \mid T_1, \ldots, T_n)$ is the orthogonal projection (in $L^2$) of $X$ on $\mathcal{T} = \text{span}\{T_1, \ldots, T_n\}$.

**proof**

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

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

- Then,

  $$E(X \mid T_1, \ldots, T_n) = E(\hat{X} \mid T_1, \ldots, T_n) + E(\varepsilon \mid T_1, \ldots, T_n)$$

  $$= \hat{X} + E(\varepsilon) = \hat{X}$$

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

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

with

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

Hence,

$$
\lambda = \frac{\sigma_{1,2}}{\sigma_2^2}$$
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 $Z_2 \mid Z_1 \sim \mathcal{N}(\mu(Z_1), \sigma(Z_1)^2) \rightarrow \mu$ ? $\sigma$ ?

$\mu = \mathbb{E}(Z_2 \mid Z_1) = \lambda Z_1$ with $\lambda = \frac{\sigma_{1,2}}{\sigma_2^2}$

Using the property of the orthogonal projection:

$\sigma^2 = \mathbb{E}((Z_2 - \mathbb{E}(Z_2 \mid Z_1))^2 \mid Z_1)$

$\perp \equiv \mathbb{E}((Z_2 - \mathbb{E}(Z_2 \mid Z_1))^2)$

$= \mathbb{E}((Z_2 - \lambda Z_1)^2)$

$\perp \equiv \mathbb{E}((Z_2 - \lambda Z_1)Z_2)$

$= \sigma_2^2 - \lambda \sigma_{1,2}$
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 $\xi$ at $x_1, \ldots, x_n \in X$

Given $x_0 \in X$, what is the conditional distrib.—or the posterior distrib. in our Bayesian framework—of

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

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

$$\xi(\cdot) \mid \xi(x_1), \ldots, \xi(x_n)?$$
Computation of the posterior distribution of a GP

Prop.

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

- mean \( \hat{\xi}_n : x \mapsto E(\xi(x) \mid \xi(x_1), \ldots, \xi(x_n)) \)
- covariance \( k_n : x, y \mapsto E((\xi(x) - \hat{\xi}_n(x))(\xi(y) - \hat{\xi}_n(y))) \)
Computation of the posterior distrib. of a GP

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

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

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

\[ k_n(x, y) := \text{cov} \left( \xi(x) - \hat{\xi}_n(x), \xi(y) - \hat{\xi}_n(y) \right) = k(x - y) - \sum_i \lambda_i(x) k(y - x_i). \]

- \( k_n \) is the covariance function of the error of prediction

- The posterior variance of \( \xi \), also called the kriging variance, is defined as

\[ \sigma^2_n(x) = \text{var}(\xi(x) - \hat{\xi}_n(x)) = k_n(x, x) \]

- \( \sigma^2_n(x) \) 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

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

proof
Posterior distrib. of a GP

- For all $x \in \mathbb{X}$, the random variable $\xi(x) \mid F_n$ with distrib. $\mathcal{N}(\hat{\xi}_n(x), \sigma_n^2(x))$ represents the residual uncertainty about $\xi(x)$ when $\xi(x_1), \ldots, \xi(x_n)$ 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
  - GPStuf: GP Models for Bayesian analysis
  - scalaGAUSS: Kriging toolbox with a focus on large datasets
  - Matlab Stat & ML toolbox: GP regression from Mathworks
  - STK: Small (Matlab/GNU Octave) Toolbox for Kriging
  - SUMO: ooDACE Surrogate Modeling Lab
  - UQLab: Uncertainty quantification framework in Matlab

- Python
  - scikit-learn: Machine learning in Python
  - OpenTURNS: Open source lib for UQ
  - Spearmint: Bayesian optimization
  - GPy: Gaussian processes framework in Python
Generalization: prediction from noisy observations

- Let $\xi \sim \text{GP}(0, k)$
- For $i = 1, \ldots, n$, we observe $Z_i = \xi(x_i) + \varepsilon_i$ at points $x_i$, where the random variables $\varepsilon_i$ model an observation noise:
  - $\varepsilon_i \overset{\text{i.i.d}}{\sim} \mathcal{N}(0, \sigma^2)$
  - independent from $\xi$
- As above, the posterior mean $\hat{\xi}_n(x)$ of $\xi(x)$ is obtained as the orthogonal projection of $\xi(x)$ on the linear subspace $\text{span}\{Z_i, i = 1, \ldots, n\}$:
  $$\hat{\xi}_n(x) = \sum_{i=1}^{n} \lambda_i(x)Z_i$$
  with $\lambda_i(x)$ such that
  $$\forall i, \quad \xi(x) - \hat{\xi}_n(x) \perp Z_i$$
Generalization: prediction from noisy observations

Thus, $\forall i$

$$E[(\xi(x) - \hat{\xi}_n(x))Z_i]$$

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

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

Under matrix form (exercise):
Generalization: prediction from noisy observations

Kriging prediction based on noisy observations
Generalization: prediction from noisy observations

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

i) The observations are noisy (obviously): the computer code is stochastic (for instance, Monte Carlo is used) and running the code twice does not produce the same output

ii) The output of the computer code is very irregular → a smooth approximation is preferred

iii) The covariance matrix is ill-conditioned → adding a small observation noise will regularize the solution of the linear system (why?)
Lecture 1: From meta-models to UQ

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

- Using the posterior distribution of $\xi$, we can address questions like
  - What are plausible values for $\xi(x)$ at a given $x$? (obviously)
  - What are plausible values for $\int g(\xi(x)) \, d\mu(x)$ for given $g$ and $\mu$?
  - What are plausible values for the minimum $M = \min_x \xi(x)$?
  - Where is the minimizer $x^* = \text{argmin}_x \xi(x)$?
  - 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 $f : X \to \mathbb{R}$
- In our Bayesian approach, we choose a GP prior $\xi$ for $f$ (in other words, $\xi$ is a model of $f$)
- Objective: construct a sequence $(X_1, X_2, \ldots) \in X$ that converges to $X^* = \arg\min_x \xi(x)$
- 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 $x \in X$ is such that $m_n - \xi(x)$ is large
- Define the excursion of $\xi$ 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

\[ +2 \hat{\sigma}_n(x) \]

\[ -2 \hat{\sigma}_n(x) \]
Example of a quantity of interest: the improvement
Example of a quantity of interest: the improvement

\[ \hat{\xi}_n(x) \]

\[ \hat{\sigma}_n(x) \]
Example of a quantity of interest: the improvement

\[ \hat{\xi}_n(x) \]

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 \( \xi \)

- The posterior mean of \( I_n \) may be written as

\[
\rho_n(x) = \mathbb{E}(I_n \mid \xi(X_1), \ldots, \xi(X_n)) \\
= \int_{z=-\inf}^{m_n} (m_n - z) \ p^{\xi}(x) \mid \xi(X_1), \ldots, \xi(X_n)(z) \ dz \\
= \gamma(m_n - \hat{\xi}_n(x), \sigma_n^2(x))
\]

with

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

- \( \rho_n \) is called the **expected improvement** [Mockus 78, Schonlau et al. 96, Jones et al. 98]
Example of a quantity of interest: the improvement

\[ \hat{\xi}_n(x) \]

\[ \rho_n(x) \]

\[ m_n \]
Insertion into an optimization algorithm

- The EI algorithm: \( X_{n+1} = \arg \max_x \rho_n(x) \)
Insertion into an optimization algorithm

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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 $f : \mathbb{X} \rightarrow \mathbb{R}$ and suppose we are interested in seeking its minimizer:

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

- Choose a GP prior $\xi$ for $f$. Given observations $\xi(x_1), \ldots \xi(x_n)$, what is the posterior distrib. of $X^* = \text{argmin}_x \xi(x)$?

- Unlike $I_n$ above, the distrib. of $X^*$ does not possess a closed-form expression → 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 $p_{x^*|F_n}$.
Empirical posterior density of the minimizer

\[ p_{x^* | F_n^+} \]
Empirical posterior density of the minimizer
Empirical posterior density of the minimizer
Empirical posterior density of the minimizer

\[ p_{x^* \mid F^+_n} \]
Empirical posterior density of the minimizer
Empirical posterior density of the minimizer

\[ p_{x^* | F_n} \]
Lecture 1: From meta-models to UQ

1.1 Introduction
1.2 Black-box modeling
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1.5 Complements on Gaussian processes
Choosing a centered Gaussian random process

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

**Def.**

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

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

**Prop.**

Let $\xi$ be a second-order random process with continuous mean function and stationary covariance function $k$. $\xi$ 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

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

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

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

Prop.

