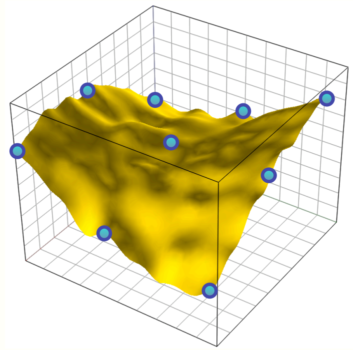


The DiceKriging and DiceOptim packages: kriging-based metamodeling and optimization for computer experiments

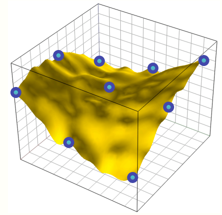
UseR! 2009 Conference - Rennes

Olivier Roustant, *Ecole des Mines de St-Etienne (France)*

David Ginsbourger, *Université de Neuchâtel (Switzerland)*

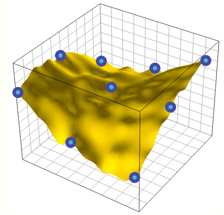
Yves Deville, *Statistical Consultant (France)*

Scientific framework



- Analysis of costly numerical simulators
  - Crash-test simulators, thermo-hydraulic simulators or neutronic simulators for nuclear safety…
  - 1 run = several hours !
- Some issues
  - Optimization (ex: minimization of the vehicle weight)
  - Risk assessment (ex: probability that the temperature exceeds a threshold ?)
  - Calibration

Scientific framework



- Some mathematical issues and tools
  - To approximate the simulator with a cheaper-to-run proxy

    -> metamodeling: linear models, PolyMars, Splines, **Gaussian processes (kriging)**, …

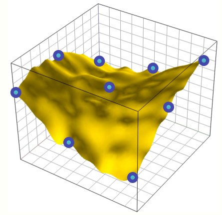
  - To choose design points in a relevant way

    -> computer experiments: space-filling designs, quality criteria, optimal designs…

  - To use metamodels to solve problems

    -> metamodel-aided optimization **with EGO method**

Some references



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- Rasmussen C.E., Williams C.K.I. (2006), ***Gaussian Processes for Machine Learning***, *the MIT Press, www.GaussianProcess.org/gpml*
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- Ginsbourger D. (2009), *Multiples Métamodèles pour l'Approximation et l'Optimisation de Fonctions Numériques Multivariables,* PHD thesis.
- Jones D.R., Schonlau M. and Welch W.J. (1998), Efficient Global Optimization of Expensive Black-Box Functions, *Journal of Global optimization*, **13**, 455-492.
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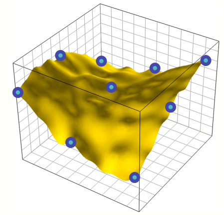
Some R packages about computer experiments



- BACCO [Bayes. Analysis of Comp. Code Output, R. Hankin]

  At least: *Bayesian modelling – Calibration – Prediction when a proxy (e.g. fast code) is available*

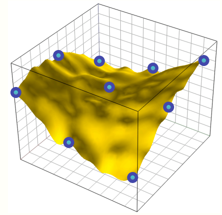
- tgp [bayesian Treed Gaussian Process models, R. Gramacy]

  At least: *Bayesian modelling – For an irregular output – EGO method*

- mlegp [Max. Lik. Estim. of Gauss. processes, G.M. Dancik]

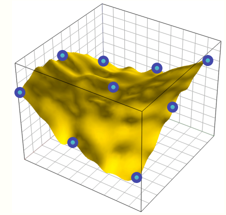
  At least: *Univariate & multidimensional outputs – Constant or 1st order polynomial trend – Gaussian covariance - Stochastic simulators – Sensitivity analysis*

The DiceKriging package



- DiceKriging (now split in DiceKriging & DiceOptim)
  - Univariate output
  - Trend is a linear model (including any transformation of inputs)
  - Max. Lik. Est. of Gaussian Processes with analytical gradients - BFGS and genetic algorithm (with rgenoud)
  - Deterministic or stochastic simulators
  - Several choices of covariance functions
  - EGO method, with analytical gradient (genetic algorithm)
  - Extension of EGO method for parallel computing
  - Prediction, validation, conditional simulations
  - Tested on several case studies (2D, 3D, … 30D)

