# Some research results of the DICE project

http://www.dice-consortium.fr/

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# OUTLINE

## 1 - The DICE project at a glance

- Organization and partners
- Scientific production and R packages

## 2 - Overview of the methodological issues

- Spotlight on 9 topics

## 3 - Focus I: Construction of Space-Filling Designs

## 4 - Focus II: Approximation of a target region

# DICE project – The participants

**Academic participants**

- Mines St-Etienne (ARMINES/3MI - size ≈ 5) PROJ. LEADER
- Université Paul Cézanne (LMRE Pr. Michelle Sergent)
- Université d'Orsay (Pr. Georges Oppenheim)
- Université Joseph Fourier (Pr. Anestis Antoniadis)

**Industrial partners**

- TOTAL – *petroleum*
- EDF - *electricity, nuclear engineering*
- IRSN - *nuclear engineering*
- Renault - *automotive*
- ONERA - *aerospatial*

# DICE project – General description

- 3 years project – Dec 2006 to Dec 2009
- Topic: analysis of time-consuming computer codes

- Sequenced in 6-months research periods
- Steering committee **(2 days)**
  - **1.5 days: presentation of scientific results**
  - **0.5 days: organization & case studies def.**
- Ticket for each "industrial" partner

# DICE project – Outputs (1/2)

- Defended PhD thesis
  - J. Franco, *research engineer at Total*
    - *Keywords: design of computer experiments, SFDs*
  - D. Ginsbourger, *ass. Prof. at Bern University*
    - *Keywords: metamodelling, Kriging-based optimization*
  - V. Picheny, *post-doc. at Ecole Centrale de Paris*
    - *Keywords: metamodelling, Reliability*

Outstanding:

- B. Gauthier, *EMSE, started in 2007*
  - *Keywords: RKHS, Continuous constraints*
- N. Durrande, *EMSE, started in 2008*
  - *Keywords: Dimension reduction, Additive functions, Kernels*

# DICE project – Outputs (2/2)

- ≈ 10 publications
- 30 internal research reports – *restricted access*
- 4 R packages
  - DiceDesign, DiceKriging, DiceOptim, DiceEval
  - Now published on CRAN, http://cran.r-project.org/
  - Supplementary materials
    - General presentation in preparation
    - Vignette for DiceKriging&DiceOptim, www.emse.fr/~roustant

# DICE project – "Closing" conference

- At least another conference dedicated only to computer experiments!


- Link: http://www.emse.fr/enbis-emse2009/

# DICE project – Publications list (1/3)


1. Sergent M., Dupuy D., Corre B., Clayes-Bruno M., Comparaison de méthodes de criblage pour la simulation numérique, HAL,
   http://hal.archives-ouvertes.fr/inria-00386602/fr/
2. Franco J., Bay X., Dupuy D. et Corre B. (2008), Planification d'expériences numériques à partir du processus ponctuel de Strauss, HAL,
   http://hal.archives-ouvertes.fr/hal-00260701/fr/
3. Ginsbourger D., Dupuy D., Badea A., Roustant O. et Carraro L. (2009), A note on the choice and the estimation of Kriging models for the analysis of deterministic computer experiments, *Applied Stochastic Models for Business and Industry*, **25** (2), 115-131.
4. Ginsbourger D., Helbert C. et Carraro L. (2008), Discrete mixtures of kernels for Kriging-based optimization, *Quality and Reliability Engineering International*, **24** (6), 681-691.
5. Ginsbourger D., Le Riche R. et Carraro L., A Multi-points Criterion for Deterministic Parallel Global Optimization based on Gaussian Processes, *Journal of Global Optimization.*

# DICE project – Publications list (2/3)


6. Helbert C., Dupuy D. et Carraro L. (2009), Assessment of uncertainty in computer experiments : from Universal to Bayesian Kriging, *Applied Stochastic Models for Business and Industry*, **25**, 99-113.
7. Picheny V., Ginsbourger D., Roustant O., Haftka R.T. et Kim, N.-H., Adaptive Designs of Experiments for Accurate Approximation of Target Regions, to appear in *Journal of Mechanical Design.*
8. Ginsbourger D., Bay X. et Carraro L., Noyaux de covariance pour le Krigeage de fonctions symétriques, to appear in *C. R. Acad. Sci. Paris, section Maths.*
9. Pujol G. (2009), Simplex-based screening designs for estimating metamodels, *Reliability Engineering and System Safety*, **94**, 1156–1160.
10. Roustant O., Franco J., Carraro L. et Jourdan A. (2010), A radial scanning statistic for selecting space-filling designs in computer experiments, in A. Gio- vagnoli, A.C. Atkinson, B. Torsney (éditeurs) et C. May (editeur) "mODa 9 – Advances in Model-Oriented Design and Analysis, Contributions to statistics", Springer (Physica-Verlag), p. 189-196.

# DICE project – Publications list (3/3)

## Submitted or in preparation

J. Franco, X. Bay, B. Corre and D. Dupuy, "Strauss Processes: A new approach in Computer Experiments"

D. Dupuy, C. Helbert, J. Franco, "DiceDesign and DiceEval: new R packages for Design and Analysis of Computer Experiments." In preparation.

O. Roustant, D. Ginsbourger, Y. Deville, "DiceKriging, DiceOptim: two R packages for the analysis of computer experiments by kriging-based metamodelling and optimization", submitted to Journal of Statistical Software,
http://hal.archives-ouvertes.fr/hal-00495766/fr/

# PART I

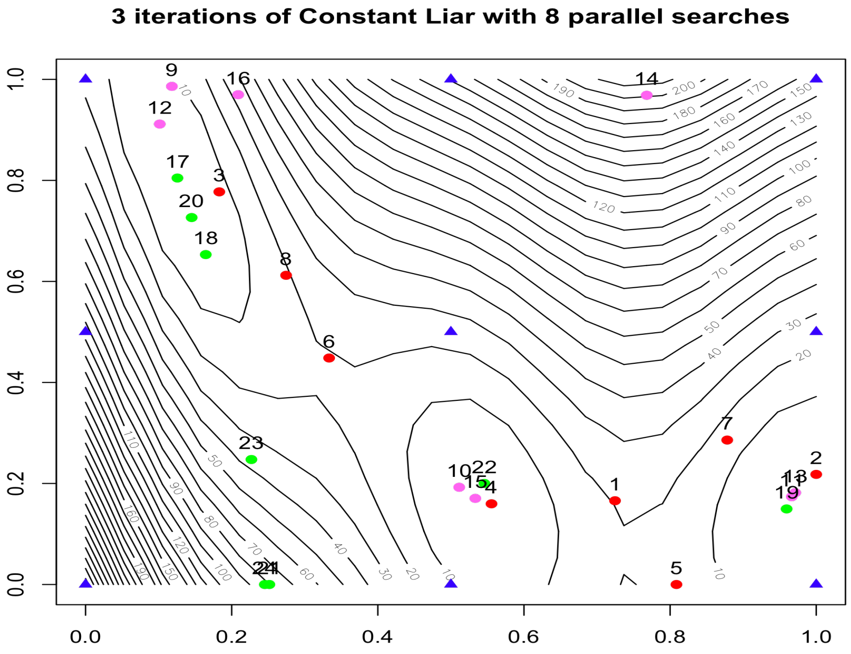
- General overview

# General overview – Kriging-based Optimization

- Extension of EGO method for parallel computing

  - EGO method: EI criterion with analytical gradient, EI maximization with a genetic algorithm

  - Parallel computing: Constant liar heuristic, multipoints EI

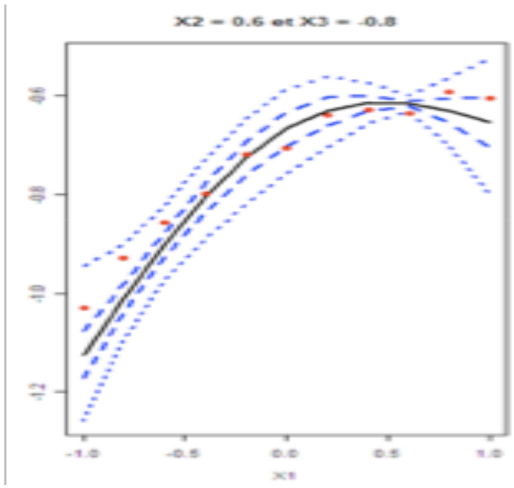



*Related package: DiceOptim*

*Scientific production.* R Package « *DiceOptim* », D. Ginsbourger thesis (part I & III), 1 deliverable, 2 publications ([4], [5]).

# General overview – Uncertainty propagation

- Uncertainty propagation in a Bayesian framework
- Bayesian interpretation of Universal Kriging



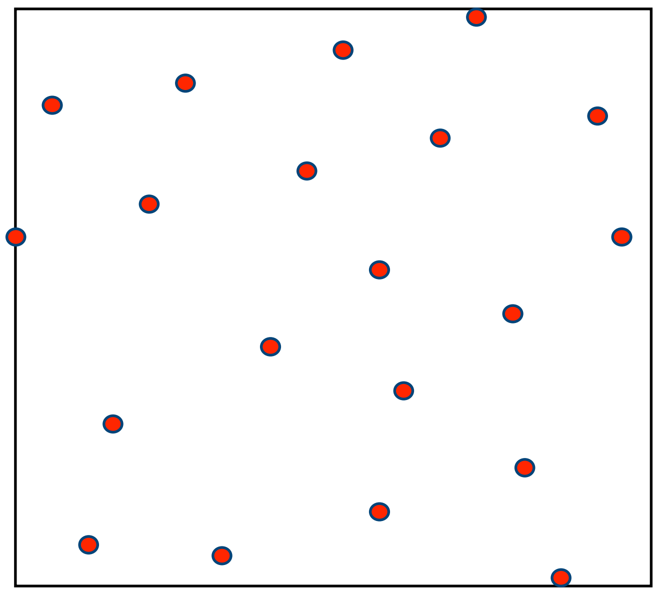
- UK formulas can be obtained assuming an improper uniform prior for beta… but constant variance and correlation
- Get informative priors from a degraded simulator. Test and comparison on a 3D case study

*Scientific production.* 1 deliverable, 1 publication ([6])

# General overview – Design of experiments (1)

- Construction of space-filling designs for a first investigation with Strauss point processes