Let \( \xi \) be a second-order random process with differentiable mean function and stationary covariance function \( k \). \( \xi \) 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 → mean-square differentiability of $\xi$
Influence of the regularity

mean-square continuity

three-time mean-square differentiability
Choice of a covariance

- A Gaussian process prior carries a high amount of information about $f$
  - it is often difficult to elicit such a prior before any evaluation is made

- Covariance function of $\xi$ is usually assumed to belong to some parametric class of positive definite functions

- Parameter values assumed to be unknown

- Two approaches:
  1. The parameters can be estimated from the evaluation results by maximum likelihood, and then used as if they were known (plug-in approach)
  2. We can assume a prior distrib. for the parameters of the covariance and use a fully Bayesian approach
Choice of a parametrized covariance function: the Matérn covariance

- The Matérn covariance function is a conventional covariance function in the literature of computer experiments
  - offers the possibility to adjust the regularity of $\xi$ with a single parameter

- The Matérn function:

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

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

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

  \[
  k_\theta(h) = \sigma^2 \kappa_\nu(|h|/\rho), \quad h \in \mathbb{R}
  \]
Choice of a parametrized covariance function: the Matérn covariance

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

$\xi$ 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 $X \subset \mathbb{R}^d$, with $d > 1$, we use the anisotropic form of the Matérn covariance:

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

where $x[i], y[i]$ denote the $i^{th}$ coordinate of $x$ and $y$, and the positive scalars $\rho_i$ 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 $\xi$ is a zero-mean Gaussian process.

- The log-likelihood of the data $\xi_n = (\xi(x_1), \ldots, \xi(x_n))^t$ can be written as

$$
\ell(\xi_n; \theta) = -\frac{n}{2} \log(2\pi) - \frac{1}{2} \log \det K(\theta) - \frac{1}{2} \xi_n^t K(\theta)^{-1} \xi_n,
$$

where $K(\theta)$ is the covariance matrix of $\xi_n$, which depends on the parameter vector $\theta$.

- The log-likelihood can be maximized using a gradient-based search method.
Prediction of a Gaussian process with unknown mean function

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

\[ m(\cdot) = \beta^t \varphi(\cdot), \]  

(5)

with

- \( \beta \) a vector of unknown parameters
- \( \varphi = (\varphi_1, \ldots, \varphi_l)^t \) an \( l \)-dimensional vector of functions (in practice, polynomials)

- Simplest case: the mean function is an unknown constant \( m \), in which case \( \beta = m \) and \( \varphi : x \in X \mapsto 1 \)
Prediction of a Gaussian process with unknown mean function

▶ Define the linear space of functions

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

▶ Define \( \Lambda \) the linear space of finite-support measures on \( X \), i.e.

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

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

\[ \langle \lambda, f \rangle = \int_X f \, d\lambda = \sum_{i=1}^{n} \lambda_i f(x_i) \]

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

\[ \lambda \in \Lambda_{\mathcal{P}^\perp} \implies \langle \lambda, f \rangle = \int_X f \, d\lambda = \sum_{i=1}^{n} \lambda_i f(x_i) = 0, \ \forall f \in \mathcal{P} \]
Prediction of a Gaussian process with unknown mean function

Let $\xi$ 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 $\hat{\xi}_n(x)$ of $\xi(x)$ from $\xi(x_1), \ldots, \xi(x_n)$ is the linear projection

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

of $\xi(x)$ onto $\text{span}\{\xi(x_i), i = 1, \ldots, n\}$ such that the variance of the error $\xi(x) - \hat{\xi}_n(x)$ 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 $\xi$ is unknown.
Prediction of a Gaussian process with unknown mean function

\( \hat{\xi}_n(x) \) is the linear projection of \( \xi(x) \) onto \( \text{span}\{\xi(x_1), \ldots, \xi(x_n)\} \) 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

\[
\begin{pmatrix}
K & \varphi^t \\
\varphi & 0
\end{pmatrix}
\begin{pmatrix}
\lambda(x) \\
\mu(x)
\end{pmatrix}
= \begin{pmatrix}
k(x) \\
\varphi(x)
\end{pmatrix},
\]  

(6)

with

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

\[
  k_n(x, y) := \text{cov} \left( \xi(x) - \hat{\xi}_n(x), \xi(y) - \hat{\xi}_n(y) \right) \\
  = k(x - y) - \lambda(x)^t k(y) - \mu(x)^t \varphi(y).
\]

**Prop.**

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

If

\[
\begin{cases}
  \xi \mid m \sim \mathcal{GP}(m, k) \\
  m : x \mapsto \beta^t \varphi(x), \beta \sim U(\mathbb{R}^l)
\end{cases}
\]

then

\[
\xi \mid F_n \sim \mathcal{GP} \left( \hat{\xi}_n(\cdot), k_n(\cdot, \cdot) \right)
\]

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

\( \rightarrow \) justifies the use of kriging in a **Bayesian framework** provided that the covariance function of \( \xi \) is known
Parameter estimation with unknown mean function

- **Objective:** estimate the covariance parameters of a Gaussian process with unknown mean.

- **Restricted Maximum Likelihood (REML) approach** → maximize the likelihood of the increments (or generalized increments) of the data.

- Let $\xi$ be a Gaussian process with an unknown mean function in $\mathcal{P}$ and $\xi_n$ the random vector of observations at points $x_i$, $i = 1, \ldots, n$.

- Let $\varphi = (\varphi_i(x_j))_{i,j=1}^{l,n}$ 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 $P$ is $l$, the dimension of the space of the measures with support $\{x_1, \ldots, x_n\}$ that cancel out the functions of $P$ is $n - l$.

Assume an $n \times (n - l)$ matrix $W$ with rank $n - l$ has been found, such that
\[
\varphi W = 0.
\]
(The columns of $W$ are in the kernel of $\varphi$.)

Then $Z = W^T \xi_n$ is a Gaussian random vector taking its values in $\mathbb{R}^{n-l}$, with zero mean and covariance matrix
\[
W^T K(\theta) W
\]
where $K(\theta)$ is the covariance matrix of $\xi_n$ 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

$$L(z \mid \theta) = -\frac{n - l}{2} \log 2\pi - \frac{1}{2} \log \det(W^t K(\theta) W) - \frac{1}{2} z^t (W^t K(\theta) W)^{-1} z.$$
Various methods may be employed to compute the matrix $W$

- We favor the QR decomposition of $\varphi^T$

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

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

- It is trivial to check that the columns of $Q_2$ form a basis of the kernel of $\varphi$

- So we may choose $W = Q_2$

- Note that $W^T W = I_{n-l}$. 
Books

- **C. Rasmussen and C. Williams**, Gaussian processes for Machine Learning, MIT Press, 2006
Lecture 1: From meta-models to UQ

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

Lecture 2: Bayesian optimization (BO)

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

References
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
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- In this lecture we adopt this second *(more constructive !)* definition
Lecture 2: Bayesian optimization (BO)

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

- 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)

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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)

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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

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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: example

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

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

Consider the following setting

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

States of nature for this setting

- $\Omega = \{ f : \mathbb{X} \rightarrow \mathbb{R}^p \mid f \text{ such that } \ldots \}$
- e.g., $d = 1$, $p = 1$, $\mathbb{X} = [0; 1]$ and $\Omega = C(\mathbb{X}; \mathbb{R})$

Until further notice, we will use this simple (but important) setting to illustrate the basics of Bayesian optimization
Uncertainty quantification (reminder from Lecture #1)

- The true state of nature $\omega^* \in \Omega$ is unknown
- Example (cont’d)
  - a function $f^* \in \Omega = C(X; \mathbb{R})$ is inside the black box ($\omega^* \equiv f^*$)
  - we don’t “know” $f^*(x)$ until we run the code with input $x$
Uncertainty quantification (reminder from Lecture #1)

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- Bayesian approach to UQ
  - our knowledge of $\omega^*$ is encoded by a probability distribution on the set $\Omega$ of all possible $\omega$’s
  - technically: proba on $(\Omega, \mathcal{F})$ for some $\sigma$-algebra $\mathcal{F}$...
Uncertainty quantification (reminder from Lecture #1)

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  - technically: proba on $(\Omega, \mathcal{F})$ for some $\sigma$-algebra $\mathcal{F}$ . . .

- Sequence of decisions $\Rightarrow$ sequence of distributions $P_0, P_1, \ldots$
  - $P_n$ 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:

  ![Graph showing a set of curves indicating function $f$]

  then we can take $P_0 = \mathcal{GP}(m, k)$

  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:

\[
\begin{array}{c|c|c|c|c|c|c|c}
-1 & -0.5 & 0 & 0.5 & 1 \\
-2.5 & -2 & -1.5 & -1 & -0.5 & 0 & 0.5 & 1 \\
\end{array}
\]

then we can take \( P_0 = \mathcal{GP}(m, k) \)

with \( m \sim U(\mathbb{R}) \) 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 $\mathbb{P}$ on $\Omega$, 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

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  - an unknown function \( f \in \Omega \) is in the black box

- Given a proba \( P \) on \( \Omega \), 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**

\[ \xi = \text{random function that represents the unknown } f \]

- we will write, e.g., \( E_n(\xi(x)) \) instead of \( \int_\Omega f(x) P_n(df) \)  😊
Decision-theoretic framework (cont’d)

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

Ingredients of a BDT problem

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

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

with \( X \) a “known” input space
Decisions: final decision

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  with \( X \) 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 ≡ evaluations (known comput. cost)
  - stopping: a budget of $N$ evaluations is given

