

# Reliability-based design optimization using adaptive kriging surrogates

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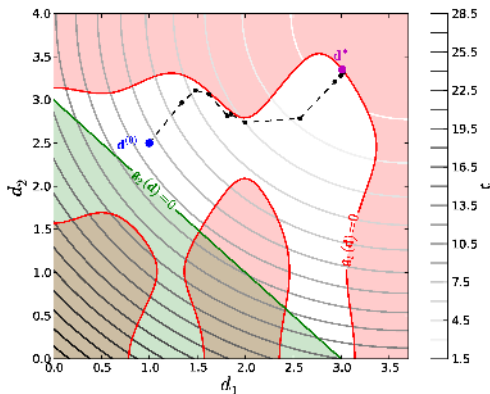
*GdR MascotNUM – Research topics day – IHP, Paris – May 11, 2012*



# Design problem formulation

## Deterministic design optimization

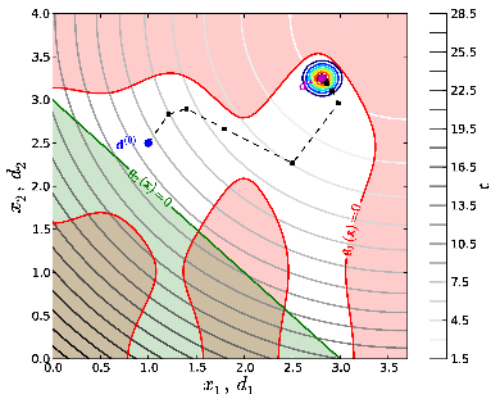
$$\mathbf{d}^* = \arg \min_{\mathbf{d} \in \mathbb{D}} c(\mathbf{d}) : \begin{cases} f_i(\mathbf{d}) < 0, i = 1, \dots, n_c \\ g_l(\mathbf{x}, \mathbf{d}) \geq 0, l = 1, \dots, n_p \end{cases}$$



# Design problem formulation

## Reliability-based design optimization

$$\mathbf{d}^* = \arg \min_{\mathbf{d} \in \mathcal{D}} c(\mathbf{d}) : \begin{cases} f_i(\mathbf{d}) \leq 0, i = 1, \dots, n_c \\ \mathbb{P}[g_l(\mathbf{X}) \leq 0 \mid \mathbf{d}] \leq p_{f,l}^0, l = 1, \dots, n_p \end{cases}$$



## Premise & objectives

- Performance models are *computationally expensive* (mostly finite-element based).
- ⇒ Replace the original expensive model with a *cheaper meta-model*.
- *Reliability approximation techniques* (such as FORM) cannot guarantee the safety level of their designs.
- ⇒ Develop a strategy that is able to *guarantee the design's safety*.
- Stakeholders target *highly reliable designs*.
- ⇒ The overall strategy should be scalable to *low failure probabilities*.

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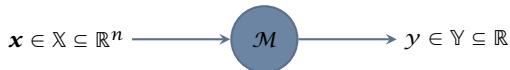
# Outline

- 1 Gaussian process meta-modelling
- 2 Adaptive designs of experiments
- 3 Reliability analysis
- 4 Reliability-based design optimization

# Meta-modelling

## Meta-modelling techniques

- aim at constructing a *predictor*  $\tilde{\mathcal{M}}$
- that *mimics* the behaviour of an existing model  $\mathcal{M}$



- from a collection of observations gathered in a *dataset*:

$$\mathcal{D} = \{(\mathbf{x}^{(i)}, y_i), i = 1, \dots, m\}, \quad y_i = \mathcal{M}(\mathbf{x}^{(i)}), i = 1, \dots, m$$

- and *statistical considerations*.

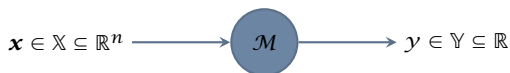
## Interest for reliability-based design

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# Gaussian process meta-modelling

The Gaussian process prior model

(Santner et al., 2003)

The function  $\mathcal{M}$  is a sample path of a Gaussian process (GP)  $Y$ :

$$Y(\mathbf{x}) = \mathbf{f}(\mathbf{x})^\top \boldsymbol{\beta} + Z(\mathbf{x}), \quad \mathbf{x} \in \mathbb{X}$$

where:

- $\mathbf{f}(\mathbf{x})^\top \boldsymbol{\beta}$  is a linear regression model;
- $Z(\mathbf{x})$  is a zero-mean, stationary GP with covariance:

$$\text{Cov}[Y(\mathbf{x}), Y(\mathbf{x}')] = \sigma^2 R(\mathbf{x} - \mathbf{x}', \boldsymbol{\theta}), \quad (\mathbf{x}, \mathbf{x}') \in \mathbb{X} \times \mathbb{X}$$

Hence, given a vector of *observations*  $Y = (Y_i = Y(\mathbf{x}^{(i)}), i = 1, \dots, m)$  and an unobserved value  $Y(\mathbf{x})$ , we have:

$$\begin{Bmatrix} Y(\mathbf{x}) \\ Y \end{Bmatrix} \sim \mathcal{N}_{1+m} \left( \begin{Bmatrix} \mathbf{f}(\mathbf{x})^\top \boldsymbol{\beta} \\ \mathbf{F} \boldsymbol{\beta} \end{Bmatrix}, \sigma^2 \begin{bmatrix} 1 & \mathbf{r}(\mathbf{x})^\top \\ \mathbf{r}(\mathbf{x}) & \mathbf{R} \end{bmatrix} \right)$$

whose parameters  $\mathbf{F}$ ,  $\mathbf{r}(\mathbf{x})$ ,  $\mathbf{R}$  are inherited from the GP's statistics ( $\mathbf{f}$  and  $R$ ).

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# Gaussian process meta-modelling

Posterior  $\equiv$  The best linear unbiased predictor (BLUP)

(Santner et al., 2003)

- Here, we are interested in the *posterior* distribution of the unobserved value given  $\mathbf{y} = (y_i = \mathcal{M}(\mathbf{x}^{(i)}), i = 1, \dots, m)$ :

$$\hat{Y}(\mathbf{x}) = [Y(\mathbf{x}) | Y = \mathbf{y}]$$

- Given  $\sigma^2$  and  $\boldsymbol{\theta}$ , the *universal Kriging* predictor is also Gaussian:

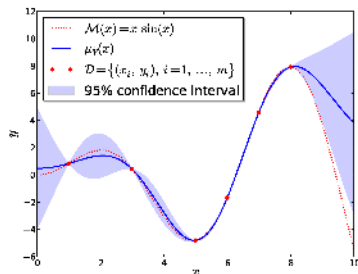
$$\hat{Y}(\mathbf{x}) = [Y(\mathbf{x}) | Y = \mathbf{y}, \sigma^2, \boldsymbol{\theta}] \sim \mathcal{N}_1(\mu_{\hat{Y}}(\mathbf{x}), \sigma_{\hat{Y}}^2(\mathbf{x}))$$

where the *mean prediction*  $\mu_{\hat{Y}}(\mathbf{x})$  and the *prediction variance*  $\sigma_{\hat{Y}}^2(\mathbf{x})$  have analytical expressions.