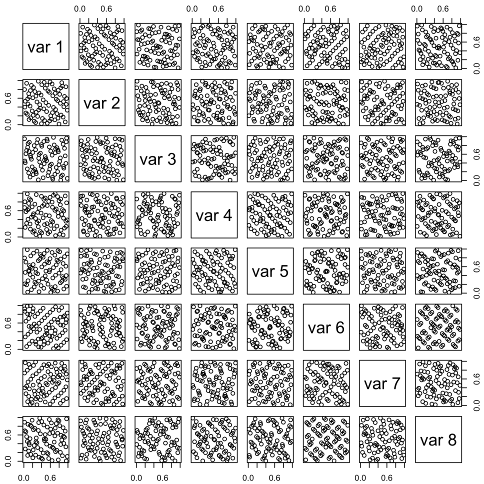
*-> see focus I*



*Related package: DiceDesign*

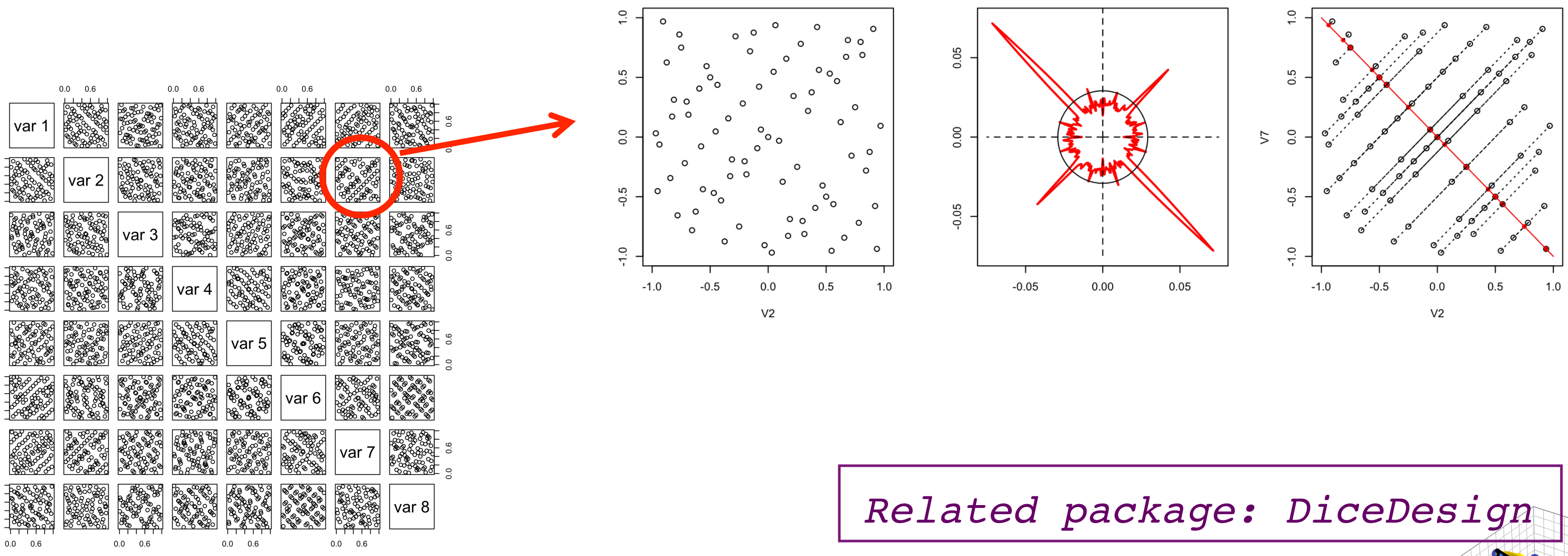
# General overview – Design of experiments (2)

- Evaluation and selection of SFDs designs with the Radial Scanning Statistic
  - Fact: dimension reduction techniques -> variables of the form $\beta' x$ -> we want more than good properties onto marginals
  - Aim: check automatically good properties of SFDs onto oblique directions



# General overview – Design of experiments (2)

- Evaluation and selection of SFDs designs with the Radial Scanning Statistic
  - Underlying maths: law of a sum of uniforms, GOF tests for uniformity based on spacings




*Related package: DiceDesign*

# General overview – Design of experiments (2)

- Evaluation and selection of SFDs designs with the Radial Scanning Statistic
  - Comparison of 80-point 8D SFDs

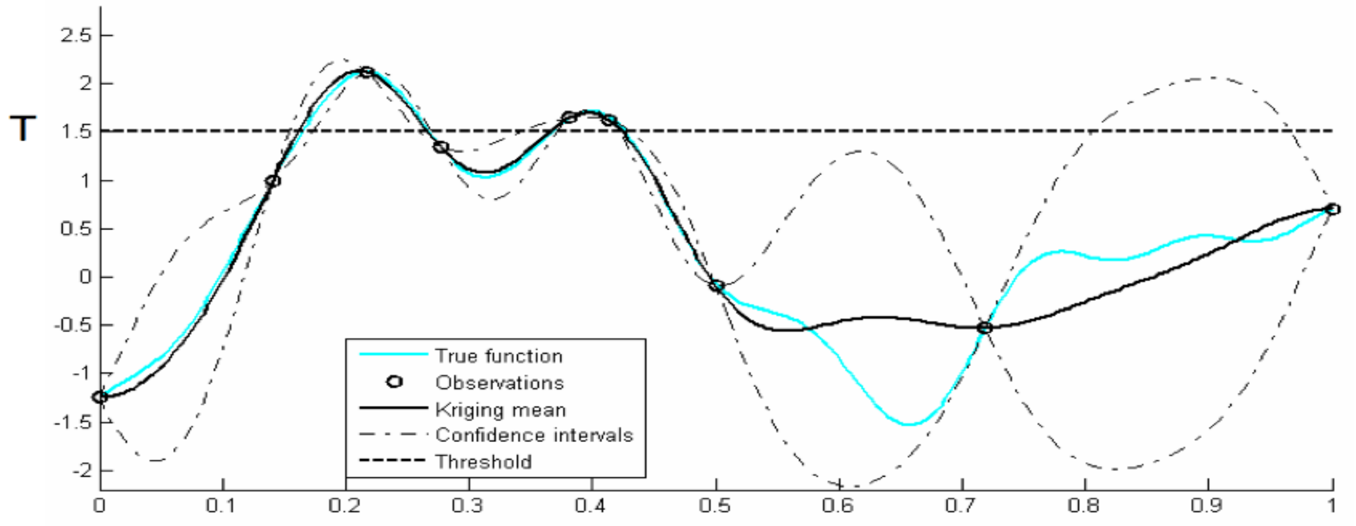
**Table 1** Worst value of Greenwood statistic for 8-dimensional SFDs of size 80

| Design type[a] | Statistic value[b] |
|---|---|
| Uniform | 0.039 (0.003) |
| Maximin Latin hypercube | 0.048 |
| Audze-Eglais Latin hypercube | 0.037 |
| Halton sequence | 0.244 |
| Faure sequence | 0.161 |
| Sobol sequence | 0.101 |
| Sobol sequence, with Owen scrambling | 0.041 (0.006) |
| Sobol sequence, with Faure-Tezuka scrambling | 0.088 (0.010) |
| Sobol sequence, with Owen + Faure-Tezuka scrambling | 0.041 (0.006) |
| Strauss | 0.040 (0.004) |

# General overview – Design of experiments (3)

- Adaptive designs for the approximation of a target region

  *-> see focus II*



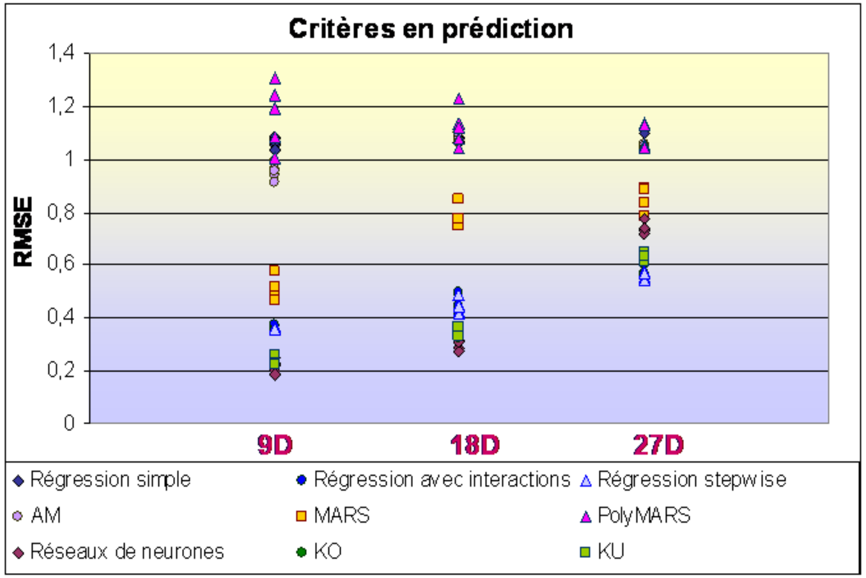

*Scientific production.* R package « *DiceDesign* », J. Franco thesis, V. Picheny thesis (chapter 5), 1 deliverable, 3 publications ([2], [7], [10])

# General overview – Kriging & other metamodels (1)

- Comparison of some famous metamodels
- Various case studies (mostly internal)

  - Kriging
  - Linear regression
  - MARS, polyMARS
  - Neural networks
  - Additive models

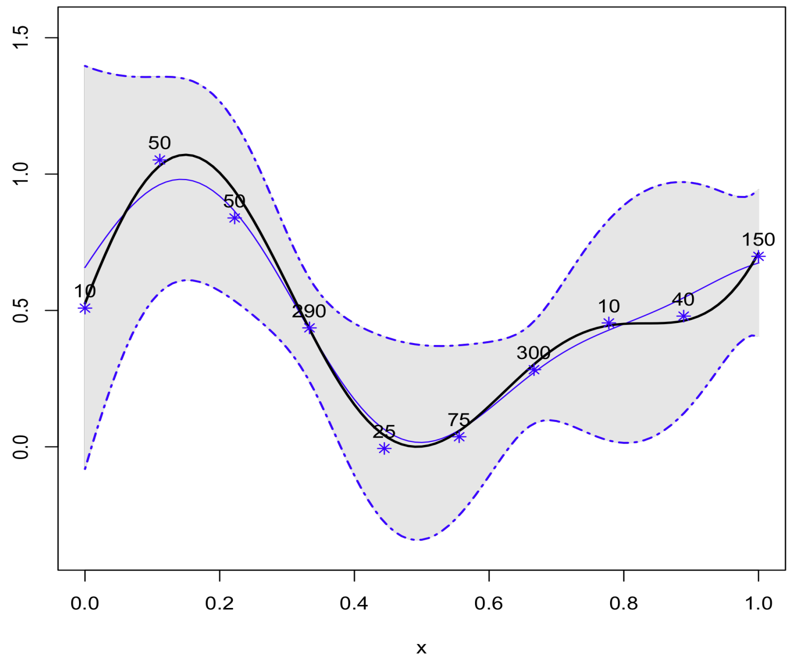
  - Case studies for d-dimensional problems (1≤d≤30)