Kriging: a stochastic metamodeling method

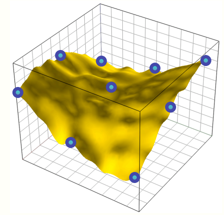


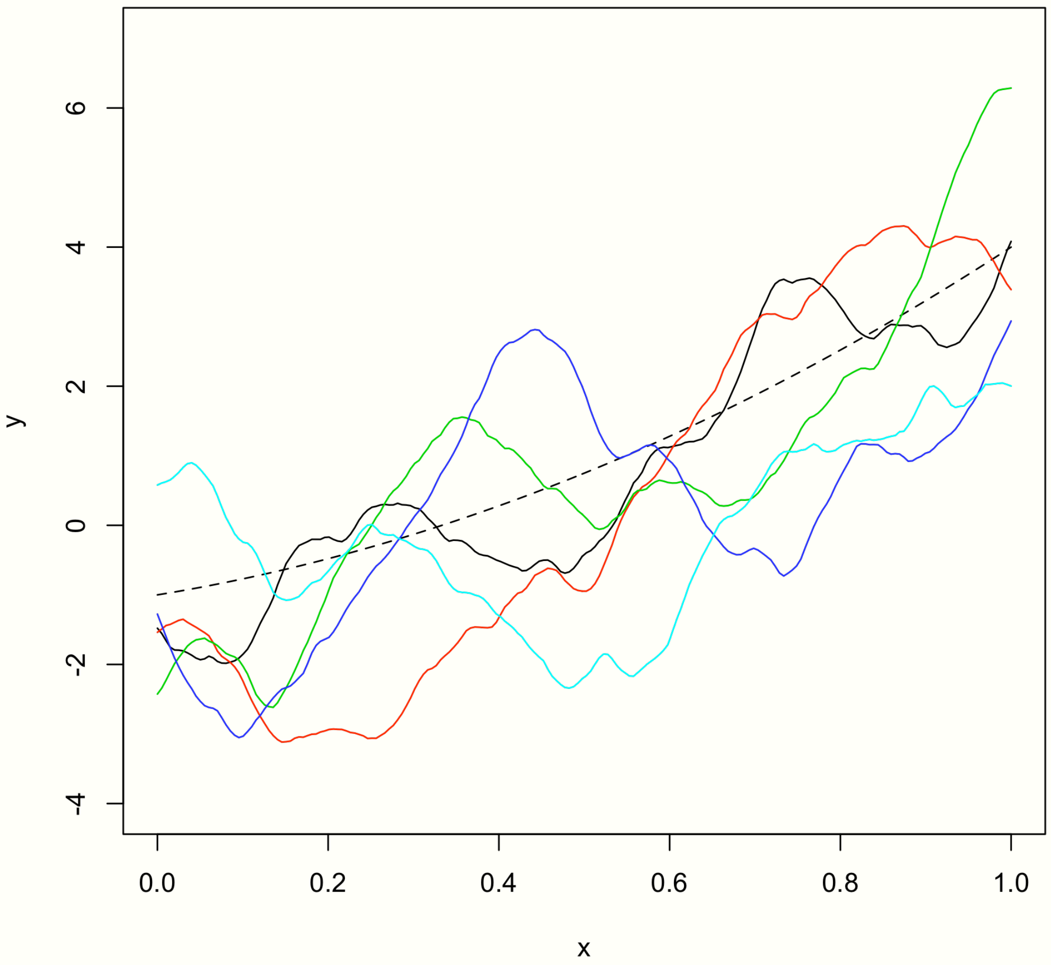
- Kriging (Gaussian processes):

$$Y(x) = F(x)\beta + Z(x)$$

with
  - $F(x)\beta$ a linear deterministic trend
  - $(Z(x))$ a centered stationary Gaussian Process with covariance kernel $C_Z(x,y)=\sigma^2 R(x-y)$

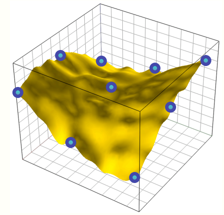
Kriging: a stochastic metamodeling method