- In practice,  $\sigma^2$  and  $\boldsymbol{\theta}$  are not known so that they must be estimated from the observations  $\mathbf{y}$  using e.g. *maximum likelihood estimation*.

(Welch et al., 1992; Marrel et al., 2008)

## Illustration on a one-dimensional regression exercise



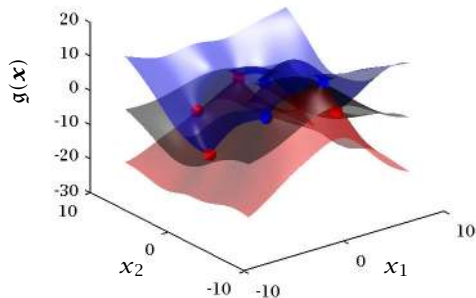
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### Interesting properties

- *interpolating*;
- *asymptotically consistent* (provided the correlation  $R$  is “compatible” with the data  $\mathbf{y}$  and the model  $M$ );  
(Vazquez, 2005)
- *Gaussian* (consequence of the prior).

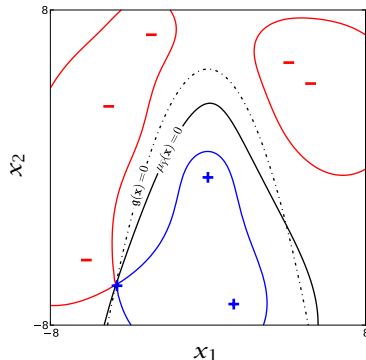
## From regression to probabilistic classification

Ex: Let  $g$  denote a quadratic limit-state function.

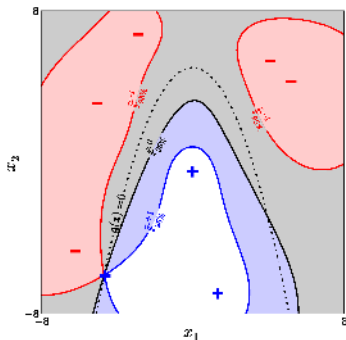


Regression

Classification ( $g \leq 0$  vs.  $g > 0$ )



## From regression to probabilistic classification



- Let  $\hat{F}_{95\%}^{-1}$ ,  $\hat{F}_{95\%}^0$ ,  $\hat{F}_{95\%}^{+1}$  denote the three following *approximate failure subsets*:

$$\hat{F}_{95\%}^i = \left\{ \mathbf{x} \in \mathbb{X} : \mu_{\hat{Y}}(\mathbf{x}) \leq i \cdot 1.96 \sigma_{\hat{Y}}(\mathbf{x}) \right\},$$

$$i = -1, 0, +1.$$

- In turns, this enables the definition of the *margin of uncertainty*:

$$\mathbb{M}_{95\%} = \hat{F}_{95\%}^{-1} \setminus \hat{F}_{95\%}^{+1}$$

- Let  $\pi$  denote the *probabilistic classification function*:

$$\pi(\mathbf{x}) = \mathcal{P} \left[ \hat{Y}(\mathbf{x}) \leq 0 \right] = \Phi \left( \frac{0 - \mu_{\hat{Y}}(\mathbf{x})}{\sigma_{\hat{Y}}(\mathbf{x})} \right)$$

$\mathcal{P}(+ | \mathbb{P})$  denotes the probability measure w.r.t. the Kriging epistemic uncertainty.

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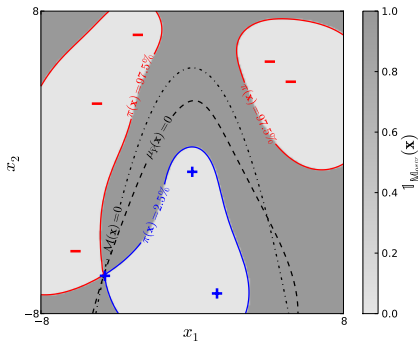
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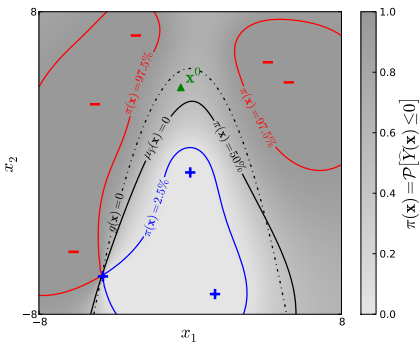
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# Designs of experiments

## Designs of experiments

- A DOE is the input part of a dataset:

$$\mathcal{X} = \{\mathbf{x}^{(i)}, i = 1, \dots, m\}$$

- Its *size*  $m$  must be minimized for the sake of *efficiency*.
- Experiments must be *selected carefully* for the sake of *accuracy* (*space-filling DOEs, Franco, 2008*).

## Adaptive designs of experiments

- are built in an *iterative* manner;
- on purpose to *refine the predictor locally* (e.g. in the vicinity of a contour);

*Sequential* adaptive DOEs for GP predictors rely on the *maximization* of a so-called *refinement criterion*.

# Sequential adaptive DOEs

## Refinement criteria for contour approximation

- Simple criteria mostly apply the *margin shrinking concept* for support vector machines

(Hurtado, 2004b; Deheeger, 2008)

- Here, we propose the “*margin probability*”:

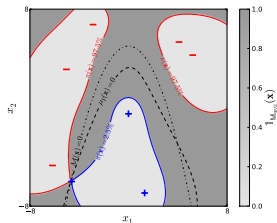
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(Dubourg et al., 2010a)

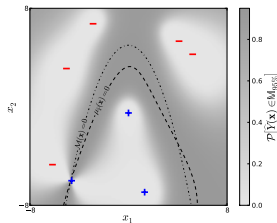
## Limitation of sequential strategies

- The multiple modes of these criteria make their *maximization difficult*;
- There does not exist *a single best point*;
- Availability of *distributed computing* platforms for  $\mathcal{M}$ .

(Ginsbourger et al., 2010)



The margin of uncertainty  $\mathbb{M}_{95\%}$



The margin probability  $\mathcal{P}[\hat{Y}(\mathbf{x}) \in \mathbb{M}_{95\%}]$

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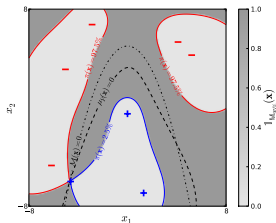
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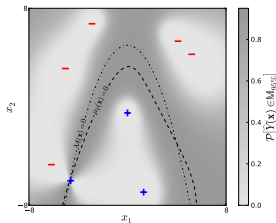
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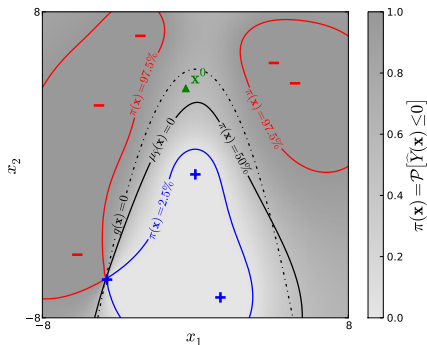
## Sampling-based adaptive DOEs