*Related packages: DiceKriging, DiceEval*

# General overview – Kriging & other metamodels (2)

- Case of stochastic simulators



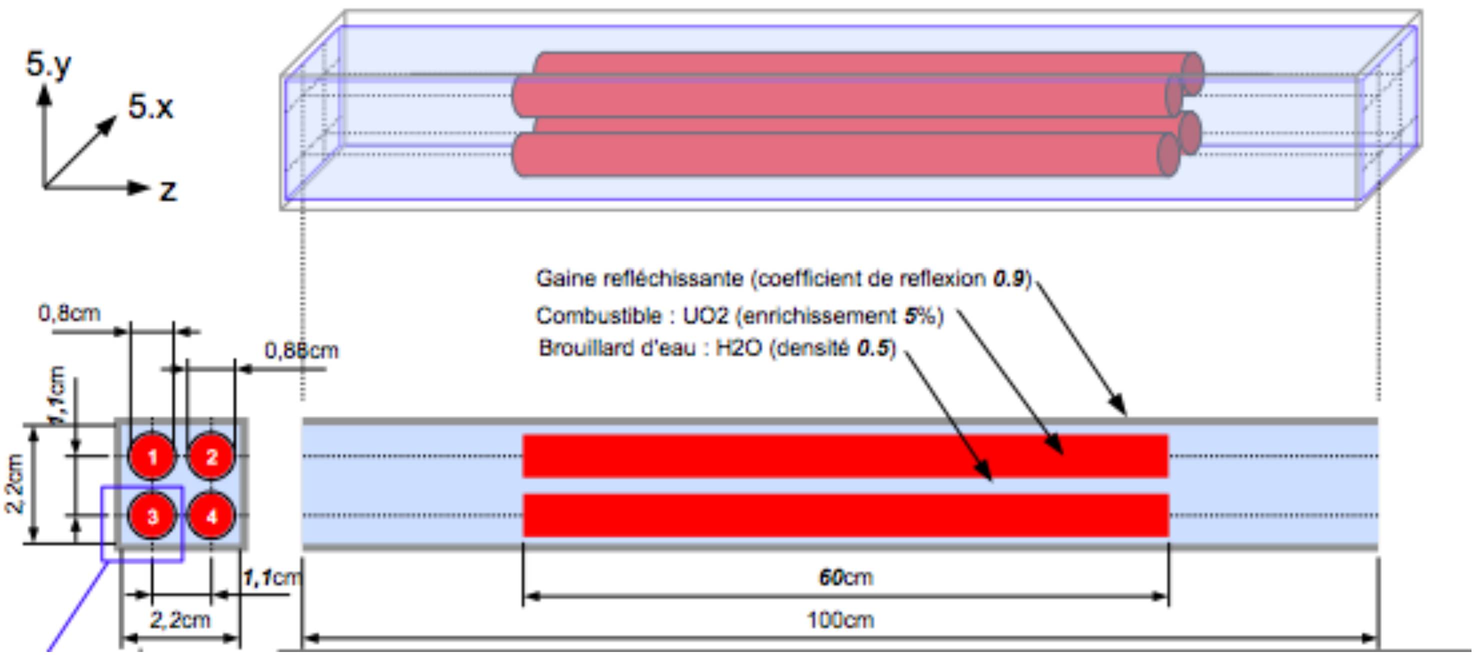

- Adaptation (and implementation) of Kriging for noisy observations
- First answer to the question: given a total budget, how do we distribute runs?

*Related package: DiceKriging*

# General overview – Kriging & other metamodels (3)

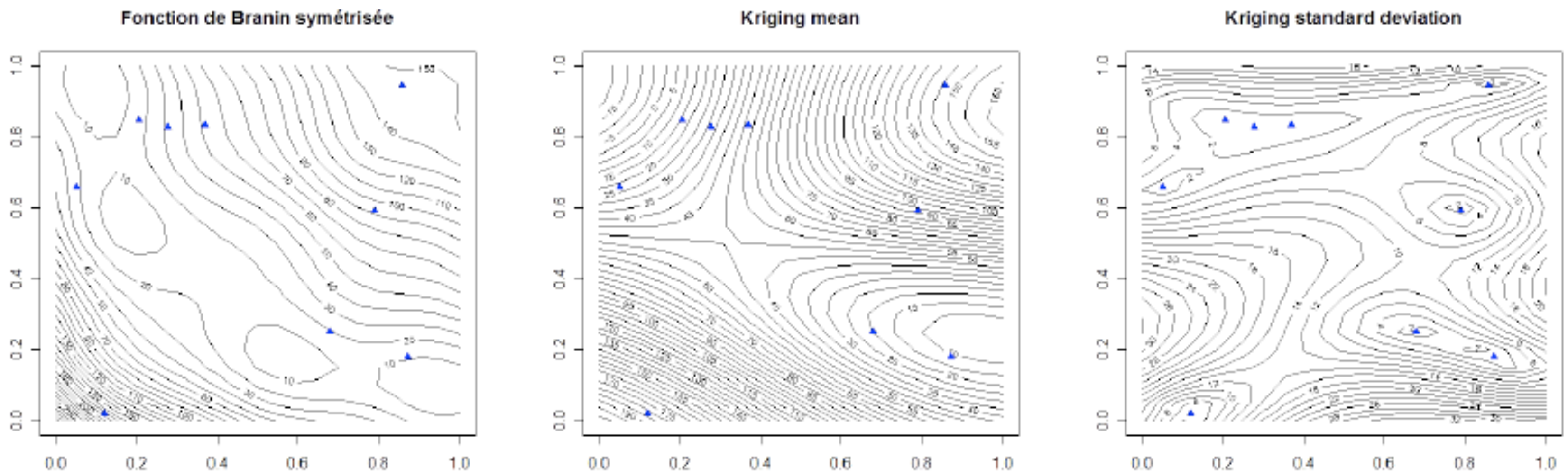
- Taking into account additional information
  - Example: symmetries with a suitable kernel

Benchmark paramétrique de réseau serré de crayons



# General overview – Kriging & other metamodels (3)

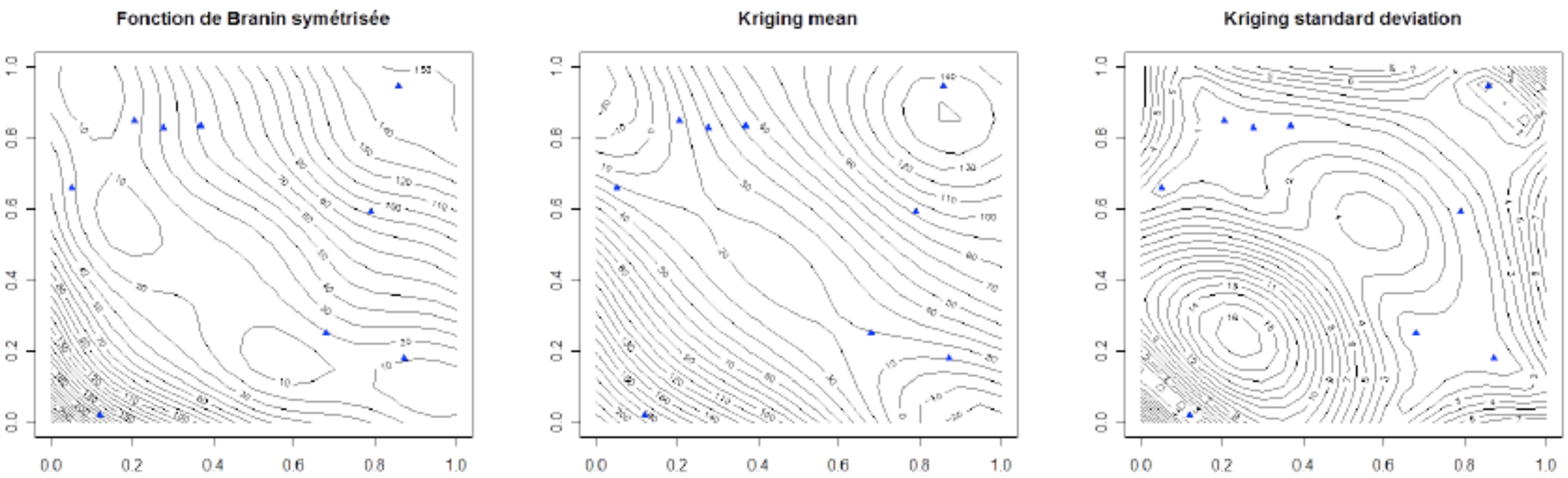
- Taking into account additional information
  - Example: symmetries with a suitable kernel




Gaussian covariance, 9-point design – IMSE over a 21-point test design: 820.93

# General overview – Kriging & other metamodels (3)

- Taking into account additional information
  - Example: symmetries with a suitable kernel

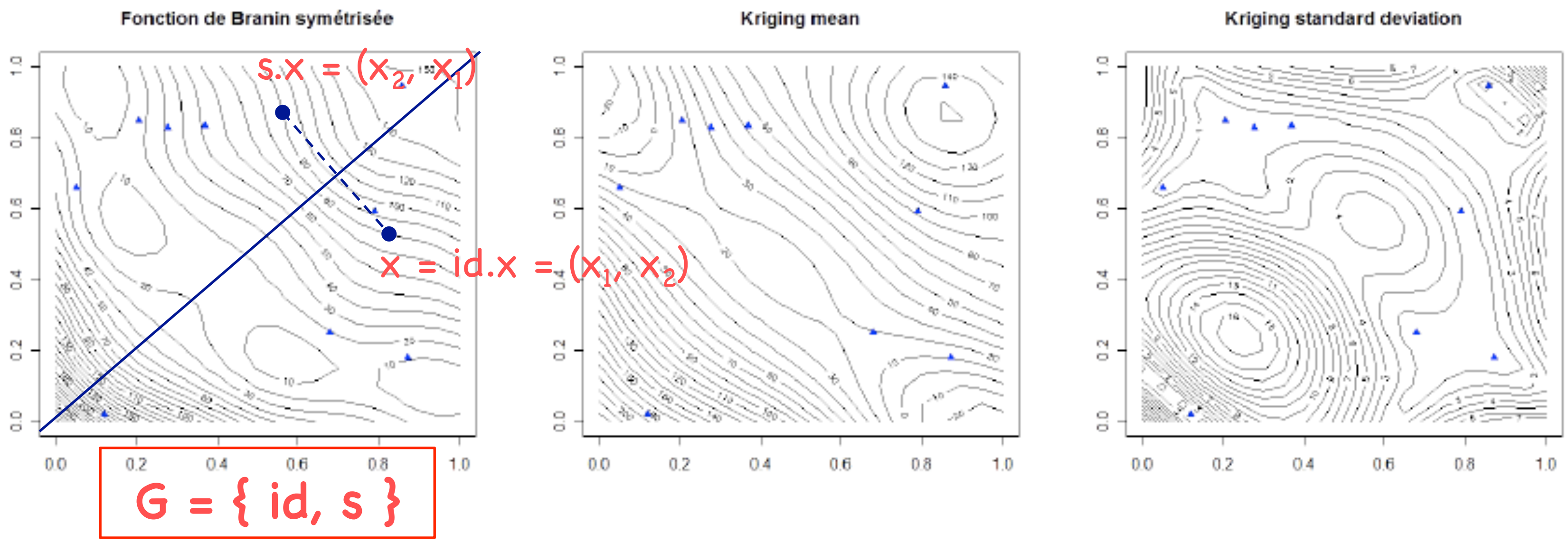



Symmeterized Gaussian covariance, 9-point design – IMSE : **330.26**

*Scientific production*. R packages *DiceEval* & *DiceKriging*, thesis: D. Ginsbourger (part II) & V. Picheny (chapter 6), B. Gauthier, N. Durrande, 2 deliverables, 2 publications ([3], [8]).