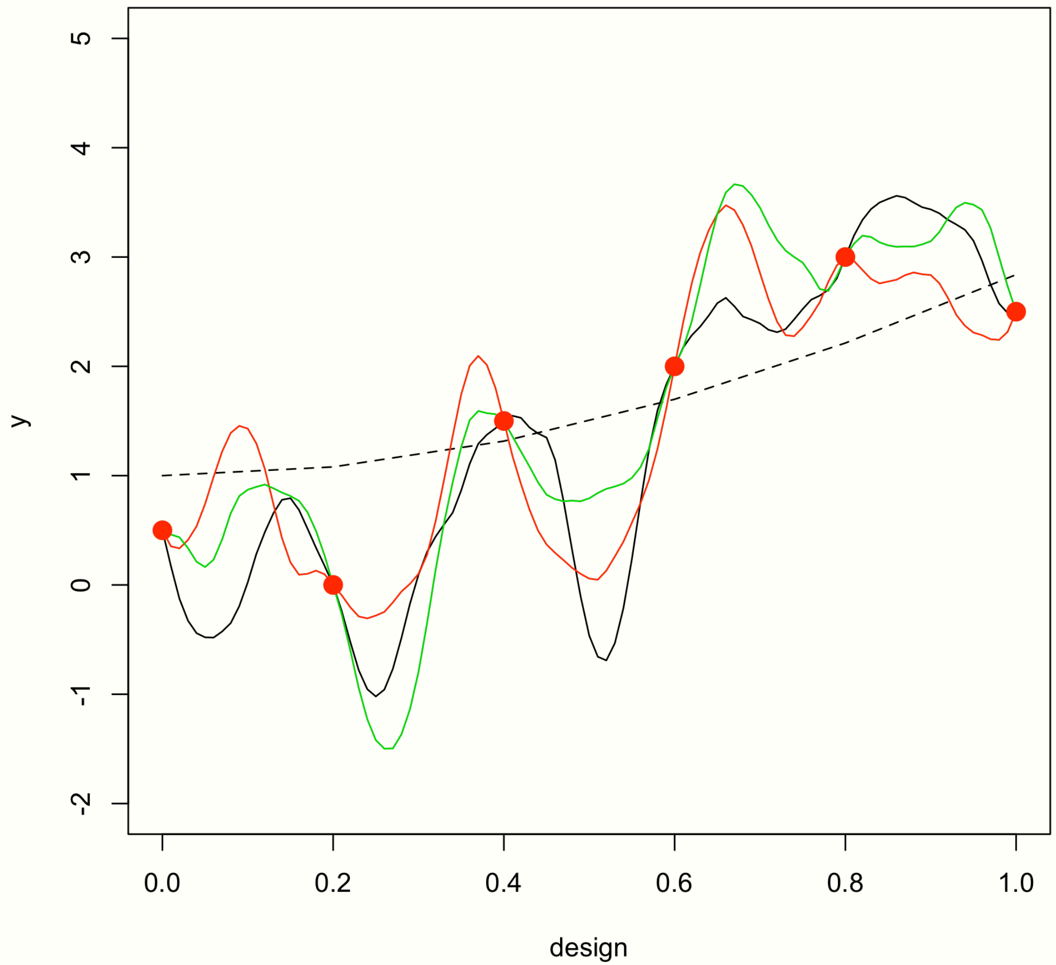




Some simulations with:
- a 2nd order poly. trend
- a Matérn covar. kernel

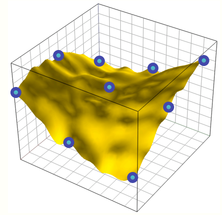
Kriging: a stochastic metamodeling method