Given an initial dataset  $\mathcal{D}$   
 and a pseudo-PDF  $w$ :

- 1 Fit a Kriging predictor  $\hat{Y}(\mathbf{x})$
- 2 Define a *weighted refinement criterion*

$$C(\mathbf{x}) = \mathcal{P} \left[ \hat{Y}(\mathbf{x}) \in \mathbb{M}_{95\%} \right] w(\mathbf{x})$$

- 3 Sample  $N$  candidates from  $C$   
*(MCMC slice sampler, Neal, 2003)*
- 4 Reduce the  $N$  candidates to  $K$  points  
*(K-means clustering, Lloyd, 1982)*
- 5 Enrich the dataset  $\mathcal{D}$  with  
 $\left\{ \left( \mathbf{x}^{(m+k)}, \mathcal{M} \left( \mathbf{x}^{(m+k)} \right) \right), k = 1, \dots, K \right\}$
- 6 Loop back to step 1



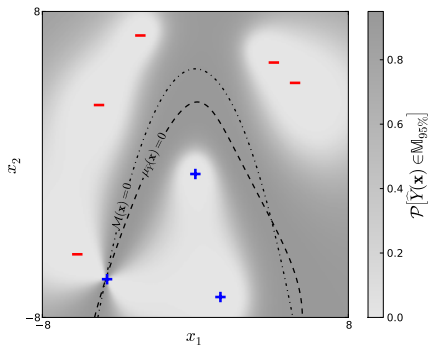
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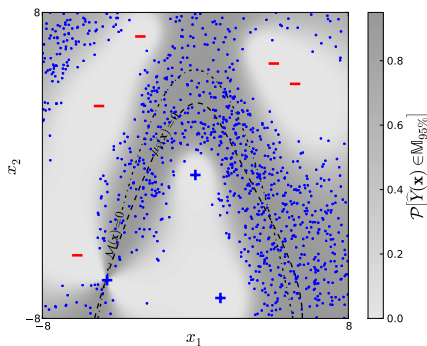
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$N$  is given (say 10,000)

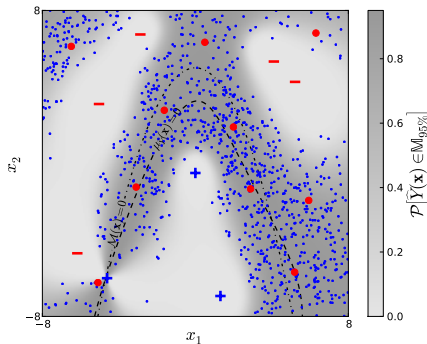
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$K$  is given (*say the number of CPUs*)

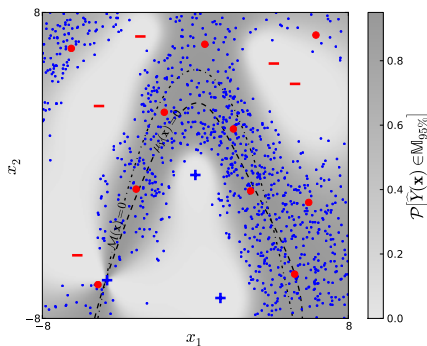
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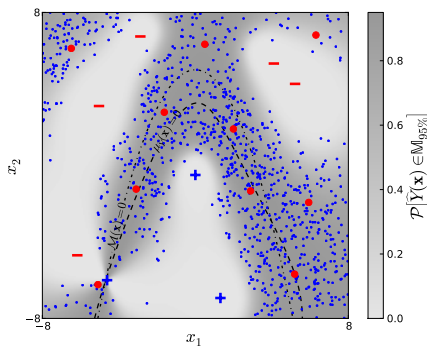
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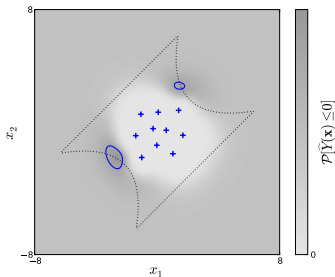
## Illustration

A four-branch series system

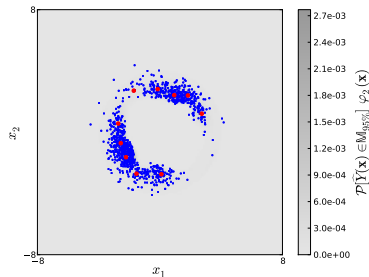
(Waarts, 2000)

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$K = 10$



Target contour, design of experiments & prediction



Sampled & clustered refinement criterion

Iteration #1

Convergence criteria depend on the *application...*

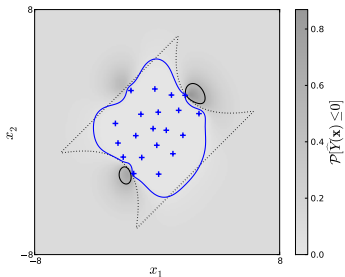
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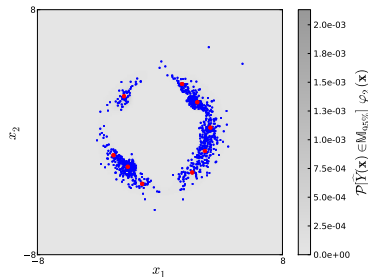
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Iteration #2

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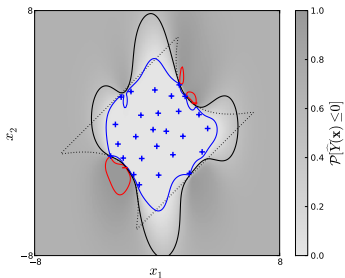
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A four-branch series system

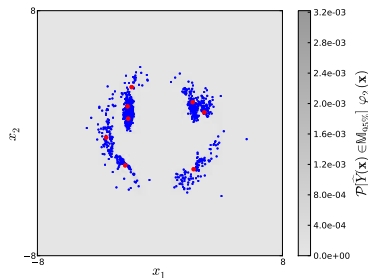
(Waarts, 2000)

$$C(\mathbf{x}) = \mathcal{P} \left[ \hat{Y}(\mathbf{x}) \in \mathbb{M}_{95\%} \right] \varphi_2(\mathbf{x})$$