### Notations

- $X_n(\omega) =$ the $n^{th}$ evaluation point
- $D_{N+1}(\omega) =$ the “final decision” (estimate of the QoI)
- $D(\omega) = (X_1(\omega), \ldots, X_N(\omega), D_{N+1}(\omega))$
Transitions: conditioning probability measures

- Recall that
  - the agent’s knowledge at time $n$ is described by $P_n$
  - the $(n + 1)^{th}$ decision induces a transition $P_n \rightarrow P_{n+1}$
Transitions: conditioning probability measures

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

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, $P_n = P_0(\cdot | F_n) = P_{n-1}(\cdot | I_n)$

- Various settings can be addressed
  - depending on what we define as $I_n$ 😊
Decisions: standard setting and notations

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  - intermediate decisions \( \equiv \) evaluations (known comput. cost)
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Notations

\[
X_n(\omega) = \text{the } n^{\text{th}} \text{ evaluation point}
\]
\[
D_{N+1}(\omega) = \text{the “final decision” (estimate of the QoI)}
\]
\[
D(\omega) = (X_1(\omega), \ldots, X_N(\omega), D_{N+1}(\omega))
\]

- We cannot use information that is not yet available
  - \( X_n(\omega) \) depends on \( \omega \) through \( F_{n-1} \) only
  - \( D_{N+1}(\omega) \) depends on \( \omega \) through \( F_N \) only
  - \( D \) 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 $F_n = (X_1, \xi(X_1), \ldots, X_n, \xi(X_n))$
  - $\xi(X_i) = f^*(X_i)$ is the true, scalar, value of the model at $X_i$
Transitions: examples

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

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  - batch setting and/or multiple outputs
Transitions: examples

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  - 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” ✓
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Loss function

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

**Notation**

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

$$(\omega, d) \mapsto L(\omega, d)$$

where $D$ 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

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

$(\omega, d) \mapsto L(\omega, d)$

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

- The Bayes-optimal strategy is, by definition:

$$D = \text{argmin} \ E_0 (L(D)) = \text{argmin} \int_{\Omega} L(\omega, D(\omega)) P_0(d\omega)$$

where $D$ ranges over all strategies
Loss function: example

- Example (cont’d)
  - Assume that we want to find the minimizer of $f$
    - $d = (x_1, \ldots, x_n, \hat{x})$
    - with $\hat{x}$ our estimate of $\text{argmin } f$
Loss function: example

Example (cont’d)

Assume that we want to find the minimizer of $f$

$\hat{d} = (x_1, \ldots, x_n, \hat{x})$

with $\hat{x}$ our estimate of $\text{argmin } f$

A standard loss function for this situation is the linear loss:

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

(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 $f$

- $d = (x_1, \ldots, x_n, \hat{x})$
- with $\hat{x}$ our estimate of $\text{argmin} \ f$

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

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

Remarks

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

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

- $L$ 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?
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Our BDT framework is complete, let’s use it 😊
Decision-theoretic framework (cont’d)

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Lecture 2: Bayesian optimization (BO)

2.1. Decision-theoretic framework

2.2. From Bayes-optimal to myopic strategies

2.3. Design under uncertainty
Problem statement

- Assume a standard BO setting
  - fixed budget $N$, terminal cost only
    - $L(\omega, d) = L(\omega, d_{N+1})$
  - 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
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    - $L(\omega, d) = L(\omega, d_{N+1})$
  - intermediate decisions ≡ 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):

  $$D^{\text{Bayes}} = \arg\min_D \mathbb{E}_0 \left( L(D_{N+1}) \right)$$
  $$= \arg\min_D \int_{\Omega} L(\omega, D_{N+1}(\omega)) P_0(\text{d}\omega)$$

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

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

Can we actually build an optimal Bayesian algorithm?
Problem statement (more precisely)

- Recall that
  - $X_{n+1}(\omega)$ must depend on $\omega$ through $F_n$ only
  - $D_{N+1}(\omega)$ must depend on $\omega$ through $F_N$ only
Problem statement (more precisely)

- Recall that
  - $X_{n+1}(\omega)$ must depend on $\omega$ through $F_n$ only
  - $D_{N+1}(\omega)$ must depend on $\omega$ 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 $\omega$ through $F_n$ only
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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 $\varphi_0, \ldots, \varphi_N$
Lecture 2: Bayesian optimization (BO)

2.2. From Bayes-optimal to myopic strategies

The optimal terminal decision

Optimal choice of the last evaluation
Bayes-optimal versus “practical Bayes” optimization
Sampling criteria for multi-objective and/or contrained optimization
Optimal terminal decision

**Notation**

\[ E_n = E(\cdot \mid F_n) = \text{conditional expectation with respect to } F_n = \text{expectation with respect to the probability } P_n \]
Optimal terminal decision

Notation

\[ E_n = E(\cdot | F_n) = \text{conditional expectation with respect to } F_n \]
\[ = \text{expectation with respect to the probability } P_n \]

Consider any incomplete strategy \( X_1, \ldots, X_N \)

Claim: the optimal terminal decision is

\[ D_{N+1} = \varphi_N^{\text{Bayes}} (X_1, Z_1, \ldots, X_N, Z_N) = \arg\min_d E_N (L(d)) \]

where \( d \) runs over all possible values for the terminal decision
Optimal terminal decision: proof

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

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

Consider the modified strategy $D' = (X_1, \ldots, X_N, D'_{N+1})$
where $D'_{N+1} = \varphi^\text{Bayes}_N(X_1, Z_1, \ldots, X_N, Z_N)$

Then, by definition of $\varphi^\text{Bayes}_N$,

$$E_N(L(D_{N+1})) = E_N(L(d))\big|_{d=D_{N+1}} \geq \min_d E_N(L(d)) = E_N(L(D'_{N+1}))$$
Optimal terminal decision: proof

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

- Consider the modified strategy $D' = (X_1, \ldots, X_N, D'_{N+1})$
  where $D'_{N+1} = \varphi^\text{Bayes}_N(X_1, Z_1, \ldots, X_N, Z_N)$

- Then, by definition of $\varphi^\text{Bayes}_N$,
  \[
  E_N(L(D_{N+1})) = E_N(L(d)) \big|_{d=D_{N+1}} \\
  \geq \min_d E_N(L(d)) = E_N(L(D'_{N+1}))
  \]

- and thus
  \[
  E_0(L(D_{N+1})) = E_0(E_N(L(D_{N+1}))) \\
  \geq E_0(E_N(L(D'_{N+1}))) = E_0(L(D'_{N+1})) \quad \blacksquare
  \]
Define the **posterior risk** at time $N$ for the decision $d$:

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

(“risk” is a synonym for “expected loss”)
Define the posterior risk at time \( N \) for the decision \( d \):

\[
R_N(d) = \mathbb{E}_N (L(d))
\]

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

Define the posterior Bayes risk at time \( N \):

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

Remember: the min attained for \( d = \varphi_N^{\text{Bayes}}(F_N) \)
Example (cont’d): linear loss

- Recall the setting
  - goal: minimize $f$
  - $d_{N+1} = \hat{x}$ is an estimate of $X^*(f) = \text{argmin } f$
  - $L(f, \hat{x}) = f(\hat{x}) - \min f$
Example (cont’d): linear loss

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

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

$$R_N(\hat{x}) = E_N (L(\xi, \hat{x})) = E_N (\xi(\hat{x}) - \min \xi)$$

$$= \hat{\xi}_N(\hat{x}) - E_N (\min \xi)$$
Example (cont’d): linear loss

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

- Compute the posterior risk at time $N$ for a given $\hat{x} \in X$:
  \[
  R_N(\hat{x}) = E_N(L(\xi, \hat{x})) = E_N(\xi(\hat{x}) - \min \xi) = \hat{\xi}_N(\hat{x}) - E_N(\min \xi)
  \]

- Thus the optimal terminal decision is
  \[
  D_{N+1}^{\text{Bayes}} = \hat{X}^{\text{Bayes}} = \arg\min_{x \in X} \hat{\xi}_N(x)
  \]
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

$$
\hat{X}^{\text{Bayes}} = \arg\min \hat{\xi}_N
$$

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

- Remark: in general, $\hat{X}^{\text{Bayes}} \notin \{X_1, \ldots, X_N\}$
  - the value of the function at $\hat{X}^{\text{Bayes}}$ is not known
Example (cont’d): the $L^1$ loss, variant

- To summarize, we have for this example

$$
\hat{X}^{\text{Bayes}} = \arg\min \hat{\xi}_N
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$$

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

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

$$
\hat{X}^{\text{Bayes},1} = \arg\min_{x \in \{X_1, \ldots, X_N\}} \xi(x)
$$

$$
R^{\text{Bayes},1}_N = \min_{i \leq N} \xi(X_i) - E_N \left( \min \xi \right)
$$
Example (cont’d): linear loss

Assume that $n = N = 5$ (a small budget indeed).
Example (cont’d): linear loss

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

Remark: the two estimates are equal when $\hat{\xi}$ does not “overshoot” (e.g., for a Brownian motion prior)
Lecture 2: Bayesian optimization (BO)