# General overview – Kriging & other metamodels (3)

- Taking into account additional information
  - The underlying maths

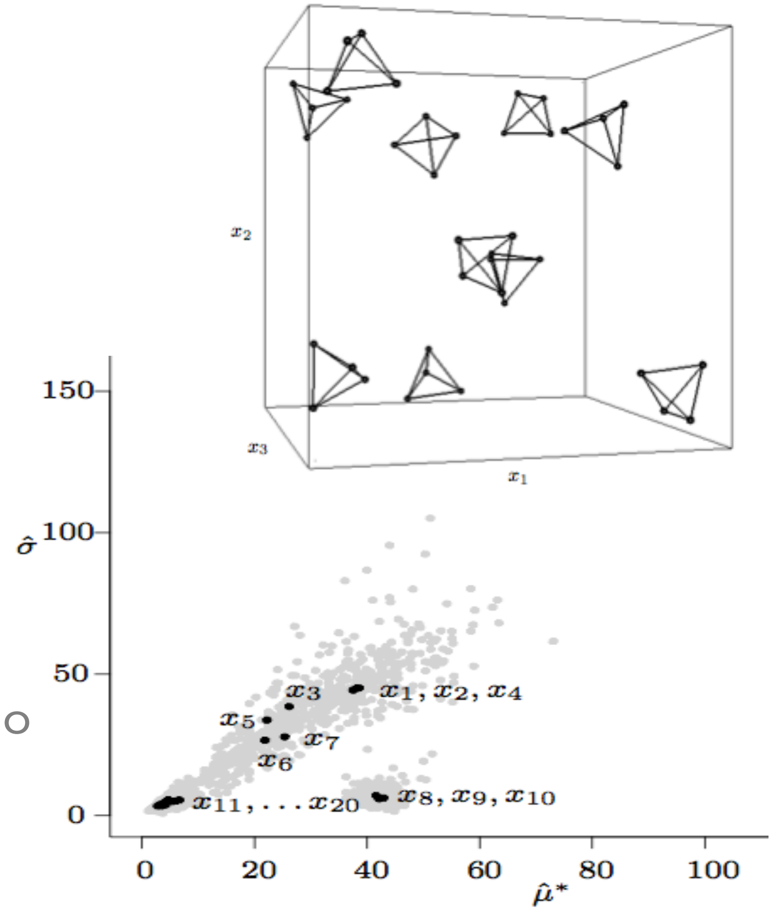



Symmeterized Gaussian covariance, 9-point design – IMSE : 330.26

$$Y_x = \sum_{g \in G} Z_{g.x} \Longrightarrow k_Y(x, x') = \sum_{(g,g') \in G^2} k_Z(g.x, g'.x')$$

# General overview – Screening & Sensitivity Analys.

- A bibliography study
  + An original method




- Simplex-based screening designs
  - Few model assumptions (in the same spirit as Morris)
  - The design can be re-used for modeling (the sample size does not collapse in projection onto subspaces)

*Scientific production.* 2 deliverables, 2 publications ([1], [9]).

# PART II

- Focus I

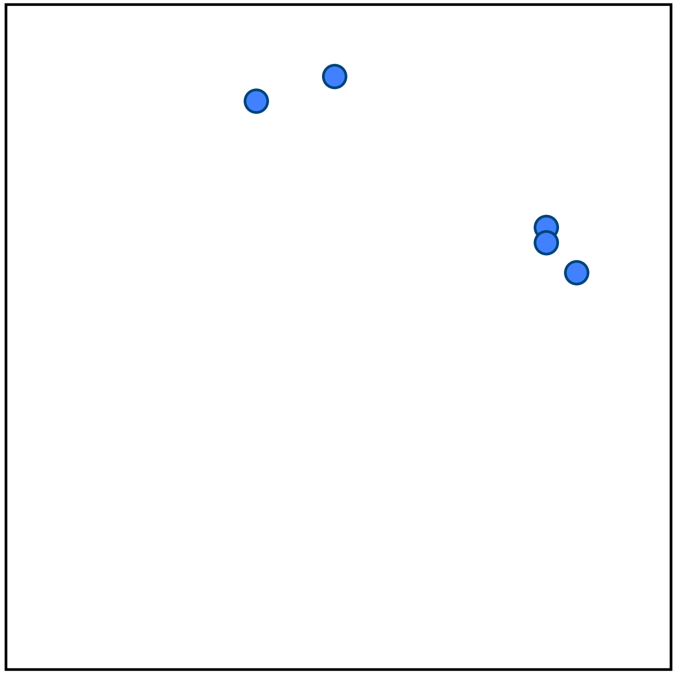
Construction of Space-Filling Designs

# Strauss designs - Objectives

- First investigation of a costly simulator
  - Space Filling Designs
- Good behavior on projections
  - Randomness reduces « aliasing » phenomenons
- Construction of designs with a fixed number of experiments
  - e.g. Wooton, Sergent, Phan-Tan-Luu designs

# Strauss designs - Algorithm and example

- Initial design : 5 points in the unit square $[0,1]^2$



**<u>Objective</u>**

**Iterative construction of a**

**« well distributed » new population**

**System of interacting particles (repulsion)**

# Strauss designs – Example, first iteration

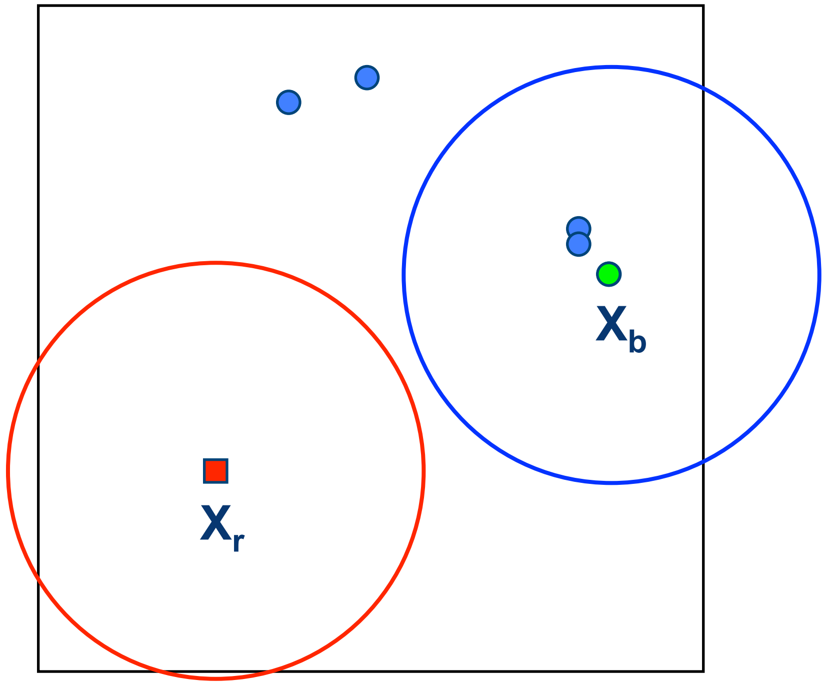
**We choose a blue point $X_b$ (he becoms green) and introduce a new random (red) point $X_r$.**