$K = 10$



Target contour, design of experiments & prediction



Sampled & clustered refinement criterion

Iteration #3

Convergence criteria depend on the *application...*

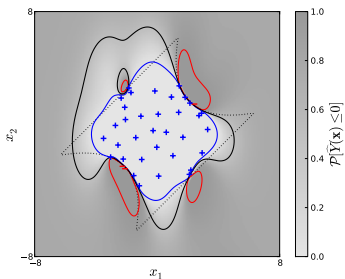
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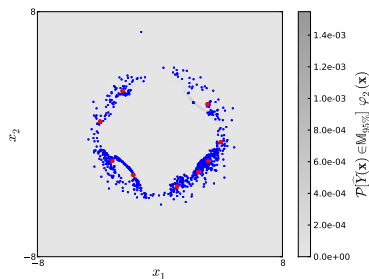
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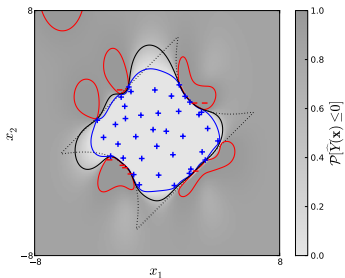
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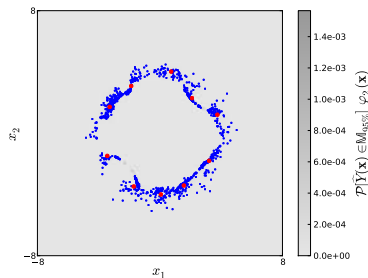
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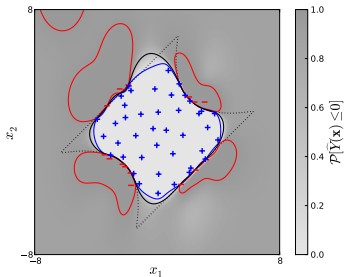
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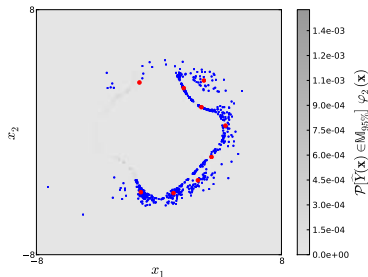
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Iteration #6

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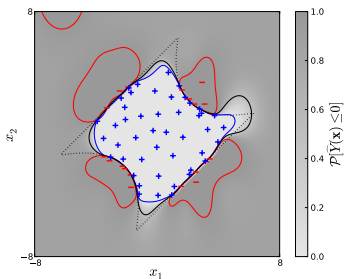
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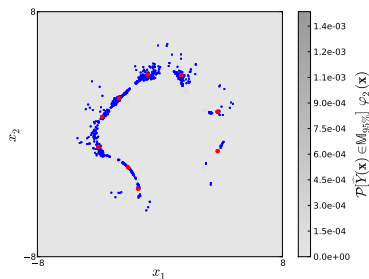
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Target contour, design of experiments & prediction



Sampled & clustered refinement criterion

Iteration #7

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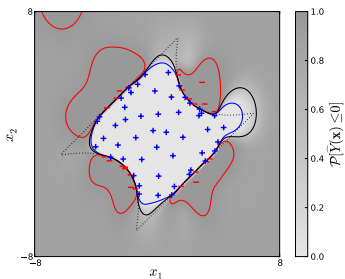
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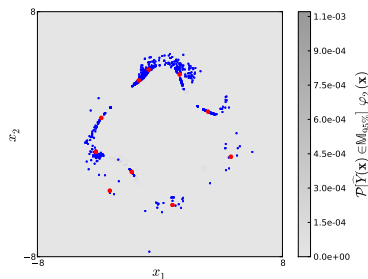
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Sampled & clustered refinement criterion

Iteration #8

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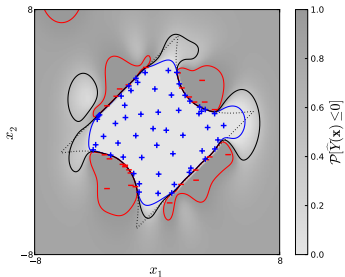
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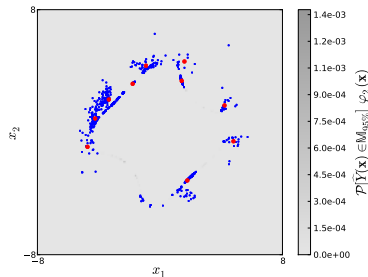
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Target contour, design of experiments & prediction



Sampled & clustered refinement criterion

Iteration #9

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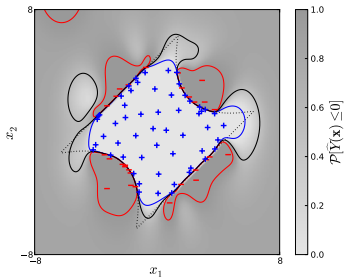
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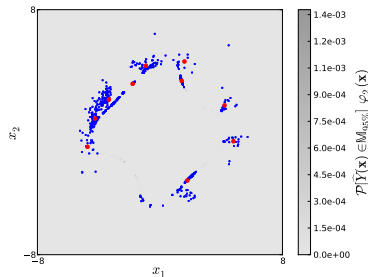
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Iteration #9

Convergence criteria depend on the *application*...

# Reliability analysis

## Introduction

(Ditlevsen & Madsen, 1996; Lemaire, 2009)

### Problem formulation

- Given a *failure domain*:

$$\mathbb{F} = \{\mathbf{x} \in \mathbb{X} : g(\mathbf{x}) \leq 0\}$$

- and a *random vector*  $X$  with known distribution:

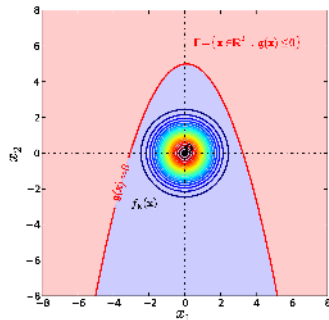
$$F_X(\mathbf{x}) = C \left( F_{X_i}(x_i), i = 1, \dots, n \right)$$

(Lebrun & Dutfoy, 2009a,b,c)

- the purpose is to quantify the reliability of a design in the form of a *failure probability*:

$$p_f = \mathbb{P}[X \in \mathbb{F}] = \int_{\mathbb{F}} f_X(\mathbf{x}) d\mathbf{x}$$

$\mathbb{P}(\neq \mathcal{P})$  denotes the probability measure w.r.t. the random vector  $X$ .



# Reliability analysis

Monte Carlo sampling as a motivation for the *structural reliability methods*

## Monte Carlo sampling

- The failure probability rewrites:

$$p_f = \int_{\mathcal{X}} \mathbb{1}_F(\mathbf{x}) f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} = \mathbb{E}[\mathbb{1}_F(\mathbf{X})]$$

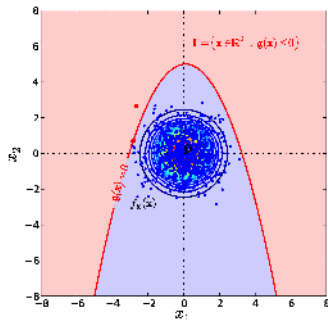
- Hence, the central limit theorem ensures that:

$$\hat{p}_f = \frac{1}{N} \sum_{i=1}^N \mathbb{1}_F(\mathbf{X}^{(i)}) \rightsquigarrow \mathcal{N}\left(p_f, \frac{p_f(1-p_f)}{N}\right)$$

- provided  $N$  is sufficiently large!*
- In order to involve  $\hat{p}_f$  in an optimization loop:

$$p_f \approx 10^{-k} \Rightarrow N \geq 10^{k+2}$$

- Structural reliability methods* aim at reducing  $N$



## Surrogate-based reliability analysis

### Principle

- A *surrogate-based* estimator:

$$\tilde{p}_f = \int_{\tilde{\Gamma}} f_X(\mathbf{x}) d\mathbf{x}$$

- where:

$$\tilde{\Gamma} = \{\mathbf{x} \in \mathbb{X} : \tilde{g}(\mathbf{x}) \leq 0\} \approx \Gamma$$

and  $\tilde{g}$  is a *meta-model* of  $g$ .