2.2. From Bayes-optimal to myopic strategies

The optimal terminal decision

Optimal choice of the last evaluation

Bayes-optimal versus “practical Bayes” optimization

Sampling criteria for multi-objective and/or constrained optimization
Finding $X_N^{\text{Bayes}}$ (last evaluation point)

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

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

**Notation**

$E_{n,x}(Y)$ will mean: “compute $E_n(Y)$, assuming that $X_{n+1} = x$”
Finding $X_N^{\text{Bayes}}$ (last evaluation point)

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

**Notation**

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

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

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

where $Z_x$ denotes the result of a new evaluation at $x$
Finding $X_N^{\text{Bayes}}$ (last evaluation point)

- Given $x_N \in X$, 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 $X_N^{\text{Bayes}}$ (last evaluation point)

- Given $x_N \in X$, 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

$$R_{N-1}(x_N) = E_{N-1,x_N} \left( L(D_{N+1}^{\text{Bayes}}) \right) = E_{N-1,x_N} \left( R_{N}^{\text{Bayes}} \right)$$
Finding $X_N^{\text{Bayes}}$ (last evaluation point)

- Given $x_N \in X$, consider the following strategy at time $N - 1$:
  1) first, evaluate at $X_N = x_N$,
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- The corresponding posterior risk at time $N - 1$ is

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

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

$$X_N^{\text{Bayes}} = \varphi_{N-1}(F_{N-1}) = \arg\min_{x_N \in X} R_{N-1}(x_N)$$
Finding $X^\text{Bayes}_N$ (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 $D^\text{Bayes}_{N+1} = \varphi_N^\text{Bayes}(F_N)$

- The corresponding posterior risk at time $N - 1$ is
  \[
  R_{N-1}(x_N) = E_{N-1,x_N} \left( L(D^\text{Bayes}_{N+1}) \right) = E_{N-1,x_N} \left( R_N^\text{Bayes} \right)
  \]

- Claim: the optimal decision rule for the last evaluation is
  \[
  X^\text{Bayes}_N = \varphi_{N-1}(F_{N-1}) = \arg\min_{x_N \in \mathbb{X}} R_{N-1}(x_N)
  \]

- Remark: $R_{N-1}$ is used as a “sampling criterion”
  (a.k.a. “infill criterion”, a.k.a. “merit function”...)
Finding $X_N^{\text{Bayes}}$: proof

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

\[
E_{N-1}(L(D_{N+1})) = E_{N-1}(R_N(F_N, D_{N+1})) \\
\geq E_{N-1}(R_N^{\text{Bayes}}(F_N)) = R_{N-1}(F_{N-1}, X_{N-1})
\]
Finding $X_N^{\text{Bayes}}$: proof

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

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

- Let $D' = (X_1, \ldots, X_{N-1}, X'_N, D'_{N+1})$,

where $X'_N = \varphi_{N-1}^{\text{Bayes}}(F_{N-1})$ and $D'_{N+1} = \varphi_N^{\text{Bayes}}(F_{N-1}, X'_N, Z'_N)$
Finding $X_N^{\text{Bayes}}$: proof

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

$$E_{N-1}(L(D_{N+1})) = E_{N-1}(R_N(F_N, D_{N+1}))$$

$$\geq E_{N-1}(R_N^{\text{Bayes}}(F_N)) = R_{N-1}(F_{N-1}, X_{N-1})$$

Let $D' = (X_1, \ldots, X_{N-1}, X'_N, D'_{N+1})$,

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

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

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

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

- Let $D' = (X_1, \ldots, X_{N-1}, X'_N, D'_{N+1})$,

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

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

- Thus $E_0(L(D_{N+1})) \geq E_0(L(D'_{N+1}))$
Finding $X^\text{Bayes}_N$: example (cont’d)

- Recall our linear loss example

\[
\hat{X}^\text{Bayes} = \arg\min \hat{\xi}_N \\
R^\text{Bayes}_N = \min \hat{\xi}_N - E_N (\min \xi)
\]
Finding $X^\text{Bayes}_N$: example (cont’d)

- Recall our linear loss example
  \[
  \hat{X}^\text{Bayes} = \arg\min \hat{\xi}_N \\
  R^\text{Bayes}_N = \min \hat{\xi}_N - E_N (\min \xi)
  \]

- Compute the posterior risk at time $N - 1$
  \[
  R_{N-1}(F_{N-1}, x_N) = E_{N-1,x_N} \left( R^\text{Bayes}_N (F_N) \right) \\
  = E_{N-1,x_N} \left( \min \hat{\xi}_N \right) - E_{N-1} (\min \xi)
  \]
Finding $X_N^{\text{Bayes}}$: example (cont’d)

- Recall our linear loss example

$$\hat{X}^{\text{Bayes}} = \arg\min \hat{\xi}_N$$

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

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

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

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

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

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

(first appears (in english) in Mockus, Tiesis & Žilinskas, 1978)
Finding $X_N^{\text{Bayes}}$: example (cont’d)

- Equivalently,

$$
X_N = \text{argmax}_{x_N} \min_\hat{\xi}_{N-1} - E_{N-1,x_N} \left( \min \hat{\xi}_N \right)
\underbrace{\rho_{N-1}^{\text{KG}}(x_N) \geq 0}_{\rho_{N-1}^{\text{KG}}(x_N) \geq 0}
$$
Finding $X_N^{\text{Bayes}}$: example (cont’d)

- Equivalently,

\[ X_N = \arg\max_{x_N} \min \hat{\xi}_{N-1} - E_{N-1,x_N} \left( \min \hat{\xi}_N \right) \]

\[ \rho_{N-1}^{\text{KG}}(x_N) \geq 0 \]

- Nowadays called the Knowledge Gradient (KG) criterion
  (Frazier, Powell & co-authors, 2008, 2009, 2011)
Finding $X_N^{\text{Bayes}}$: example (cont’d)

- Equivalently,

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

$$\rho_{N-1}^{\text{KG}}(x_N) \geq 0$$

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

- Remarks
  - applicable to “noisy” observations as well
    - a.k.a. simulation-based optimization
Finding $X_N^{\text{Bayes}}$: example (cont’d)

- Equivalently,

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

- 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, $\rho_{\text{KG}}^N$ is not exactly computable in general
  
    - idea: approx. max over a finite grid (more about that later)
Finding $X_{N}^{\text{Bayes}}$: example (cont’d)

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

![Graph of response $z$ vs. input $x$]

![Graph of sampling criterion $\rho$ vs. final point $x_N$]
Finding $X^\text{Bayes}_N$: example (cont’d)

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

Graph showing the response $z$ and sampling criterion $\rho$ against input $x$ and final point $x_N$. The graph illustrates the relationship between the response and input, with shaded regions indicating variability.
Finding $X_N^{\text{Bayes}}$: example (cont’d)

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

Warning: $X_N \neq \arg\max \hat{\xi}_{N-1}$ (uncertainty is taken into account)
Finding $X^\text{Bayes}_N$: example, variant (cont’d)

- Recall the following variant

\[
\hat{X}^\text{Bayes, 1} = \arg\min_{x \in \{X_1, \ldots, X_N\}} \xi(x)
\]

\[
R_{N}^{\text{Bayes, 1}} = \min_{i \leq N} \xi(X_i) - E_N(\min \xi)
\]
Finding $X^\text{Bayes}_N$: example, variant (cont’d)

- Recall the following variant

\[
\hat{X}^{\text{Bayes},1} = \arg\min_{x \in \{X_1, \ldots, X_N\}} \xi(x)
\]

\[
R^{\text{Bayes},1}_N = \min_{i \leq N} \xi(X_i) - E_N (\min \xi)
\]

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

\[
X_N = \arg\max_{x_N} M_{N-1} - E_{N-1,x_N} (M_N)
\]
Finding $X_N^{\text{Bayes}}$: example, variant (cont’d)

- Recall the following variant

$$\hat{X}_{\text{Bayes}, 1} = \arg\min_{x \in \{X_1, \ldots, X_N\}} \xi(x)$$

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

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

$$X_N = \arg\max_{x_N} M_{N-1} - E_{N-1,x_N}(M_N)$$

$$= \arg\max_{x_N} E_{N-1} \left( (M_{N-1} - \xi(x_N))_+ \right)$$

$$\rho_n^{\text{EI}}(x_N) \geq 0$$

- This is the Expected Improvement (EI) criterion

(Mockus et al 1978; Jones, Schonlau & Wlech, 1998)
Finding $X_N^{\text{Bayes}}$: example, variant (cont’d)

- Recall the following variant

$$\hat{X}^{\text{Bayes},1} = \arg\min_{x \in \{X_1, \ldots, X_N\}} \xi(x)$$
$$R_N^{\text{Bayes},1} = \min_{i \leq N} \xi(X_i) - E_N(\min \xi)$$

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

$$X_N = \arg\max_{x_N} M_{N-1} - E_{N-1,(x_N)}(M_N)$$
$$= \arg\max_{x_N} E_{N-1}\left((M_{N-1} - \xi(x_N))_+\right)$$
$$\geq 0$$

- 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 $X_{N}^{\text{Bayes}}$: example (cont’d)