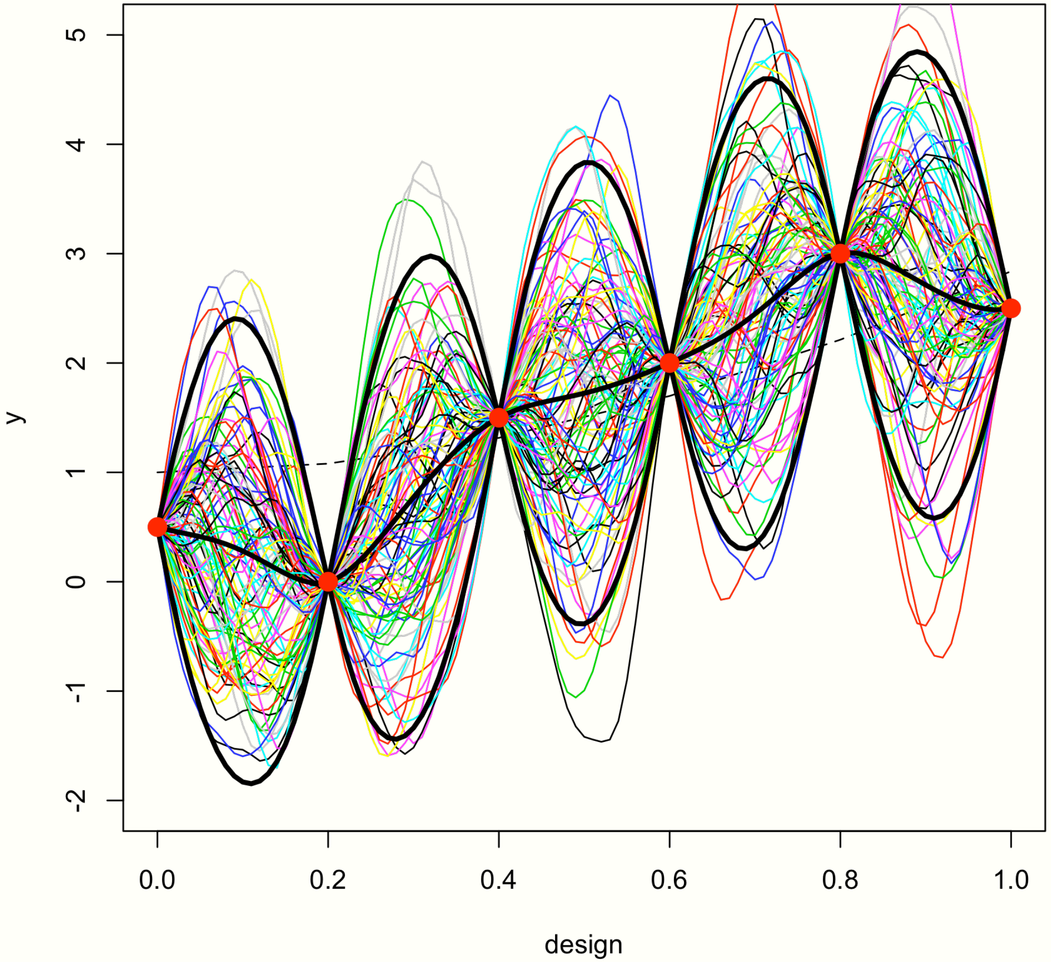




Some conditional simulations with:
- a 2nd order poly. trend
- a Matérn covar. kernel