- $\tilde{g}$  is built from  $m \ll N$  runs of  $g$ .

### Error (bias) quantification?

- Provided  $\tilde{g}$  is a *Kriging predictor*:

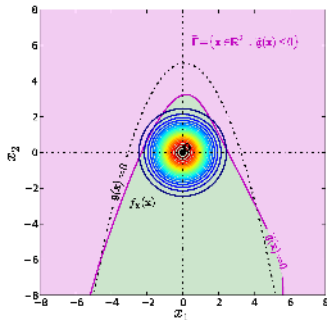
$$\hat{F}_{95\%}^{-1} \leq \hat{F}_{95\%}^0 \leq \hat{F}_{95\%}^{+1} \Rightarrow p_{f,95\%}^{-1} \leq p_{f,95\%}^0 \leq p_{f,95\%}^{+1}$$

- Hence the following *empirical error*:

$$\Delta p_{f,95\%} = \log_{10} \left( \frac{p_{f,95\%}^{-1}}{p_{f,95\%}^{+1}} \right)$$

$$\Delta p_{f,95\%} \leq \Delta_0$$

For the sake of *efficiency*  
*low probabilities* can be handled by  
*subset sampling* (Au & Beck, 2001)



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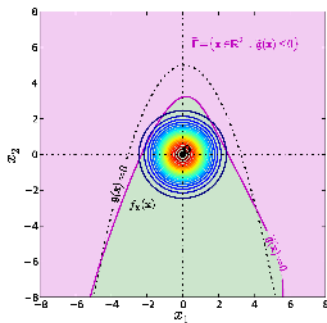
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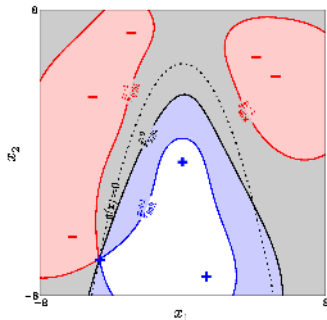
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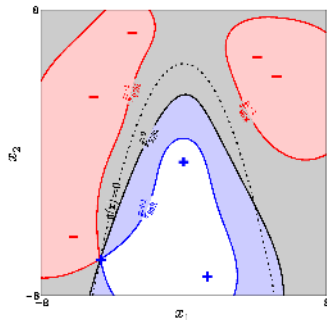
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# Reliability-based design optimization

## Introduction

(Tsompanakis et al., 2008)

### Problem formulation

$$\mathbf{d}^* = \arg \min_{\mathbf{d} \in \mathbb{D}} c(\mathbf{d}) : \begin{cases} f_i(\mathbf{d}) \leq 0, & i = 1, \dots, n_c \\ p_{fl}(\mathbf{d}) \leq p_{fl}^0, & l = 1, \dots, n_p \end{cases}$$

where  $\mathbf{d}$  is exclusively involved in the definition of the random vector  $\mathbf{X}$  (e.g. *mean values*).

### Bottlenecks

- The *repeated* reliability estimations are *computationally expensive*;
- Most NLP constrained optimization algorithms require *the gradients of the failure probabilities*.

### Solutions

- Nested approaches
- Sequential approaches
- Surrogate-based approaches

(Enevoldsen & Sørensen, 1994)

(Du & Chen, 2004)

(Eldred et al., 2002)

## Surrogate-based RBDO

The augmented reliability space

(Taflanidis & Beck, 2008, 2009a,b)

### Motivation

Building the Kriging surrogates *from scratch* for each nested reliability analysis would be particularly inefficient.

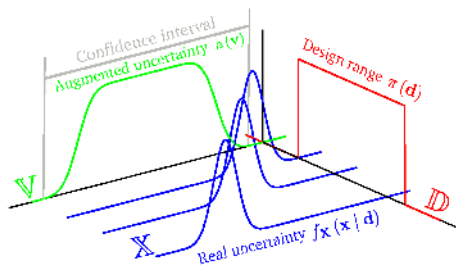
### Definition

- The admissible range  $\mathbb{D}$  simply *augments the spread* of  $f_X$ :

$$h(x) = \int_{\mathbb{D}} f_X(x | d) \pi(d) dd$$

where  $\pi$  is the uniform distribution over  $\mathbb{D}$ .

- The idea is to work on a *sufficiently large confidence region* of  $h$ .



# Surrogate-based RBDO

## Reliability sensitivity analysis

### Motivations

- NLP optimization algorithms require *the gradient of the failure probabilities*;
- How to compute these derivatives with *Monte Carlo* techniques?

### The score function approach

(Rubinstein, 1976, 1986)

Given a random vector  $X$  with parameter  $d$ , *provided its support  $\mathbb{X}$  does not depend on  $d$* :

$$\frac{\partial p_f(d)}{\partial d} = \mathbb{E}_X \left[ \mathbb{1}_F(X) \frac{\partial \log f_X(X | d)}{\partial d} \right]$$

### Interesting properties

- *A simple post-processing* of a reliability analysis!
- The **score function** comes *analytically* when the copula formalism is used.  
(Lee et al., 2011a,b)
- The approach extends to *reduction variance techniques* such as:
  - subset sampling  
(Song et al., 2009)
  - (meta-model-based) importance sampling  
(Dubourg, 2011)

## Surrogate-based RBDO

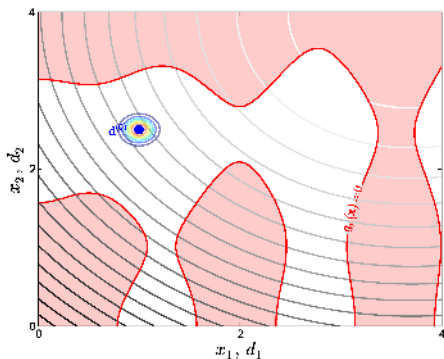
### Overview of the proposed algorithm

Given an initial design  $\mathbf{d}^{(0)} \in \mathbb{D}$  (*bounded*):

- 1 Determine the *augmented reliability space*;
- 2 Fit an *adaptive Kriging surrogate* with target local accuracy;
- 3 Compute  $\hat{p}_{f,95\%}^0(\mathbf{d}^{(i)})$  and its *gradient*;
- 4 Compute *search direction*  $\mathbf{h}^{(i)}$  using min-max formulation;
- 5 Perform *approximate line-search* using Goldstein-Armijo step size rule;

$$\mathbf{d}^{(i+1)} = \mathbf{d}^{(i)} + s^{(i)} \mathbf{h}^{(i)}$$

- 6 Loop back to step 2 until the *optimizer converges*.