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

Warning: $X_{N} \neq \text{argmax} \hat{\xi}_{N-1}$ (uncertainty is taken into account)
Finding $X_N^{\text{Bayes}}$: example (cont’d)

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

Warning: $X_N \neq \arg\max \hat{\xi}_{N-1}$ (uncertainty is taken into account)
Lecture 2: Bayesian optimization (BO)

2.2. From Bayes-optimal to myopic strategies

- The optimal terminal decision
- Optimal choice of the last evaluation
- Bayes-optimal versus “practical Bayes” optimization
- Sampling criteria for multi-objective and/or contrained optimization
The Bayes-optimal strategy

Recall the optimal terminal decision rule:

\[
\varphi_{\text{Bayes}}^N (F_N) = \arg\min_d E_N (L(d)) \\
R_{\text{Bayes}}^N (F_N) = \min_d E_N (L(d))
\]
The Bayes-optimal strategy

Recall the optimal terminal decision rule

\[ \varphi^\text{Bayes}_N(F_N) = \arg\min_d E_N(L(d)) \]

\[ R^\text{Bayes}_N(F_N) = \min_d E_N(L(d)) \]

Recall the optimal rule for the last evaluation

\[ \varphi^\text{Bayes}_{N-1}(F_{N-1}) = \arg\min_{x_N} E_{N-1,x_N}(R^\text{Bayes}_N(F_N)) \]

\[ R^\text{Bayes}_{N-1}(F_{N-1}) = \min_{x_N} E_{N-1,x_N}(R^\text{Bayes}_N(F_N)) \]
The Bayes-optimal strategy

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

\[
\varphi_{n-1}^{\text{Bayes}}(F_{n-1}) = \arg\min_{x_n} E_{n-1,x_n} \left( R_n^{\text{Bayes}}(F_n) \right)
\]

\[
R_{n-1}^{\text{Bayes}}(F_{n-1}) = \min_{x_n} E_{n-1,x_n} \left( R_n^{\text{Bayes}}(F_n) \right)
\]

- This is called **backward induction** (or dynamic programming)
The Bayes-optimal strategy

- The entire Bayes-optimal strategy can be written similarly: \( \forall n, \)
  \[
  \varphi_{n-1}^{\text{Bayes}}(F_{n-1}) = \arg\min_{x_n} E_{n-1,x_n} \left( R_n^{\text{Bayes}}(F_n) \right)
  \]
  \[
  R_{n-1}^{\text{Bayes}}(F_{n-1}) = \min_{x_n} E_{n-1,x_n} \left( R_n^{\text{Bayes}}(F_n) \right)
  \]

- This is called backward induction (or dynamic programming)

- So what? Can we use this?
The Bayes-optimal strategy

More explicitly, the optimal decision for the first evaluation is

\[
X_1 = \arg\min_{x_1} E_{0,x_1} \left( \min_{x_2} E_{1,x_2} \left( \ldots \right. \right.
\[
\left. \left. \min_{x_N} E_{N-1,x_N} \left( \min_d E_N(L(d)) \right) \right) \right)
\]
The Bayes-optimal strategy

More explicitly, the optimal decision for the first evaluation is

$$X_1 = \arg\min_{x_1} E_{0,x_1} \left( \min_{x_2} E_{1,x_2} \left( \ldots \right. \right.$$

$$\left. \min_{x_N} E_{N-1,x_N} \left( \min_d E_N \left[L(d)\right] \right) \right)$$

Very difficult to use in practice beyond $N = 1$ or 2

- each “min” is an optim. problem that needs to be solved...
- each “$E_{n,x}$” is an integral that needs to be computed...
- none of them are tractable, even for the nicest (GP) priors 😞
Practical Bayesian optimization: myopic strategies

- Practical BO algorithms use, in general, **myopic strategies**
  - a.k.a. one-step look-ahead strategies
  - principle: make each decision as if it were the last one
  - Bayes-optimal if $N = 1$, sub-optimal otherwise
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- For any $n \leq N$, let $\overline{L}_n = \min_d E_n (L(d))$

**Generic myopic BO algorithm**

- For $n$ from 0 to $N - 1$
  - Compute $X_{n+1} = \arg\min_x E_{n,x_{n+1}} (\overline{L}_{n+1})$
  - Make an evaluation at $X_{n+1}$
- Output $D_{N+1} = \arg\min E_N (L(d))$
Practical Bayesian optimization: hyper-parameters

- GP models have **hyper-parameters** $\theta$ (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
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  - **plug-in** approach
    - use $P_n^\theta \approx \delta_{\hat{\theta}_n}$, with $\hat{\theta}_n$ an estimator of $\theta$ (MML, LOO-CV, ...)
    - enough initial data is needed for this approach
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    - enough initial data is needed for this approach

Generic myopic BO algorithm with hyper-parameter estimation

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

STK demo

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

- Each iteration involves an auxiliary optimization problem
Practical Bayesian optimization: optimization

- Each iteration involves an auxiliary optimization problem

- Various approaches to solve it
  - Fix grid or IID random search
    - OK for low-dimensional, simple problems
    - if accurate convergence is not needed
Practical Bayesian optimization: optimization

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

- **Bayesian optimization** ⇒ run-time overhead
  - depends on the model, sampling criterion, optimizer, etc.
  - BO is appropriate for expensive-to-evaluate numerical models
Lecture 2 : Bayesian optimization (BO)

2.2. From Bayes-optimal to myopic strategies
   - The optimal terminal decision
   - Optimal choice of the last evaluation
   - Bayes-optimal versus “practical Bayes” optimization
   - Sampling criteria for multi-objective and/or constrained optimization
Multi-objective problems

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

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

Pareto domination relation

$z \prec z'$ if (def)

\[
\begin{align*}
\begin{cases}
z_j & \leq z_j' & \text{for all } j \leq p, \\
z_j & < z_j' & \text{for at least one } j \leq p.
\end{cases}
\end{align*}
\]
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 \( P = \{ x \in \mathbb{X} : \forall x' \in \mathbb{X}, f(x') \prec f(x) \} \)
    (a.k.a. set of Pareto-efficient solutions)
Multi-objective problems

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

**Pareto domination relation**

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

- The goal is to find (estimate)
  - the Pareto set \( \mathbb{P} = \{ x \in \mathbb{X} : \not\exists x' \in \mathbb{X}, f(x') \prec f(x) \} \)
    (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
```

```
f_2

\( z_1 \)

\( z_2 \)