Kriging: a stochastic metamodeling method

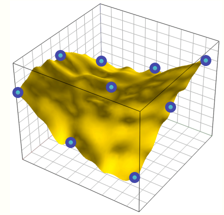


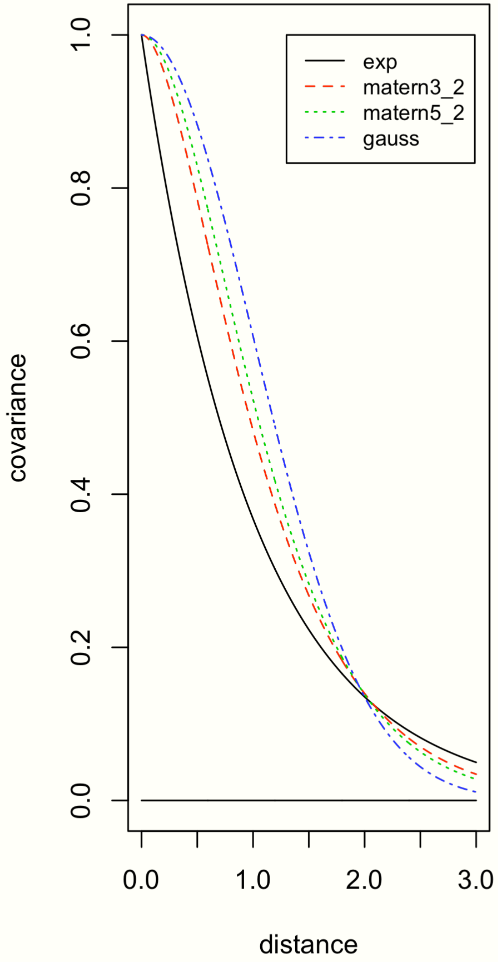


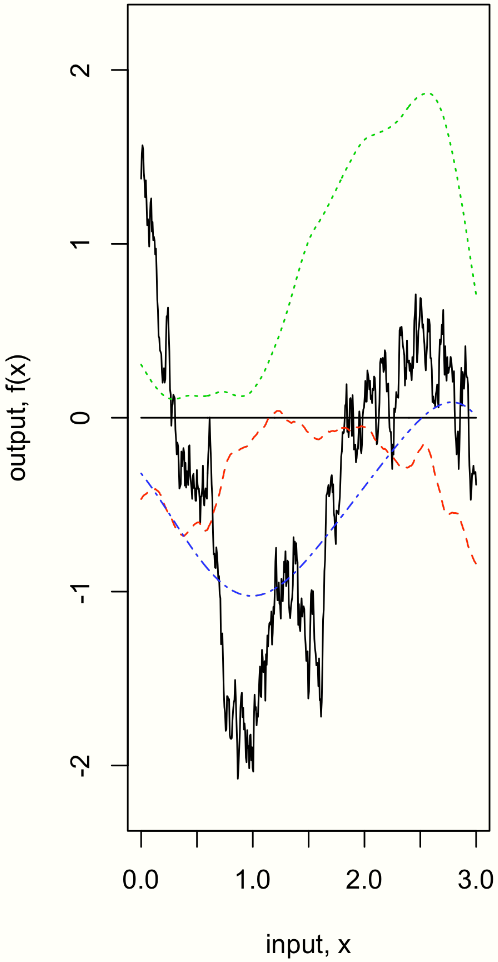
More conditional simulations with:
- a 2nd order poly. trend
- a Matérn covar. Kernel

In bold:
- Kriging mean
 -> BLUP interpolator
- kriging variance
 -> measure of uncertainty

Kriging: a stochastic metamodeling method

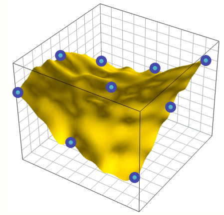






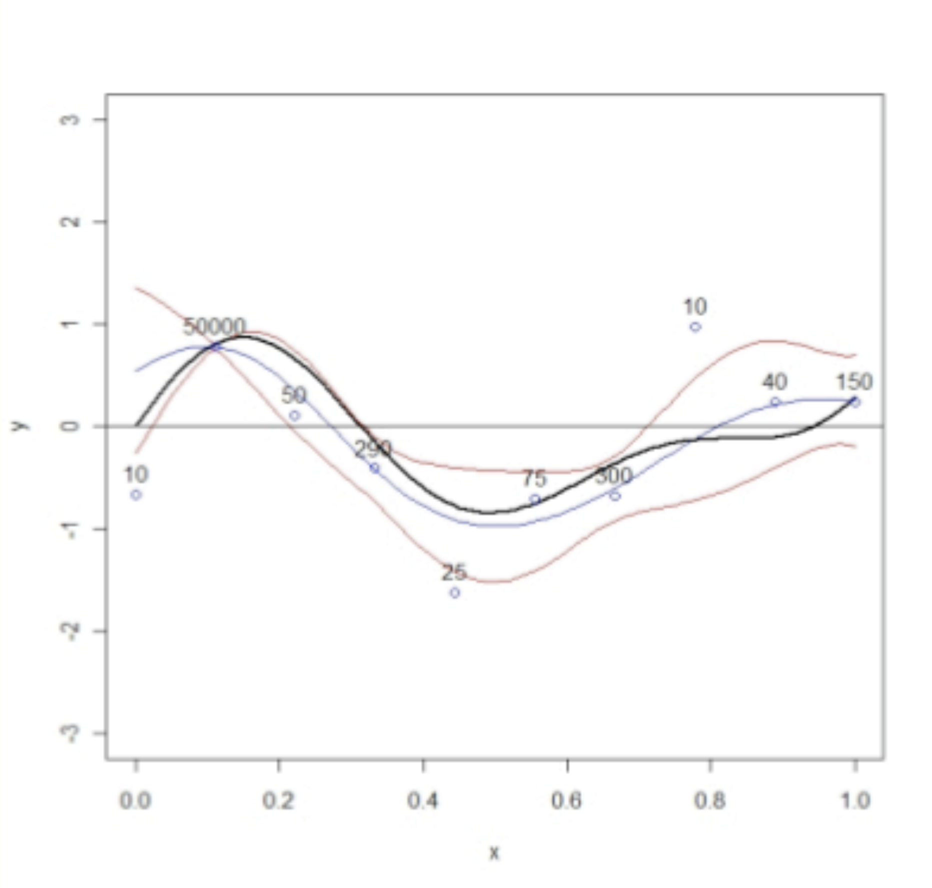
Smoothness and choice of covariance kernels