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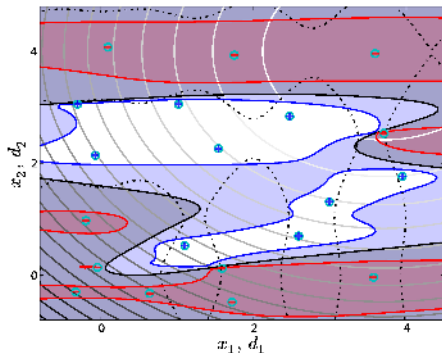
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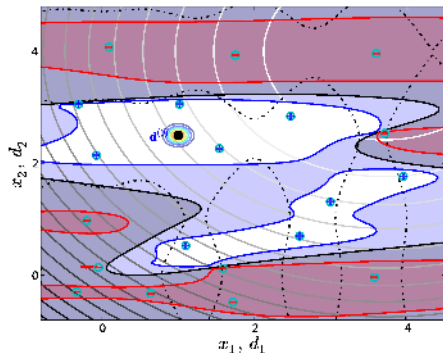
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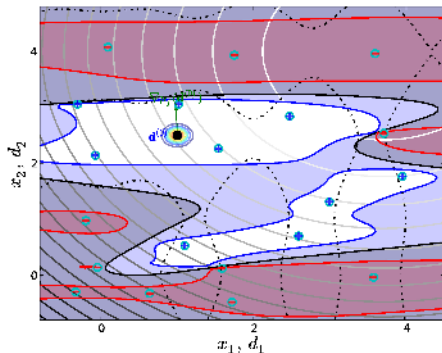
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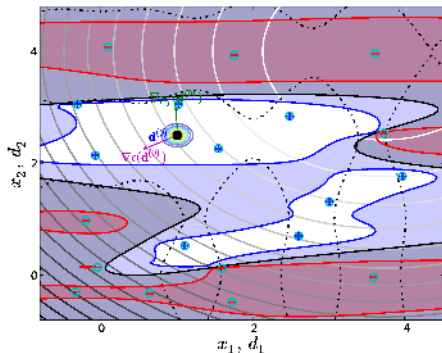
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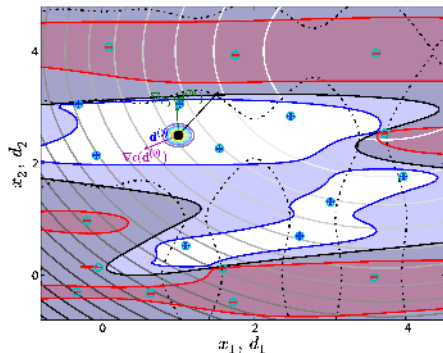
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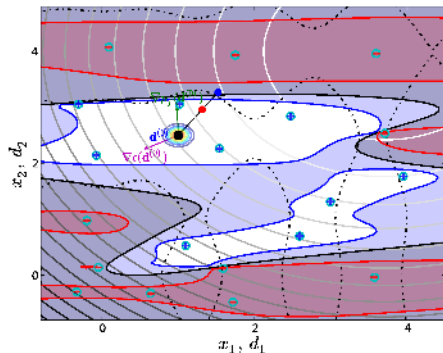
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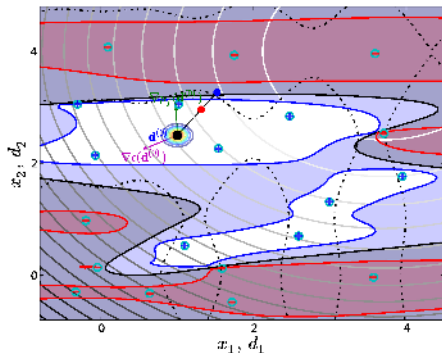
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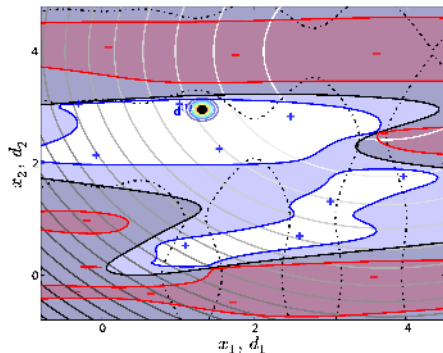
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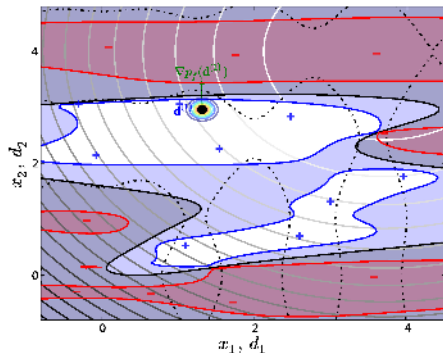
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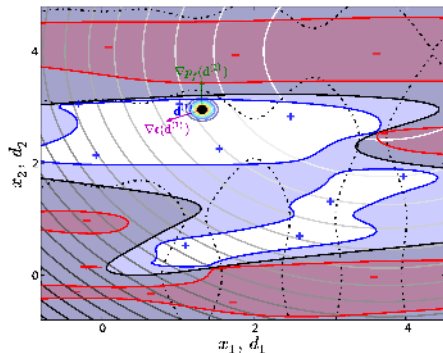
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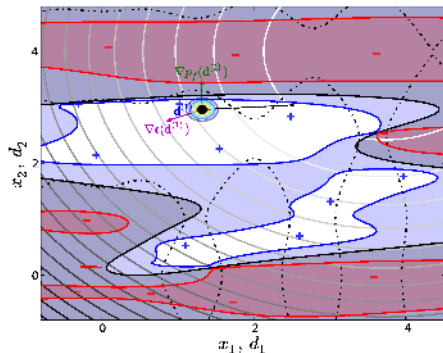
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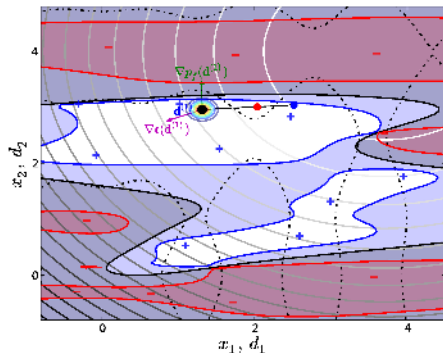
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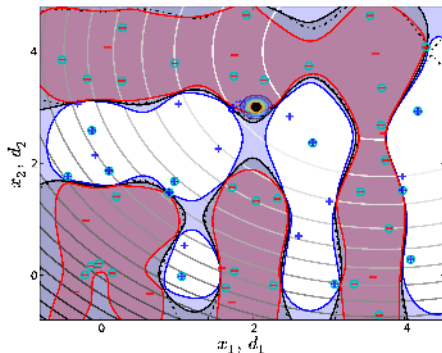
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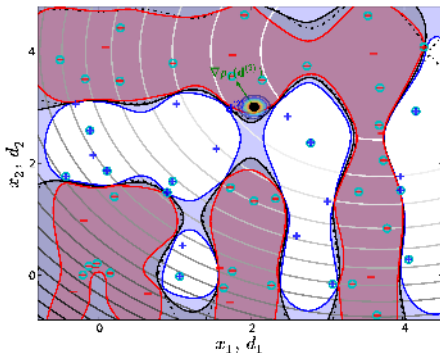
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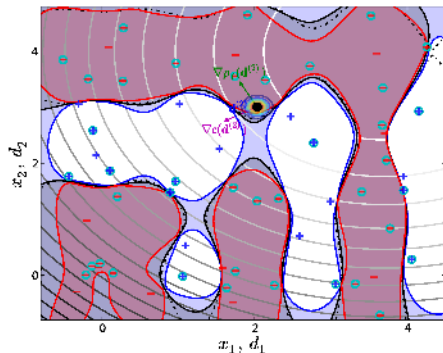