**New point is accepted with probability 1 if :**

$$n(S_{X_r}) \leq n(S_{X_b})$$

**Otherwise, acceptance probability of $X_r$ is given by :**

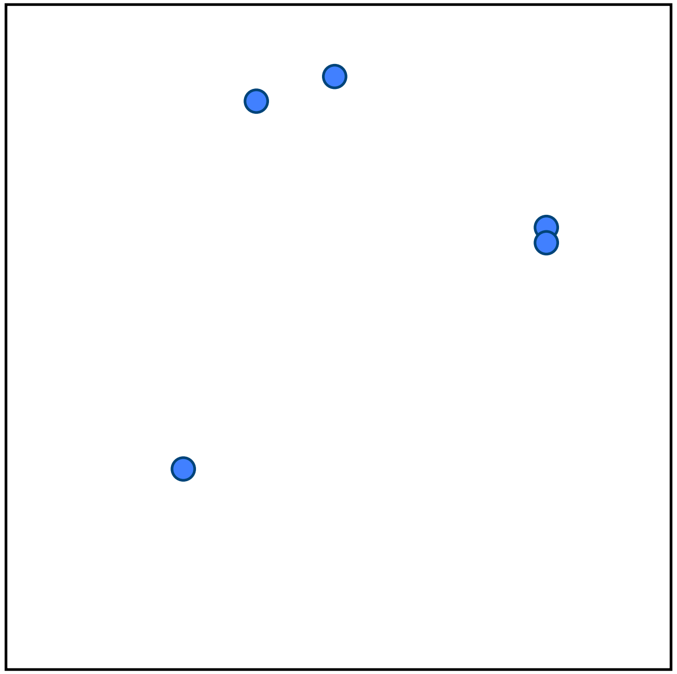
$$\gamma^{n(S_{X_r}) - n(S_{X_b})}$$




*$n(S_X)$ is the number of points in a ball of radius R centered on X.*

# Strauss designs – Example, after first iteration

**Here is the new design**



# Strauss designs – Example, second iteration

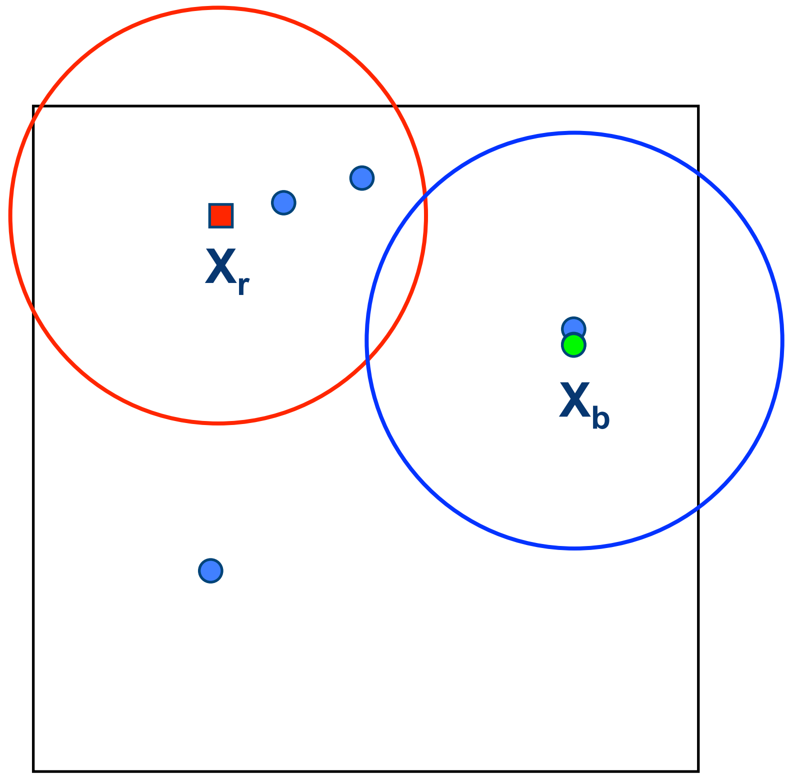
<u>**New iteration**</u>

**Interaction between $X_r$ and $X_b$**

**For $\gamma$ = 0.1**

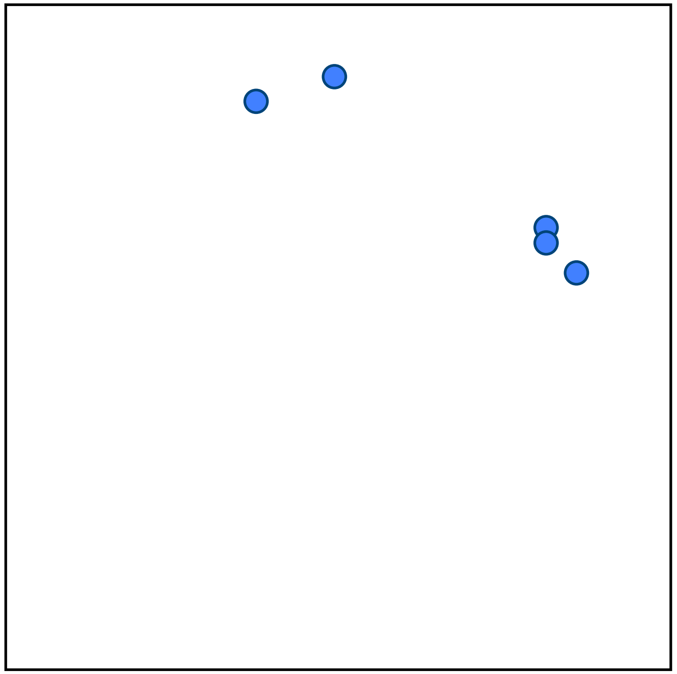
**Acceptance probability of $X_r$ is 0.1 ($\gamma^{2-1}$).**

**Here, $X_r$ is rejected.**

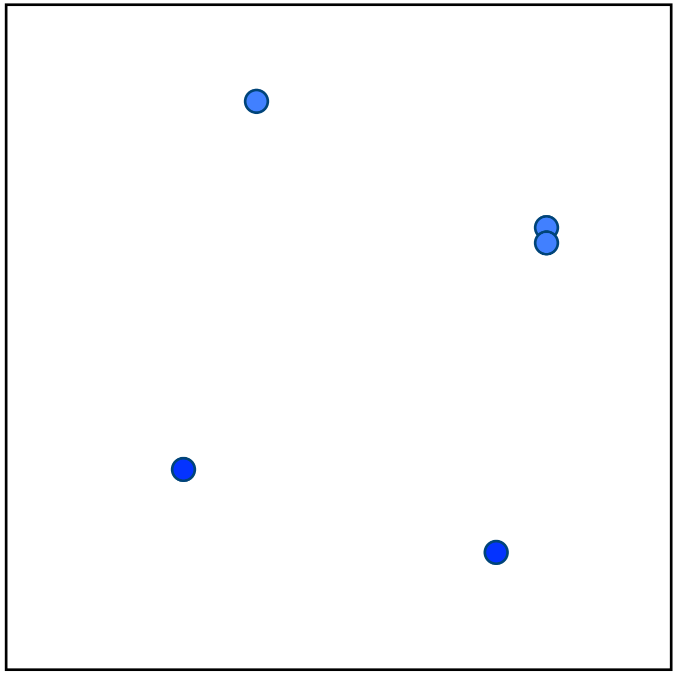


# Strauss designs – Example, after 5 iterations

**Initial design**

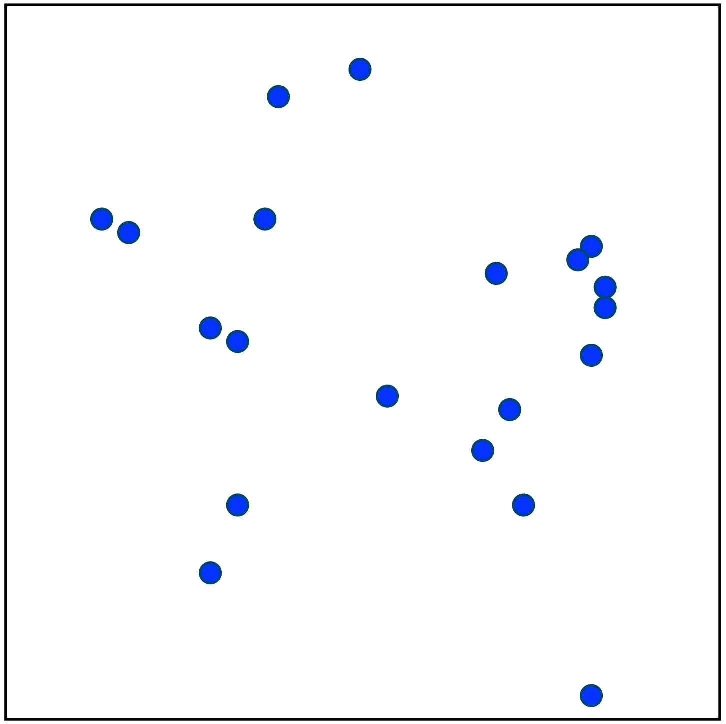


**After 5 iterations**

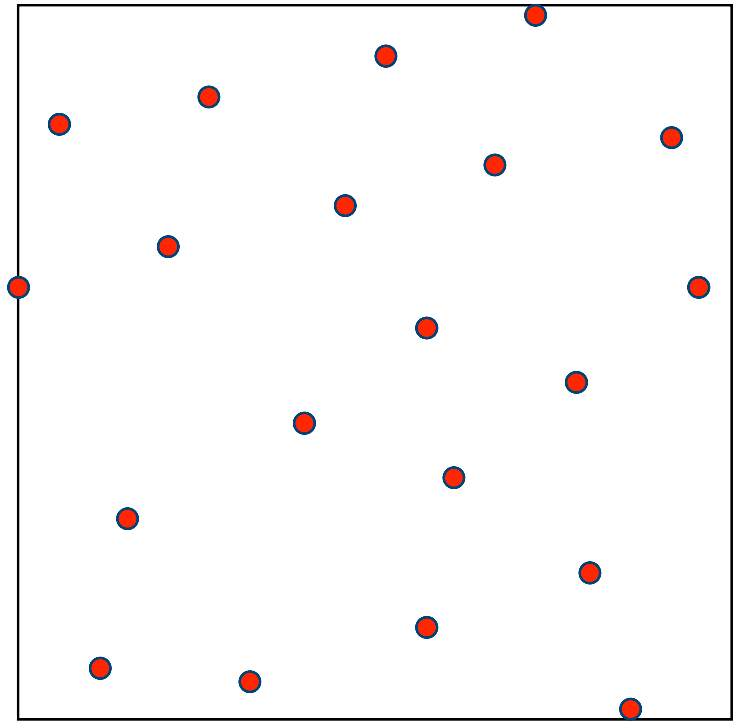


**Here, only two points have been changed.**

# Strauss designs – A more realistic example



Initial design



Stationnary state

# Strauss designs – Mathematical framework

**The pdf of a Strauss design is, conditionally to the number of points in the hypercube is given by :**

$$x = (x_1, \ldots, x_N),\ x_i \in \mathrm{R}^d$$

$$f(x_1, \ldots, x_N) = c\gamma^{S(x)} \ où\ S(x) = \sum_{i<j} 1_{\|x_i - x_j\| \le R}$$

**Strauss design is a particular case of Gibbs point process :**

$$f(x_1, \ldots, x_N) = c.\exp\left(-\beta . U(x)\right)$$

$$où \begin{cases} \beta = -\ln \gamma \\ U(x) = S(x) \end{cases}$$

**Metropolis-Hastings algorithm (MCMC method)**

**U is the so-called potential**

**- interactions on 1-dimensional margins are possible**

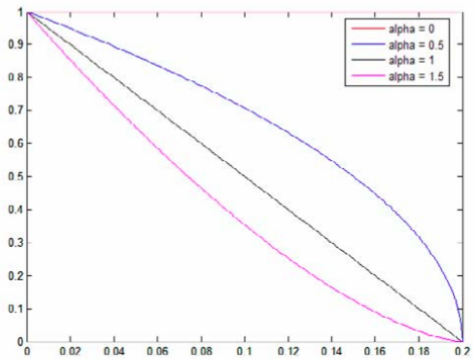
# Strauss designs – With 1D margins interaction

$$\pi(x)\,\alpha\, e^{-U(x)}$$

$$U(x) = \beta \sum_{i<j} \varphi\left(\left\| x^i - x^j \right\|\right) + \sum_{k=1}^{d} \beta_k \sum_{i<j} \varphi_k\left(\left| x_k^i - x_k^j \right|\right)$$

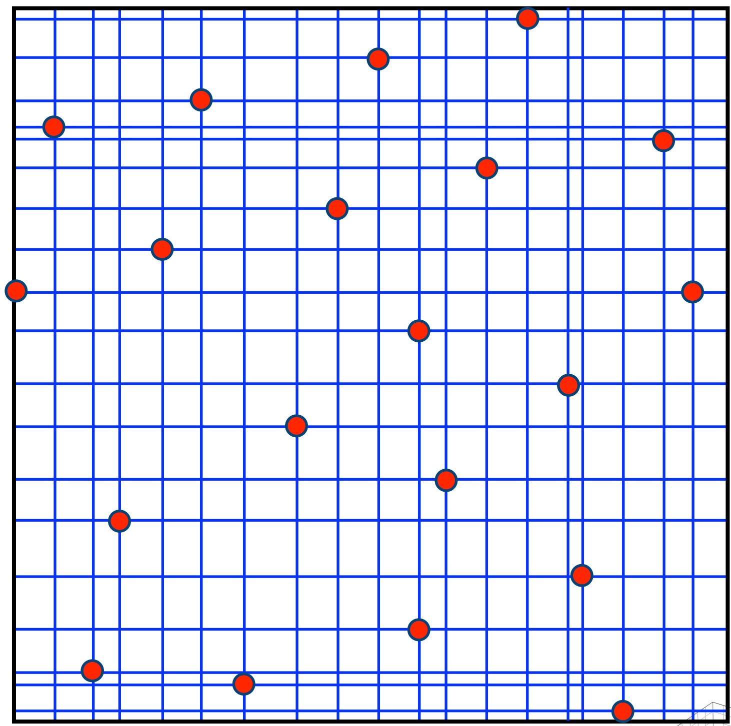
$$\beta = -\ln\gamma > 0\,; \quad \beta_k = -\ln\gamma_k > 0, \quad k = 1,\dots,d$$

$$\varphi(r) = \left(1 - \frac{r}{R}\right)^{\alpha}$$




**Projections on margins are approximately uniform**

**Note so far from LH designs**



# Strauss designs - Conclusion

- Stochastic designs, governed by the potential U
  - Regular U gives better designs
  - Designs in constrained domains
- Good results on synthetic and industrial cases
- Package DiceDesign