\rightarrow f_1
```
Multi-objective problems

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

Noiseless evaluations

\[ B = \prod_{j=1}^{p} \left[ -\infty; z_{j}^{\text{ref}} \right] : \text{bounding box} \]
Multi-objective problems

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

Noiseless evaluations

\[ \mathcal{B} = \prod_{j=1}^{p} \left[ −\infty; z_{j}^{ref} \right] : \text{bounding box} \]

True dominated region:

\[ H^*(f) = \{ z \in \mathcal{B}, \exists x \in \mathcal{X}, f(x) \preceq z \} \]
Multi-objective problems

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Noiseless evaluations

\( \mathbb{B} = \prod_{j=1}^{p} [-\infty; z_{j}^{\text{ref}}] \): bounding box

True dominated region:

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

Loss function:

\[ L(f, \hat{H}) = |H^*(f) \triangle \hat{H}| \]
Multi-objective problems

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Best "safe" estimator:

\[ H_n = \{ z \in \mathcal{B}, \exists i \leq n, f(X_i) \preceq z \} \]
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Best “safe” estimator:

\[ H_n = \{ z \in \mathcal{B}, \exists i \leq n, f(X_i) \preceq z \} \]

\[
\rho_{n}^{\text{EHVI}}(x_{n+1}) = E_{n,x_{n+1}}( |H_{n+1} \setminus H_n| )
\]
Multi-objective problems

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

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

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

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

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

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

- Consider the following loss function
  \[
  L(f, \hat{x}) = \begin{cases} 
    f_o(\hat{x}) - f_o^* & \text{if } f_c(\hat{x}) \leq 0, \\
    +\infty & \text{otherwise}. 
  \end{cases}
  \]

where \( f_o^* = \min_{x : f_c(x) \leq 0} f_o(x) \)
Inequality-constrained problems

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

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

\[
\rho_n^{EIC}(x_{n+1}) = \rho_{o,n}^{EI}(x_{n+1}) \cdot \prod_{j=1}^{q} P_n(\xi_{c,j}(x_{n+1}) \leq 0).
\]

Proba of Feasibility (PF)
Inequality-constrained problems

- Assuming
  - noiseless evaluations,
  - independent priors on objective and constraint functions,
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$$\rho^\text{EIC}_n(x_{n+1}) = \rho^\text{EI}_{o,n}(x_{n+1}) \cdot \prod_{j=1}^q P_n(\xi_{c,j}(x_{n+1}) \leq 0).$$

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

- Assuming
  - noiseless evaluations,
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\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
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 !

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    - SMC = Sequential Monte Carlo
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**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
Miscellaneous references for further reading

- Information-based BO: a different approach
  - Risk = entropy of the minimizer

- Aggregation-based approaches
  - Multi-objective: ParEGO (Knowles, 2006)
  - Constrained: Augmented Lagrangian methods (Gramacy et al, 2016; Picheny et al, 2016)
- Information-based BO: a different approach
  - Risk = entropy of the minimizer

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- Batch of evaluations: multi-point criteria
Miscellaneous references for further reading

▶ Information-based BO: a different approach
  ▶ Risk = entropy of the minimizer

▶ 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

▶ Noisy evaluations / stochastic simulators
  ▶ will be discussed in the next part 😊
Lecture 2: Bayesian optimization (BO)

2.1. Decision-theoretic framework
2.2. From Bayes-optimal to myopic strategies
2.3. Design under uncertainty
Lecture 2 : Bayesian optimization (BO)

2.3. Design under uncertainty

Overview of possible approaches

Optimization of a mean response

RBDO (and other formulations)
Design under uncertainty

- Standard design optimization problem:
  - Minimize one objective ("cost") function $f_0(x)$
  - or several objective functions $f_{o,1}(x), \ldots, f_{o,p}(x)$
  - under the constraints $f_{c,j}(x) \leq 0$, $1 \leq j \leq q$

- Some objective/constraint functions are expensive to evaluate
Design under uncertainty

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  - under the constraints $f_{c,j}(x) \leq 0, 1 \leq j \leq q$

- Some objective/constraint functions are expensive to evaluate

“Design under uncertainty” framework

- objective functions: $f_{o,j}(x, u), 1 \leq j \leq p$
- constraint functions: $f_{c,j}(x, u), 1 \leq j \leq q$
- where $u$ denotes factors that the designer cannot control
(a few words on the) Worst-case approach

- Principle of the worst-case (minimax) approach
  - Define an uncertainty set \( \mathbb{U} \)
  - Optimize by considering the worst \( u \in \mathbb{U} \)
(a few words on the) Worst-case approach

- 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:

$$\minimize \max_{u \in \mathbb{U}} f_o(x, u)$$
(a few words on the) Worst-case approach

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

- For instance, assuming a single-objective problem:

  \[
  \text{minimize } \max_{u \in \mathcal{U}} f_o(x, u)
  \]

- If the problem has constraints, they become:

  \[
  \forall j \leq q, \forall u \in \mathcal{U}, f_{c,j}(x, u) \leq 0
  \]
Example 1: Illustration of the worst-case approach

Example: \( f_0(x, u) = \tilde{f}(x + u) \), with \( u \in \mathbb{U} = [-\delta; \delta], \ \delta = 5 \)
Example 1: Illustration of the worst-case approach

Example: $f_o(x, u) = \tilde{f}(x + u)$, with $u \in \mathbb{U} = [-\delta; \delta], \delta = 5$
Example 1: Illustration of the worst-case approach

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

Remark: very conservative, the nominal performance is ignored
Example 2: Illustration of the worst-case approach

Example: \( f_o(x, u) = \tilde{f}(x + u) \), with \( u \in \mathbb{U} = [-\delta; \delta], \ \delta = 5 \)
Example 2: Illustration of the worst-case approach

Example: \( f_\circ(x, u) = \tilde{f}(x + u) \), 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 $\rightarrow U \sim P^U$
  - 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 $\rightarrow U \sim P_U$
  - can be a random vector ($\in \mathbb{R}^m$), or a more complicated object

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

where $f = (f_{o,1}, \ldots, f_{o,p}, f_{c,1}, \ldots, f_{c,q})$
The “stochastic simulator” setting

\[ Z = f(x, U) \]

- 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 explicitly
The "stochastic simulator" setting

\[ Z = f(x, U) \]

- **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 explicitly

- **“State of nature” (the things that we don’t know)**
  - the family \( (P^Z_x) \) 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 \( U_{\text{real}} \) that defines the \( f(x, U_{\text{real}}) \) ultimately realized
The “environmental variables” setting

\[ z = f(x, u) \]

Features of the black box

- the simulator remains deterministic
- \( P^U \) is specified separately, usually explicitly
- 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 explicitly
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“State of nature” (the things that we don’t know)

- the deterministic function \( f : (x, u) \mapsto f(x, u) \)
- the RV \( U_{\text{real}} \) that defines the \( f(x, U_{\text{real}}) \) ultimately realized
The “environmental variables” setting

- Features of the black box
  - the simulator remains deterministic
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- “State of nature” (the things that we don’t know)
  - the deterministic function \( f : (x, u) \mapsto f(x, u) \)
  - the RV \( U_{\text{real}} \) that defines the \( f(x, U_{\text{real}}) \) 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 $U_{\text{real}}$. 

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 $U_{\text{real}}$.

In the following, we focus on
- single objective problems
- in the “environmental variables” setting

and discuss two important cases:
- optimization of the averaged objective function
- reliability-based design optimization (RBDO), a.k.a. “chance constrained” optimization, and other formulations
Lecture 2: Bayesian optimization (BO)

2.3. Design under uncertainty

- Overview of possible approaches
- Optimization of a mean response
- RBDO (and other formulations)
Assume

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

- Assume
  - single objective $f = f_0$, expensive to evaluate
  - no (expensive-to-evaluate) constraints
  - remark: cheap constraints allowed in the definition of $X \subset \mathbb{R}^d$
  - “environmental variables” setting

- Consider once again the $L^1$ loss function

\[
L \left( (f, u_{\text{real}}), \hat{x} \right) = \left| f(\hat{x}, u_{\text{real}}) - \min_x f(x, u_{\text{real}}) \right|
\]
\[
= f(\hat{x}, u_{\text{real}}) - \min_x f(x, u_{\text{real}})
\]
Optimization of a mean response

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

\[
E_N \left( L \left( (\xi, U_{\text{real}}), \hat{x} \right) \right) = E_N \left( \xi(\hat{x}, U_{\text{real}}) \right) - E_N \left( \min \xi(\cdot, U_{\text{real}}) \right)
\]
Optimization of a mean response

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

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

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

where $\bar{\xi}(x) = \int \xi(x, u) P^U(u) \, du$
Optimization of a mean response

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

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

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

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

**Equivalent “deterministic” problem**

$$
\min_{\hat{x}} \overline{f}(x), \quad \text{with} \quad \overline{f}(x) = \int f(x, u) P^U(du)
$$

(Remark: this formulation occurs very naturally in a BO framework 😊)
Example 1: Illustration of the worst-case approach

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

Remark: very conservative, the nominal performance is ignored
Example 1: Worst-case versus probabilistic approach

Example: \( f_0(x, u) = \tilde{f}(x + u) \), with \( u \in \mathbb{U} = [-\delta; \delta] \), \( \delta = 5 \)

\[ \bar{f}_0 = \mathbb{E}(f_0(\cdot, U)), \text{ with } U \sim \mathcal{N}(0, s^2), \text{ s.t. } \mathbb{P}(|U| \leq \delta) = 99.9\% \]
Example 2: Illustration of the worst-case approach

Example: \( f_o(x, u) = \tilde{f}(x + u) \), with \( u \in \mathbb{U} = [-\delta; \delta], \ \delta = 5 \)
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Example 3: Three-bar truss (Koski, 1985; Das, 1997)
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Design variables: \( x = (a_1, a_2, a_3, w) \)
- \( a_j \): cross-section of bar \( j \)