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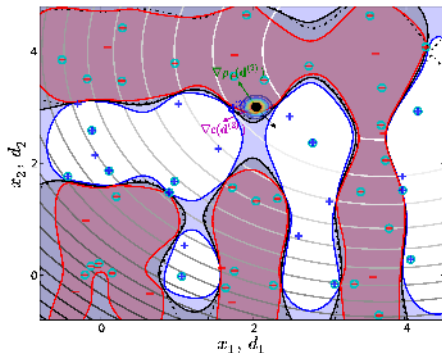
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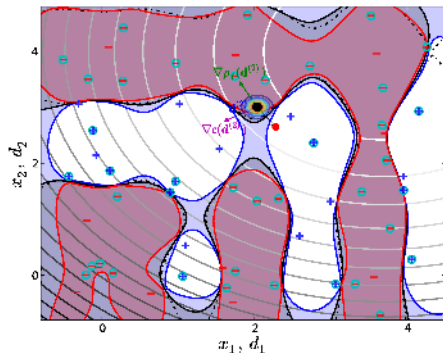
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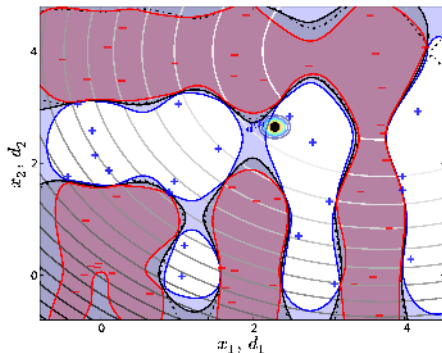
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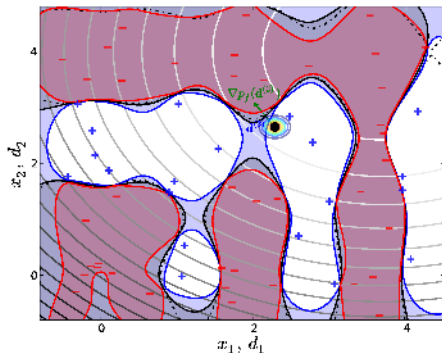
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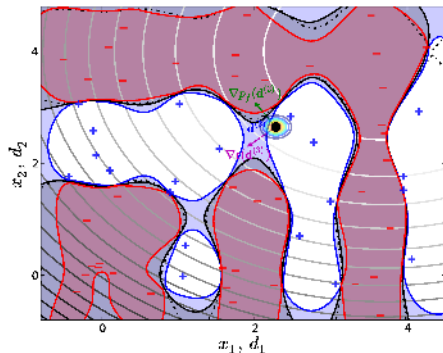
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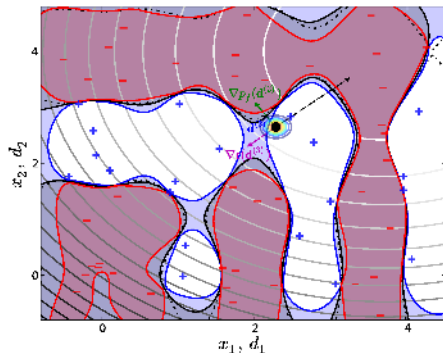
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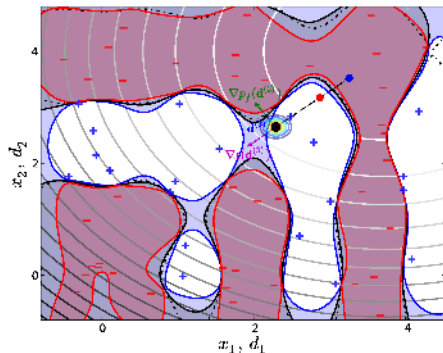
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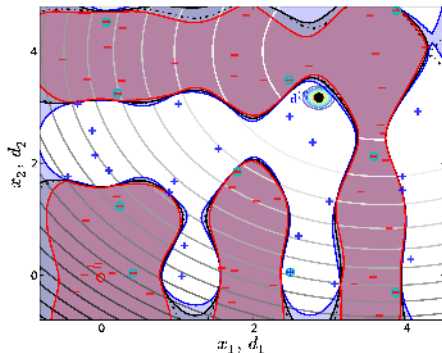
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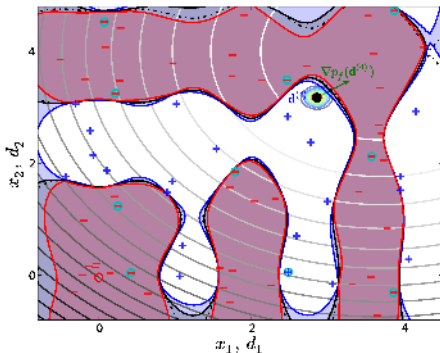
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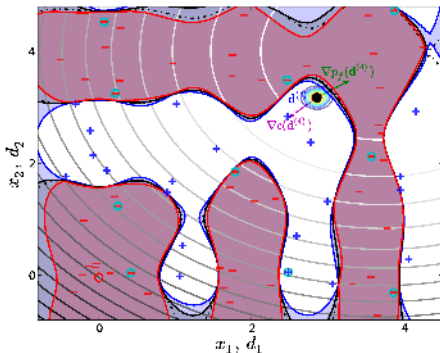
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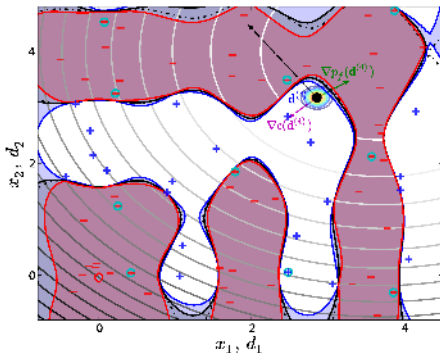
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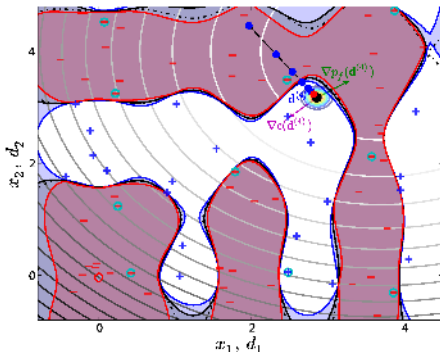
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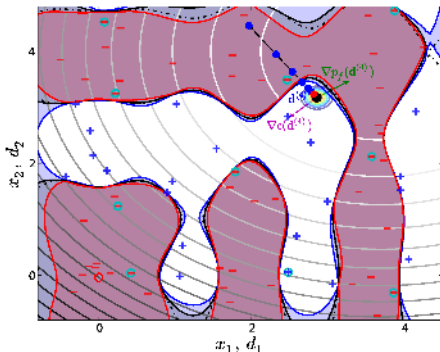
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Shrink  $\mathbb{D}$  and decrease  $\Delta_0$