# PART II

- Focus II

Approximation of a target region

# Approximation of a target region

- In frequent situations, global accuracy of metamodels is not required

- Example:

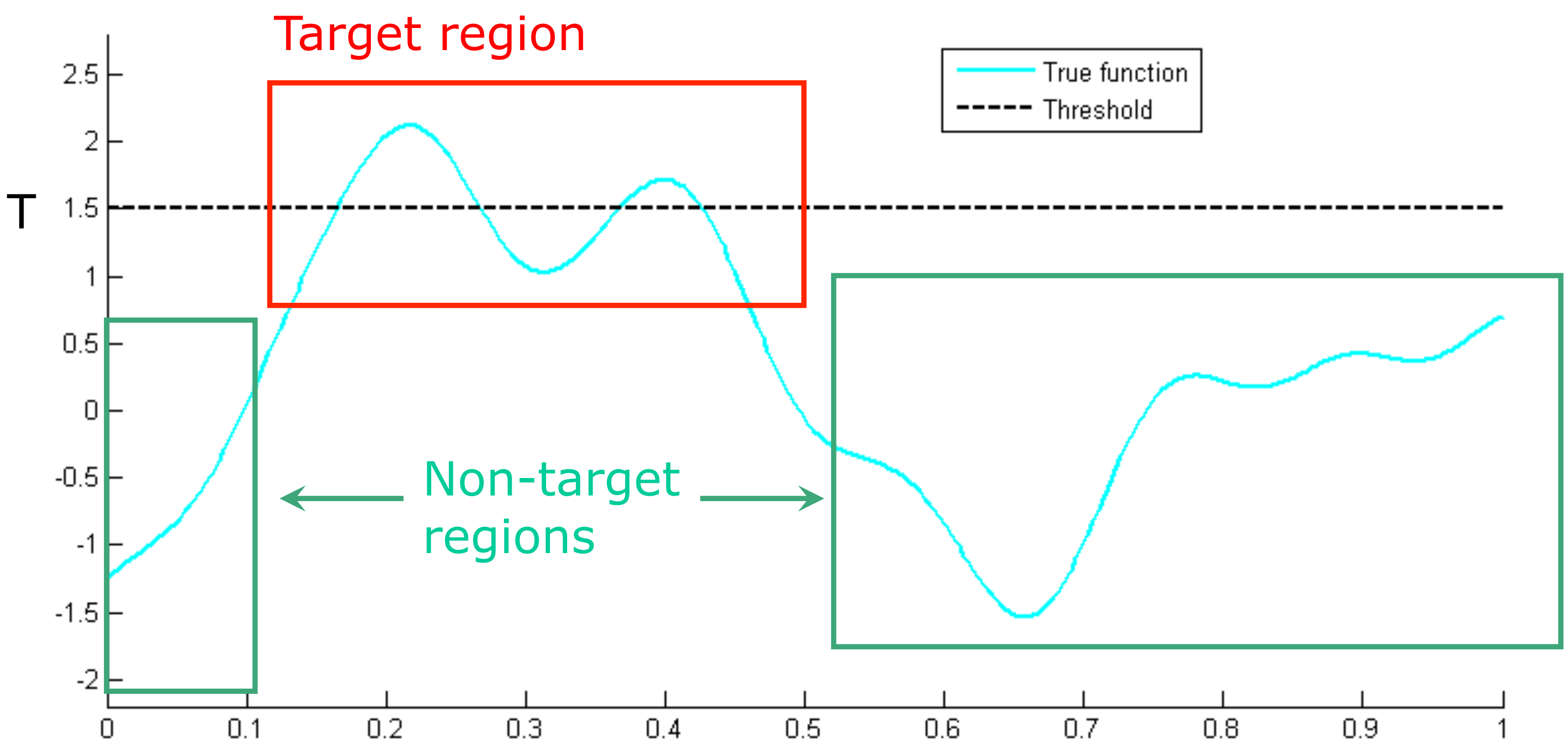
$$\operatorname*{Min}_{\mathbf{x}} \quad F(\mathbf{x}) \qquad \text{s.t.} \quad G(\mathbf{x}) \leq T$$

$$\mathrm{P_f} = \mathrm{Prob}\left(G\left(\mathbf{X}\right) \geq T\right)$$

Good accuracy for G(x) ≈ T

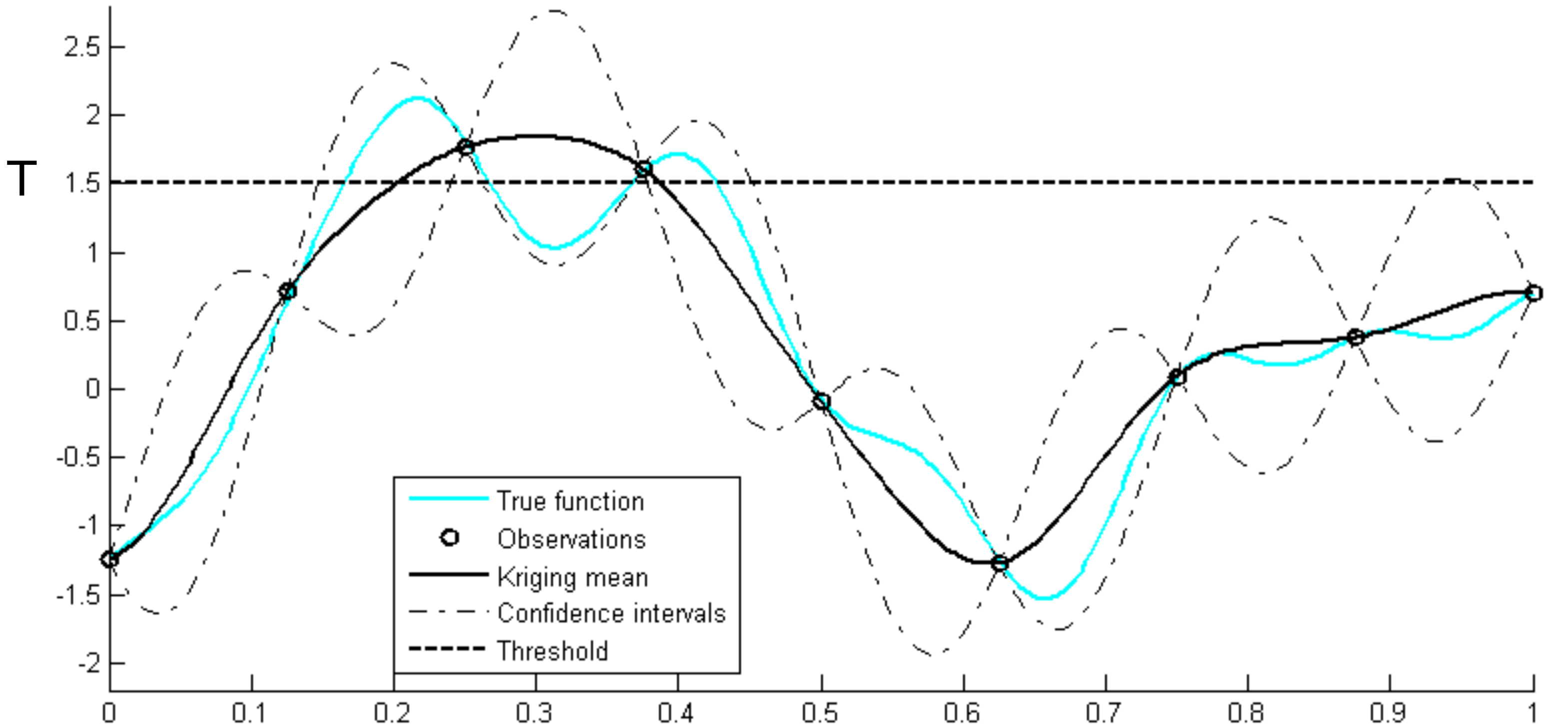
# Approximation of a target region – Example (1)

Function to approximate:



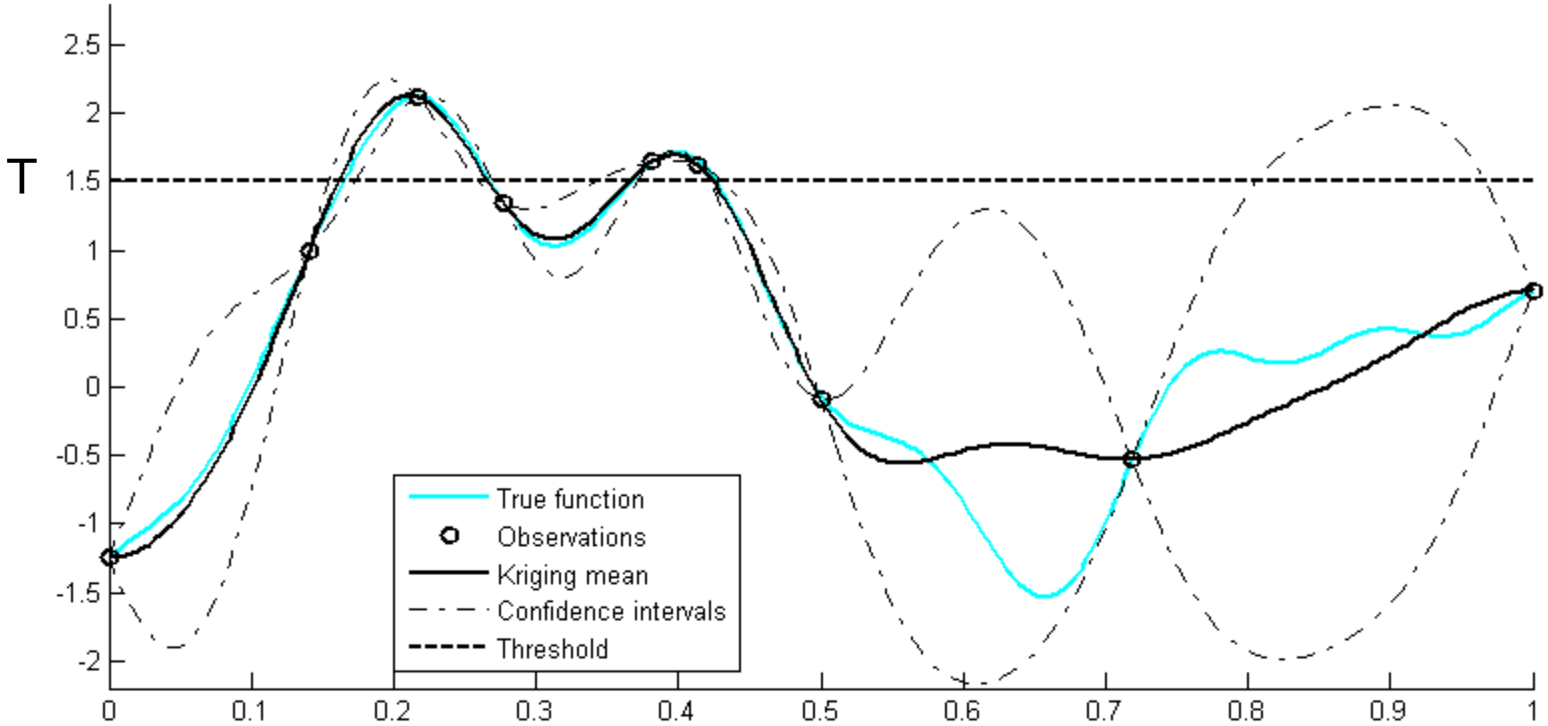
# Approximation of a target region – Example (2)