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- 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 \( \sigma_j \) in each bar \( (1 \leq j \leq 3) \).
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We will consider the following problem:

- minimize \( E_U (\|y\|) \)
- under the constraints: \( x_{\text{min}} \leq x \leq x_{\text{max}}, \ V \leq V_{\text{max}} \)
Example 3: Three-bar truss (Koski, 1985; Das, 1997)

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  - minimize $E_U(\|y\|)$
  - under the constraints: $x_{\text{min}} \leq x \leq x_{\text{max}}$, $V \leq V_{\text{max}}$

- Remark about constraints
  - The constraint $V \leq V_{\text{max}}$ 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: $|\sigma_j| \leq \sigma_{\text{max}}$ can be checked a posteriori
Breaking the “double loop”

- Natural “double loop” approach
  - outer loop: ordinary optimization algorithm applied to $\tilde{f}$
  - inner loop: integration (MC, quadrature...) to compute $\tilde{f}$
Breaking the “double loop”

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- Drawback: typically require large number of evaluations
Breaking the “double loop”

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

- Drawback: typically require large number of evaluations

- Bayesian optimization breaks the double loop 😊
  - Construct a Bayesian model for $f$, not $\bar{f}$
  - Remark: can be achieved using other surrogate-model based approaches (see 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: \( \bar{f} = \int f(\cdot, u) P^U(du) \)

- \( \bar{f} \) is a function of \( f \)
  - priors cannot be specified independently
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  - priors cannot be specified independently

Gaussian process priors are, again, very convenient

If \( \xi \sim \mathcal{GP}(m, k) \), then \( \bar{\xi} \sim \mathcal{GP}(m_{\bar{\xi}}, k_{\bar{\xi}}) \),

with

\[
\begin{align*}
m_{\bar{\xi}}(x) &= \int m(x, u) P^U(du) \\
k_{\bar{\xi}}(x, y) &= \int \int k((x, u), (y, v)) P^U(du) P^U(dv)
\end{align*}
\]
Proof

- \(\overline{\xi}\) is Gaussian by linearity of the integral

- Computation of the mean function: exchange \(\int\) and \(E\)

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

- Computation of the covariance function: idem with bilinearity

\[
k_{\overline{\xi}}(x, y) = \text{cov}\left(\overline{\xi}(x), \overline{\xi}(y)\right) = \text{cov}\left(\int \xi(x, u) P^U(du), \int \xi(x, v) P^U(dv)\right) = \iint k((x, u), (y, v)) P^U(du)P^U(dv)
\]

\[\blacksquare\]
Actual, we can say much better:

**Jointly Gaussian processes**

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

$$k_{\xi, \bar{\xi}}((x, u), (y, v)) = \text{cov}(\xi(x, u), \bar{\xi}(y)) = \int k((x, u), (y, v)) P_U(dv)$$
Prior model (cont’d)

- Actually, we can say much better:

**Jointly Gaussian processes**

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

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

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

**Jointly Gaussian processes**

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

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

Remark: $m_{\xi}$, $k_{\xi}$ and $k_{\xi, \xi}$ can be computed exactly

- if $P^U$ is discrete ($P^U = \sum_{j=1}^{n_U} w_j \delta_{u_j}$)
- if $P^U$ is (a mixture of) Gaussian(s), for some particular $k$
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Important special case: $\xi(x, u) = \tilde{\xi}(x + u)$

- If $\xi$ is a GP iff $\tilde{\xi}$ is a GP
- $m_{\xi}(x, u) = m_{\tilde{\xi}}(x + u)$ and $k_{\xi}((x, u), (u, v)) = k_{\tilde{\xi}}(x + u, y + v)$
Examples 1 and 2: discretization of $P^U$

- In the two examples, $Prob^U = \mathcal{N}(0, s^2)$, with $s = 1.52$
- $P(|U| \leq 5) \approx 99.9\%$
Examples 1 and 2: discretization of $P^U$

- In the two examples, $Prob^U = \mathcal{N}(0, s^2)$, with $s = 1.52$
  - $P(|U| \leq 5) \approx 99.9\%$
- We choose to use a regular discretization with $n_U = 11$ points
  - points regularly spaced on $[-5; 5]$
  - weights computed using the normal cdf (using mid-points)
Example 3: discretization of $P^U$

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

Monte Carlo sample of size $n_U = 50$
Example 3: discretization of $P^U$

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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 $X \times U$
  - at each step, we must select a pair $(X_{n+1}, U_{n+1}) \in X \times U$
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  - numerical model $f : (x, u) \mapsto f(x, u)$, defined on $X \times U$
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- Important special case
  - $f(x, u) = \tilde{f}(x + u)$
  - in this case, we must simply select a point $X_{n+1} \in X$

- 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?

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  - other strategies are proposed in the literature
    - Williams et al 2000; Janusevkis et Le Riche 2013
    - Entropy-based methods could be used as well
      (Villemonteix et al 2009, Hennig & Schueller 2012...)
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- Assume now the $L^1$ loss

- Recall the posterior risk at time $N$ for an estimate $\hat{x} \in X$:
  \[
  E_N \left( L((\xi, U_{\text{real}}), \hat{x}) \right) = E_N \left( \bar{\xi}(\hat{x}) \right) - E_N \left( \min_x \xi(\cdot, U_{\text{real}}) \right)
  \]
Sampling strategy: one step look-ahead

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

$$
\bar{L}_n = \min_x E_n \left( \tilde{\xi}(x) \right) - E_n \left( \min_x \xi(\cdot, U_{\text{real}}) \right)
$$

$$
= \min_x m^{-\xi,n} - E_n \left( \min_x \xi(\cdot, U_{\text{real}}) \right)
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\]

\[
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\]

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

\[
(X_{n+1}, U_{n+1}) = \arg\min_{x_{n+1}, u_{n+1}} E_n, (x_{n+1}, u_{n+1}) \left( \bar{L}_{n+1} \right)
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- The one-step look-ahead (myopic) strategy is

\[
(X_{n+1}, U_{n+1}) = \arg\min_{x_{n+1}, u_{n+1}} E_{n, (x_{n+1}, u_{n+1})} \left( \bar{L}_{n+1} \right) \\
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Sampling strategy: one step look-ahead

- Equivalently,

$$(X_{n+1}, U_{n+1}) = \arg\max_{x_{n+1}, u_{n+1}} \rho_n(x_{n+1}, u_{n+1})$$

where $\rho_n$ denotes the corresponding “expected improvement”

$$\rho_n(x_{n+1}, u_{n+1}) = \bar{L}_n - E_{n,(x_{n+1},u_{n+1})}(\bar{L}_{n+1})$$

$$= \min_{x_\xi} m_{\xi,n} - E_{n,(x_{n+1},u_{n+1})}(\min_{x_\xi} m_{\xi,n+1})$$
Sampling strategy: one step look-ahead

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\[\rho_n(x_{n+1}, u_{n+1}) = \bar{L}_n - E_n,(x_{n+1}, u_{n+1})\left(\bar{L}_{n+1}\right)\]

\[= \min_X m_{\xi,n} - E_n,(x_{n+1}, u_{n+1})\left(\min_X m_{\xi,n+1}\right)\]

- Formally, looks like the KG criterion of Frazier & co, but...
Sampling strategy: one step look-ahead

- Comparison with KG as presented in the literature

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- There is no real difference mathematically: in both cases
  1. the function to be optimized is not observable directly,
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## Sampling strategy: one step look-ahead

- **Comparison with KG as presented in the literature**

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- **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:

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

where the min runs over $\mathbb{X}_n^{\text{ref}} \cup \{\tilde{x}_{n+1}\}$.
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- Initially proposed by Scott et al (2011)
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  - 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**.
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.

  - AKG emerges has one of the most efficient criteria
  - Huang et al (2006)'s “augmented EI” also performs well
  - (Entropy-based criteria not benchmarked)
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  - 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)
Lecture 2: Bayesian optimization (BO)

2.3. Design under uncertainty

- Overview of possible approaches
- Optimization of a mean response
- RBDO (and other formulations)
Reliability-based (design) optimization (RBO, RBDO)

- Assume
  - a single objective $f = f_0$, often cheap to evaluate
  - one or several expensive-to-evaluate constraints $f_{c,1}, \ldots, f_{c,q}$
  - “environmental variables” setting
Reliability-based (design) optimization (RBO, RBDO)

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  - one or several expensive-to-evaluate constraints $f_{c,1}, \ldots, f_{c,q}$
  - “environmental variables” setting

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

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

Minimize

$$
\overline{f_o}(x), \quad \text{where } f_o(x) = \mathbb{E}_U (f_o(x, U))
$$

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

$$
\forall j \leq q, \quad P_U (f_{c,j}(x, U) > 0) \leq p_{j}^{\text{tol}}
$$
Reliability-based (design) optimization (RBO, RBDO)

- See Valdebenito & Schuëller (2010) for a survey
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- $f_o$ is often cheap to evaluate
  - e.g. volume / mass / manufacturing cost / . . .
  - Expectation often computed (or approximated) analytically
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- 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
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- Again, algorithms with a “double loop” structure can be used
  - outer loop: ordinary optimization algorithm with constraints
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- Again, surrogate-based methods should be able to “break the double loop” by building a model on $\mathbb{X} \times \mathbb{U}$
Why RBDO is harder than mean-response optimization

- because the thresholds $p_j^{tol}$ are usually small
  - MC-type approx. $P^U \approx \frac{1}{m} \sum_j \delta_{u_j}$ becomes very expensive or infeasible
  - Dedicated techniques (e.g., FORM/SORM, IS, subset simulation) needed for an efficient evaluation of the constraints
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- BO: the distribution of $P_U (\xi_{c,j}(x, U) > 0)$ is intractable
  - Posterior mean/variance can be written as integrals (see, e.g., Villemonteix 2008 chap III), but...
  - ...the posterior distribution is not Gaussian even if $\xi_c$ 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:
  - Dubourg and co-authors (2011a, 2011b): RBDO-N2LA
Bayesian RBDO algorithms?

- A few GP-based algorithms have been proposed, notably:
  - Dubourg and co-authors (2011a, 2011b): RBDO-N2LA

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