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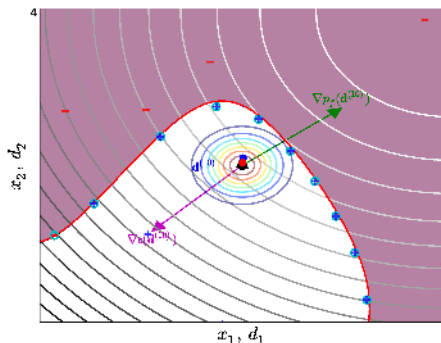
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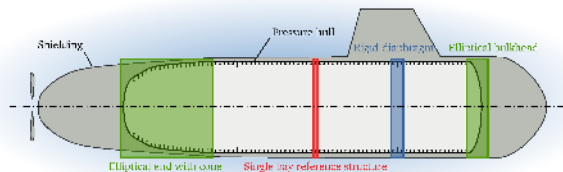
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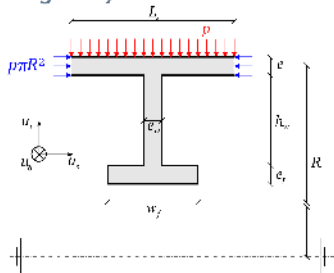
Converged!

# Application to the design of an imperfect submarine hull

## Problem formulation



### Single bay reference structure



### Design objectives

- The design should minimize the following *weight ratio*:

$$c(\mathbf{d}) = \frac{\rho_{\text{sea water}} V_{\text{sea water}}(\mathbf{d})}{\rho_{\text{steel}} V_{\text{steel}}(\mathbf{d})}$$

- while ensuring structural integrity for an *accidental depth charge*:

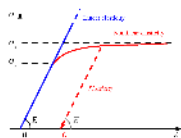
$$g(\mathbf{x}) = p_{\text{collapse}}(\mathbf{x}) - p_{\text{acc}}$$

# Application to the design of an imperfect submarine hull

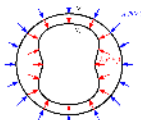
## Mechanical and probabilistic modelling

### Mechanical modelling (Noirfalise, 2009)

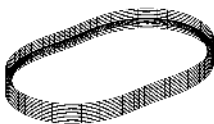
- Nonlinear finite element model (geometry, material and load);
- Shape imperfections distributed according to *two critical buckling patterns*



Nonlinear elasticity



Follower forces



Mode 2 ( $A_2$ )



Mode 14 ( $A_{14}$ )

### Probabilistic model

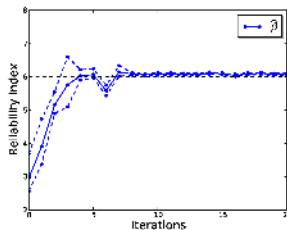
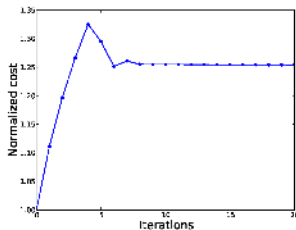
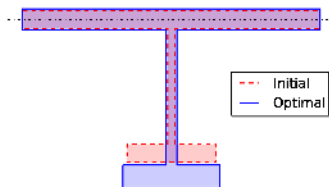
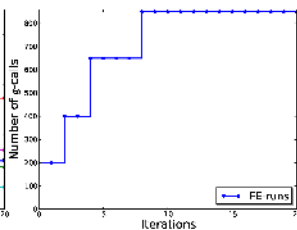
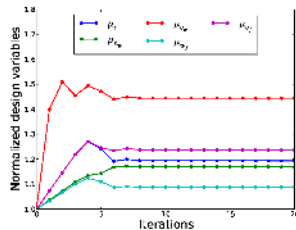
Variable	Distribution	Mean	C.o.V.
$E$ (MPa)	Lognormal	200,000	5%
$\sigma_y$ (MPa)	Lognormal	390	5%
$\sigma_u$ (MPa)	Lognormal	370	3%
$e$ (mm)	Lognormal	$\mu_e$	3%
$h_w$ (mm)	Lognormal	$\mu_{h_w}$	3%
$e_w$ (mm)	Lognormal	$\mu_{e_w}$	3%
$w_f$ (mm)	Lognormal	$\mu_{w_f}$	3%
$e_f$ (mm)	Lognormal	$\mu_{e_f}$	3%
$A_2$ (mm)	Lognormal	$\frac{1}{3} \frac{5R}{1,000}$	50%
$A_{14}$ (mm)	Lognormal	$\frac{1}{3} \frac{1.5}{100}$	50%

### Probabilistic constraint

$$\mathbb{P} \left[ p_{\text{collapse}}(X) \leq p_{\text{acc}} \mid \mathbf{d} \right] \leq 10^{-9}$$

# Application to the design of an imperfect submarine hull

## Results



- +25% on the weight ratio
- but the failure probability was drastically reduced ( $10^{-3}$  →  $10^{-9}$ ):

$$\hat{p}_{f, \text{metaIS}}(\mathbf{d}^*) = 10^{-9}$$

with a C.o.V.  $\delta_{\text{metaIS}} < 5\%$

- The whole procedure required about **1,000 FE runs**.

# Conclusions & Open questions

## Conclusions

- Universal Kriging enable an objective *quantification of the substitution error*;
- Sampling-based adaptive DOEs enabled a *reduction of this error*, while making the *use of distributed computing platforms* possible.
- The *augmented reliability space* ensures the coupling “optimization–reliability–surrogates” is efficient;
- *Subset sampling* still reveals *unavoidable* to deal with the *possibly low* failure probabilities encountered during the optimization;
- The score function approach revealed efficient for *reliability sensitivity analysis*;

## Open questions

- Real engineering problems feature a *large number of parameters* (> 10): how to extend the use of kriging surrogates to such cases?
- Search for the *optimum optimorum*: use of global optimization techniques and/or better initialization of gradient-based optimizers?
- Some manufactured products benefits from *100% quality control*: how to deal with *truncated distributions* (zero probability, reliability sensitivity)?

# Conclusions & Open questions

## Conclusions

- Universal Kriging enable an objective *quantification of the substitution error*;
- Sampling-based adaptive DOEs enabled a *reduction of this error*, while making the *use of distributed computing platforms* possible.
- The *augmented reliability space* ensures the coupling “optimization–reliability–surrogates” is efficient;
- *Subset sampling* still reveals *unavoidable* to deal with the *possibly low* failure probabilities encountered during the optimization;
- The score function approach revealed efficient for *reliability sensitivity analysis*;

## Open questions

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# Thank you for your attention!



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