- Kriging based on a uniform design:
  - Reeasonable variance everywhere
  - Large errors in the target region



# Approximation of a target region – Example (2)

- Customized design:
  - Large variance in non-target regions
  - Good accuracy in target regions



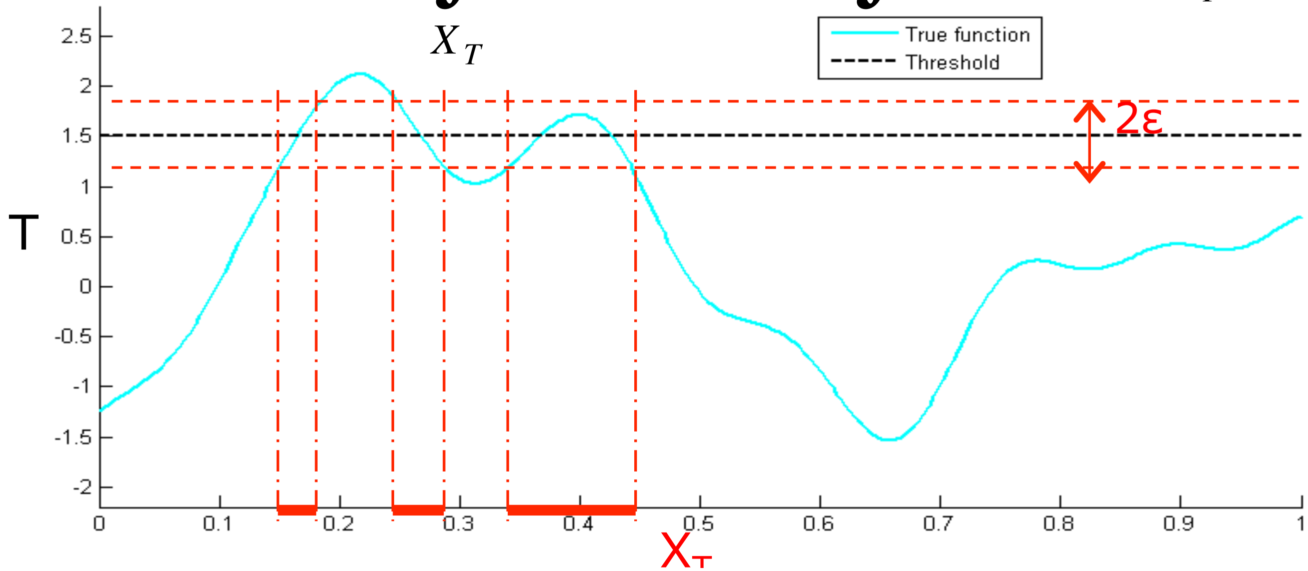
# Approximation of a target region – Criterion (1)

- Target region = close to the threshold T

$$X_T = \{\mathbf{x} \in D \,/\, |G(\mathbf{x}) - T| \le \varepsilon\}$$

- Ideal criterion: MSE, with integration over $X_T$ only:

$$IMSE_T = \int_{X_T} MSE(x)dx = \int MSE(x)1_{X_T}(x)dx$$




⇒ Problem: $X_T$ is unknown!

# Approximation of a target region - Criterion (2)

- Idea: replace $1_{X_T}(x)$ by $E(1_{X_T}(x)) = P(x \in X_T) = P(|G(x) - T| < \varepsilon)$

  the probability of belonging to the target region, and replace G by the conditional Gaussian Process.

- Using the properties of Gaussian process, we get:

$$W_\varepsilon(x) := P(x \in X_T) = \Phi\left(\frac{T + \varepsilon - m_k(x)}{s_k(x)}\right) - \Phi\left(\frac{T - \varepsilon - m_k(x)}{s_k(x)}\right)$$

  where $m_k(x)$ and $s_k(x)$ are the kriging mean and s.d.

# Approximation of a target region – Criterion (3)

- The criterion: $IMSE_T = \int MSE(x) W_\varepsilon(x) dx$

- Limit case: ε -> ∞, $IMSE_T$ -> IMSE

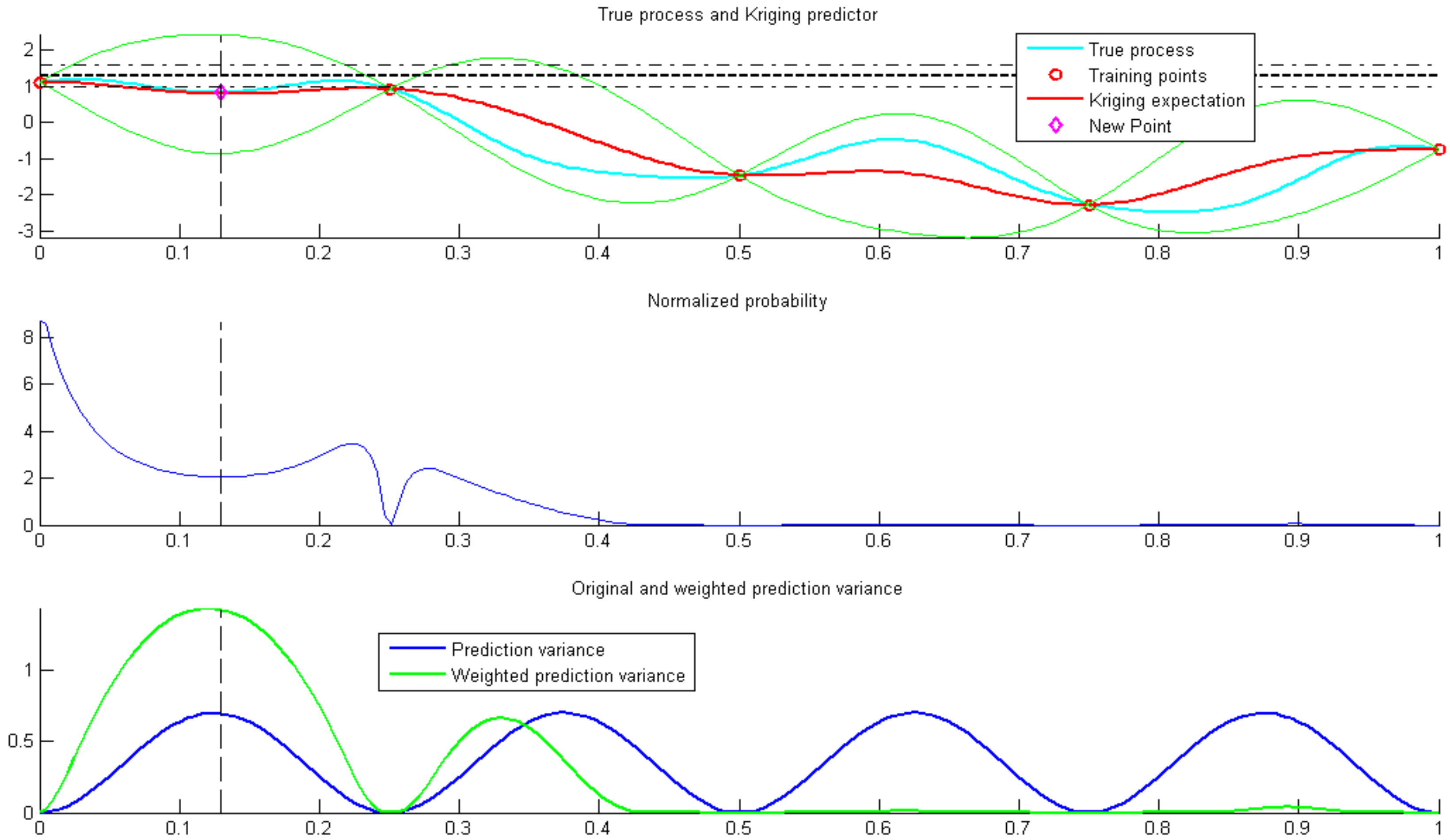
- Limit case: ε -> 0, replace $W_\varepsilon$ by the pure local W where

$$W(x) = \lim_{\varepsilon \to 0} \frac{W_\varepsilon(x)}{2\varepsilon} = f_{N(m_k(x), s_k(x)^2)}(T)$$

the density of the conditional distribution of the Gaussian Process.