```
Algorithm 1 Population-based adaptive refinement strategy
1: F := ∅, F := ∅
2: w := w + w(x)
3: k := k + 1
4: Refine := true
5: P(x ∈ M) := x := 1
6: while Refine do
7:  F := MCMCAlgorithm(F)
8:  F := KMeansAlgorithm(F, K)
9:  F := F ∪ F
10:  F := F ∪ F
11:  G := MaximumLikelihoodKrigingModel
12:  F := F ∪ F
13:  P(x ∈ M) := x := 1
14:  for i := 1, 0, +1 do
15:  ̃F := F \ {x : μ̃(x) + ikσ̃(x) ≤ 0}
16:  ̃F := ReliabilityAnalysis(̃F)
17:  Refine := max(̃F \ {x : μ̃(x) + ikσ̃(x) ≤ 0}) > 0
18:  Optimize := ̃F \ {x : μ̃(x) + ikσ̃(x) ≤ 0}
19:  end while

Algorithm 2 Adaptive surrogate-based nested RBDO strategy
1: θ(0), g(0), F(0), j := 0
2: for i = 0 to n do
3:  q(i) := min F(i) (x, θ)
4:  q(i) := max F(i) (x, θ)
5:  end for
6: w := w + w(x)
7: k := k + 1
8: Refine := true
9: Optimize := true
10: while Refine do
11:  G := RefineKrigingModel(w, k, cp) \ Use Algorithm 1
12:  end while
13: ̃F := F ∪ F
14: ̃F := ReliabilityAnalysis(̃F)
15: ̃F := KMeansAlgorithm(F(i), F(i))
16: ̃F := F ∪ F
17: ̃F := F ∪ F
18: ̃F := SolveQuasiSQP(c, F(i), F(i), F(i), F(i), F(i))
19: ̃F := GoldsteinArmijoStepSizeRule(c, f, F(i), F(i))
20: for j := 1, 0, +1 do
21:  ̃F := F \ {x : μ̃(x) + ikσ̃(x) ≤ 0}
22:  ̃F := ReliabilityAnalysis(̃F)
23:  end for
24: Refine := max(̃F \ {x : μ̃(x) + ikσ̃(x) ≤ 0}) > cp
25: Optimize := ̃F \ {x : μ̃(x) + ikσ̃(x) ≤ 0} or f(j+1) − f(j) > cp
26: end while
```
Bayesian RBDO algorithms?

- A few GP-based algorithms have been proposed, notably:
  - Dubourg and co-authors (2011a, 2011b): RBDO-N2LA

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

<table>
<thead>
<tr>
<th>Algorithm 2</th>
<th>Adaptive surrogate-based nested RBDO strategy</th>
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</thead>
<tbody>
<tr>
<td>1: ( q_0, \theta_0, \theta^t_e, j := 0 )</td>
<td></td>
</tr>
<tr>
<td>2: for ( i = 1 ) to ( n ) do</td>
<td></td>
</tr>
<tr>
<td>3: ( q_i := \min_{\theta} F_1^{-1}(q_i, \theta) )</td>
<td></td>
</tr>
<tr>
<td>4: ( q_i := \max_{\theta} F_1^{-1}(q_i, \theta) )</td>
<td></td>
</tr>
<tr>
<td>5: end for</td>
<td></td>
</tr>
<tr>
<td>6: ( w := \frac{1}{1 \times \beta} )</td>
<td></td>
</tr>
<tr>
<td>7: ( k := \Phi^{-1}(\Phi(0.95)), \epsilon_f := 10^{-1} )</td>
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</tr>
<tr>
<td>8: Refine := true, Optimize := true</td>
<td></td>
</tr>
<tr>
<td>9: while Refine and Optimize do</td>
<td></td>
</tr>
<tr>
<td>10: while Refine do</td>
<td></td>
</tr>
<tr>
<td>11: ( \hat{G} := \text{RefineKrigingModel}(w, k, \epsilon_f) )</td>
<td></td>
</tr>
<tr>
<td>12: end while</td>
<td></td>
</tr>
<tr>
<td>13: ( \tilde{F} := { x : \mu_0(x) &lt; 0 } )</td>
<td></td>
</tr>
<tr>
<td>14: ( \tilde{F} := \text{ReliabilityAnalysis} )</td>
<td></td>
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<tr>
<td>15: ( \tilde{F} := \text{ReliabilityAnalysis} )</td>
<td></td>
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<tr>
<td>16: ( \tilde{F} := \text{ReliabilityAnalysis} )</td>
<td></td>
</tr>
<tr>
<td>17: ( \tilde{F} := \text{ReliabilityAnalysis} )</td>
<td></td>
</tr>
<tr>
<td>18: ( \tilde{F} := \text{GoldsteinArmijoStepSizeRule(c, f, d^{f})} )</td>
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</tr>
<tr>
<td>19: ( f^{(i+1)} := \hat{F}^{(i)} + d^{f} )</td>
<td></td>
</tr>
<tr>
<td>20: for (\epsilon := 1, 0, +1 ) do</td>
<td></td>
</tr>
<tr>
<td>21: ( \tilde{F} := { x : \mu_0(x) + \epsilon \sigma_0(x) \leq 0 } )</td>
<td></td>
</tr>
<tr>
<td>22: ( \tilde{F} := \text{ReliabilityAnalysis} )</td>
<td></td>
</tr>
<tr>
<td>23: end for</td>
<td></td>
</tr>
<tr>
<td>24: Refine := max ( (\tilde{F}^{(i)} - \tilde{F}^{(i-1)}, \tilde{F}^{(i)} - \tilde{F}^{(i-1)}) &gt; \epsilon_f )</td>
<td></td>
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<tr>
<td>25: Optimize := ( | F^{(i+1)} - \theta^t_e | &gt; \epsilon_0 ) or ( | F^{(i+1)} - \theta^t_e | &gt; \epsilon_0 )</td>
<td></td>
</tr>
<tr>
<td>or ( g^f &gt; 0 ) or ( \beta &lt; \beta_f )</td>
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<tr>
<td>26: end while</td>
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</table>

<table>
<thead>
<tr>
<th>Algorithm 1</th>
<th>Population-based adaptive refinement strategy</th>
</tr>
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<tbody>
<tr>
<td>1: ( \mathcal{X} := \emptyset, \mathcal{F} := \emptyset )</td>
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</tr>
<tr>
<td>2: ( x := x \times \mathcal{X} )</td>
<td></td>
</tr>
<tr>
<td>3: ( \epsilon := \Phi^{-1}(\Phi(0.95)), \epsilon_f := 10^{-1} )</td>
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<tr>
<td>4: Refine := true</td>
<td></td>
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<tr>
<td>5: ( \mathcal{F} := { x \in \mathcal{F} : x \times \mathcal{X} } )</td>
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</tr>
<tr>
<td>6: while Refine do</td>
<td></td>
</tr>
<tr>
<td>7: ( \mathcal{F} := \text{MCMCAlgorithm}(\mathcal{F}) )</td>
<td></td>
</tr>
<tr>
<td>8: ( \mathcal{F} := \text{KMeansAlgorithm}(\mathcal{F}, K) )</td>
<td></td>
</tr>
<tr>
<td>9: ( \mathcal{F} := { x \times \mathcal{F} } )</td>
<td></td>
</tr>
<tr>
<td>10: ( \mathcal{X} := { x \times \mathcal{F} } )</td>
<td></td>
</tr>
<tr>
<td>11: ( \tilde{G} := \text{MaximumLikelihoodKrigingModel} )</td>
<td></td>
</tr>
<tr>
<td>12: ( \mathcal{F} := \text{ReliabilityAnalysis} )</td>
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</tr>
<tr>
<td>13: ( \mathcal{F} := \text{ReliabilityAnalysis} )</td>
<td></td>
</tr>
<tr>
<td>14: while ( f^t ) do</td>
<td></td>
</tr>
<tr>
<td>15: ( \tilde{F} := { x : \mu_0(x) + \epsilon \sigma_0(x) \leq 0 } )</td>
<td></td>
</tr>
<tr>
<td>16: ( \tilde{F} := \text{ReliabilityAnalysis} )</td>
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</tr>
<tr>
<td>17: end while</td>
<td></td>
</tr>
<tr>
<td>18: Refine := max ( (\tilde{F}^{(i)} - \tilde{F}^{(i-1)}, \tilde{F}^{(i)} - \tilde{F}^{(i-1)}) &gt; \epsilon_f )</td>
<td></td>
</tr>
<tr>
<td>19: end while</td>
<td></td>
</tr>
</tbody>
</table>

- RBDO-N2LA is available in FERUM (Bourrinet et al, 2009)
A general alternative approach in two steps

1. Explore the design space efficiently using multi-objective BO,
2. Evaluate probabilities of failure, quantiles, etc. \textit{a posteriori} for non-dominated (and possibly other) solutions,
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. \textit{a posteriori} for non-dominated (and possibly other) solutions,
3. optionally \textbf{Reduce the uncertainty} on the most promising designs.
A general alternative approach in two (or three) steps

1. Explore the design space efficiently using multi-objective BO,
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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 $P_U (f_{c,j}(x, U) > 0) \leq p_j^{tol}$
- becomes: $\min_x f_{c,j}(x, u_0) \text{ u.c. } f_{c,j}(x, u_0) \leq 0$
RBDO and other formulations: alternative approach

A general alternative approach in two (or three) steps

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In step 1. constraints can be taken into account as objectives

i.e., the contraint $P_U(f_{c,j}(x,U) > 0) \leq p^{\text{tol}}_j$

becomes: $\min_x f_{c,j}(x,u_0)$ u.c. $f_{c,j}(x,u_0) \leq 0$

In step 2. no new evaluations need to be carried out

the posterior distribution of $\xi$ is used to assess uncertainties
RBDO and other formulations: alternative approach

STK demo

... Robust design through multi-objective optimization ...
Lecture 1 : From meta-models to UQ

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

Lecture 2 : Bayesian optimization (BO)

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

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