- W(x) is large if:
  - G(x) is near the target region
  - x belongs to an unexplored area

# Approximation of a target region – Illustration



# Approximation of a target region – Algorithm

- Iterative procedure:
  - Create an initial design, compute the observations
  - Estimate the Kriging model, and compute *W(x)*
  - Find x* that minimize the practical criterion

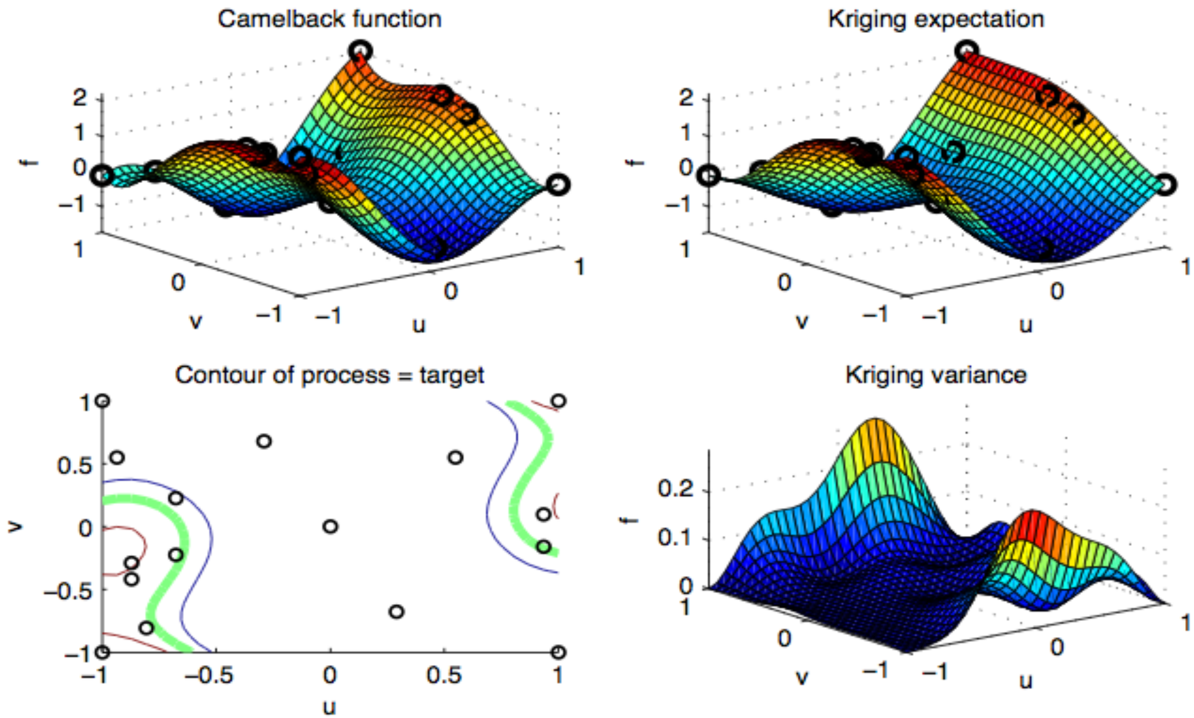
$$IMSE_T(x^*) = \int MSE(x \mid X_i, x^*) W(x \mid X_i, Y_i) dx$$

  - Run the simulator at x*
  - Continue until the maximal number of iterations is reached

- Kriging model parameters:
  - Estimated at the beginning, or re-estimated at each step

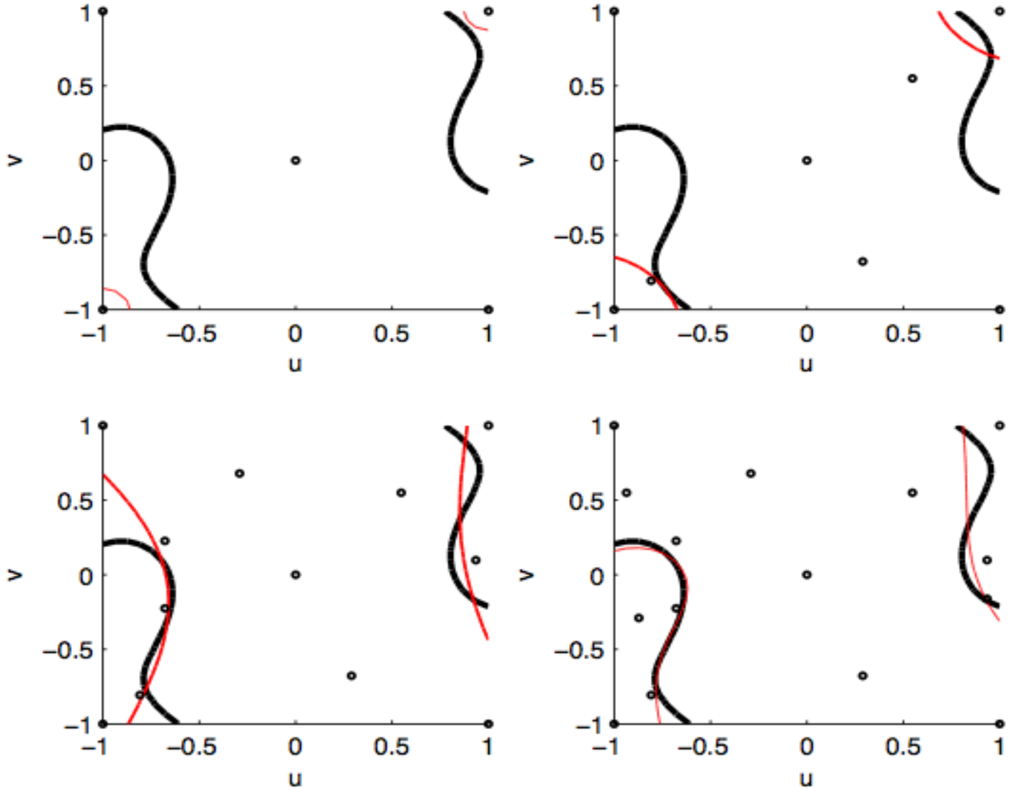
# Approximation of a target region – 2D-example

- A 2-dimensional example (Camelback function)
  - Target region G(x,y) = 1.3
  - Optimal design after 11 iterations



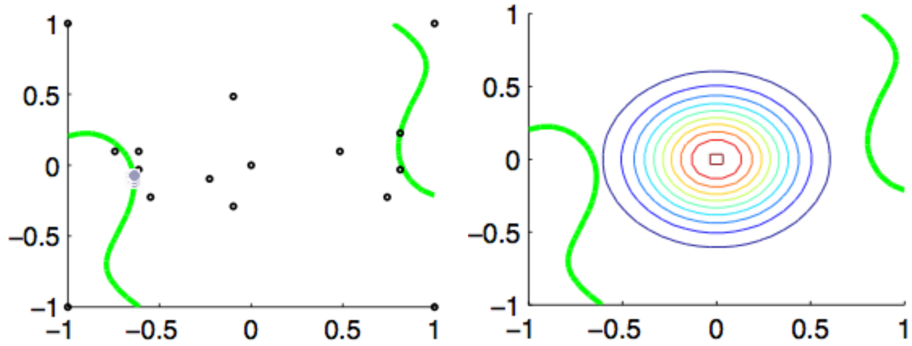
# Approximation of a target region – 2D-example

- A 2-dimensional example (Camelback function)
  - Evolution of Kriging target contour line



# Approximation of a target region – 2D-example

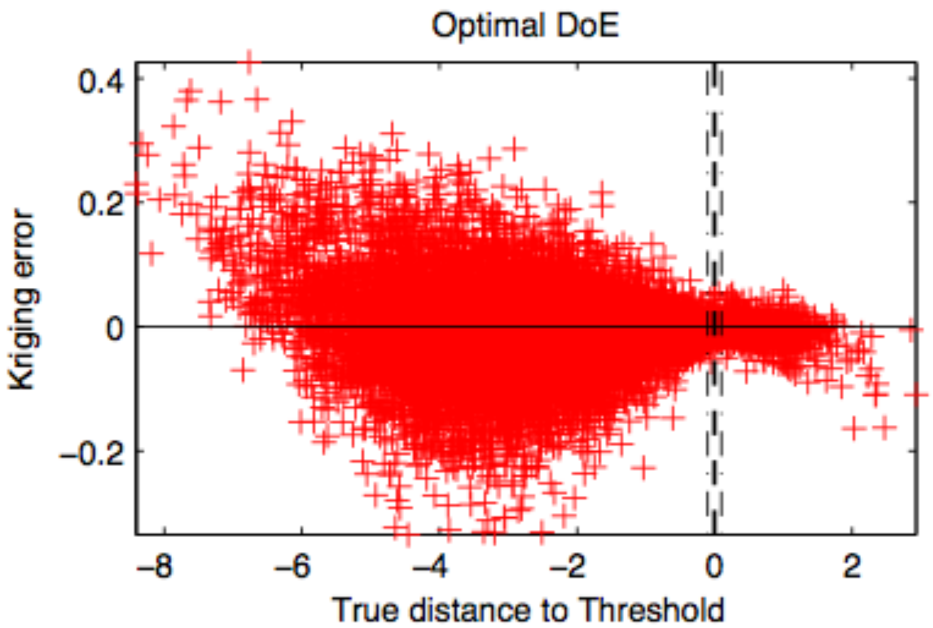
- Application to the assessment of probability of failure
  - P(G(U,V)>1.3) with U, V, i.i.d. $N(0, 0.028^2)$

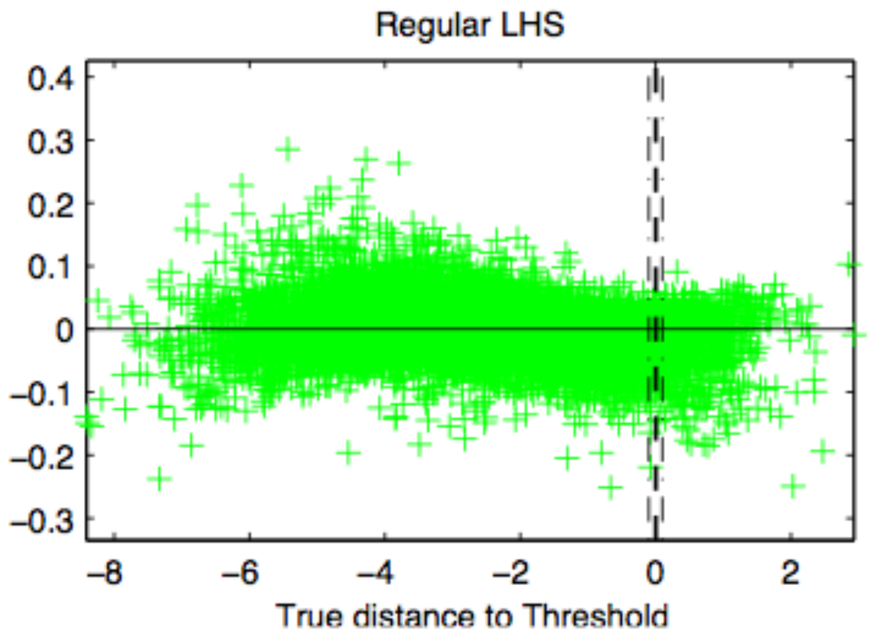



| DoE | Full Factorial | Optimal without input distribution | Optimal with input distribution | Probability estimate based on $10^7$ MCS |
|---|---|---|---|---|
| Probability of failure (%) | 0.17 | 0.70 | 0.77 | 0.75 |
| Relative error | 77 % | 7 % | 3 % | |

# Approximation of a target region – 6D-example

- A 6-dimensional example
  - Function = 1 sample function of a Gaussian Process with linear trend and isotropic Gaussian covariance (known parameters)



# Approximation of a target region - Comparison

- Good results in a numerical study comparing 4 methods -> see the poster of Ling Li in UCM 2010
  - Targeted IMSE performs as well as Stepwise Uncertainty Reduction, when W corresponds to the limit case ($\varepsilon$ -> 0)
  - Both tIMSE and SUR seem to outperform the two other ones
  - Future research: theoretical link between tIMSE & SUR ?

# Approximation of a target region – Conclusion

- An adaptive strategy
  - Trade-off between exploration of target regions and global uncertainty reduction
  - Model-believer
- Applications to the assessment of probability of failure
- Future research:
  - Influence of parameter estimation in Kriging
  - Adaptation for dimensions ≥ 10
  - A R-package is in preparation

Thank you for your attention !