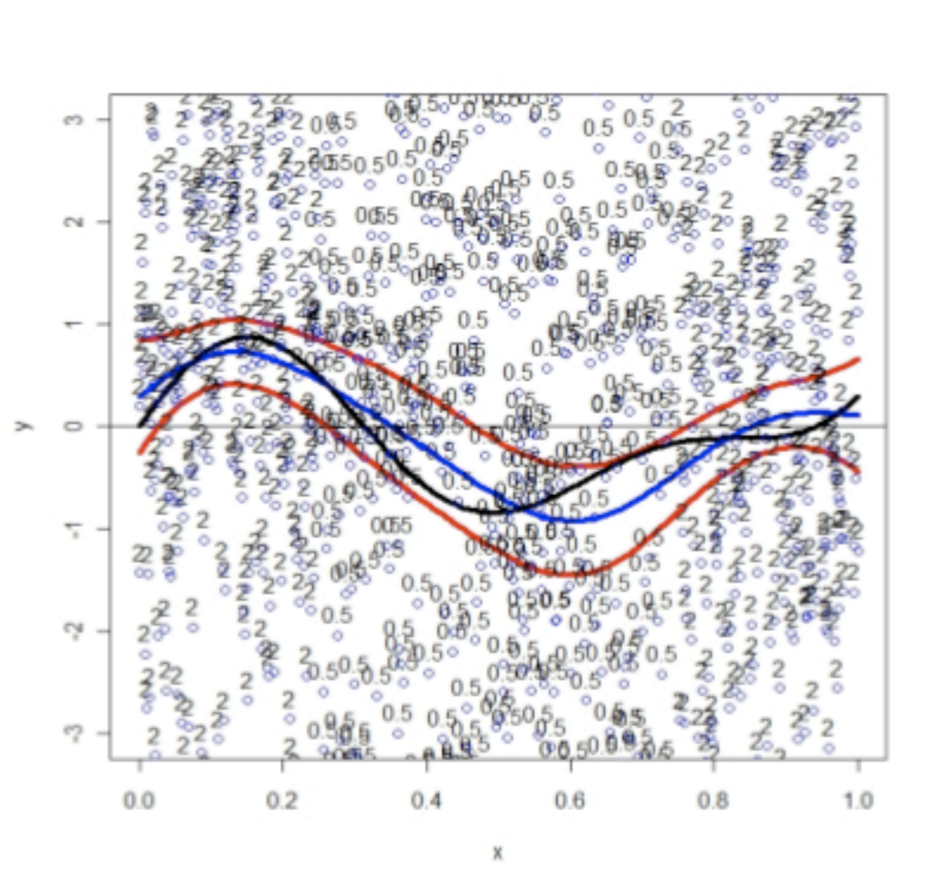
Kriging: a stochastic metamodeling method



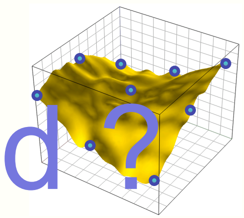
Can also be used to deal with stochastic simulators

Below: kriging estimation with noisy observations (constant budget)





Kriging – What is implemented ?

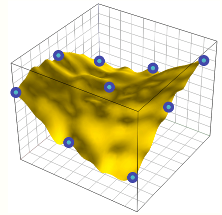


- Simulation: conditional or non-conditional simulations
- Parameter estimation including nugget effect (if wished). By Maximum Likelihood, with analytical gradients.

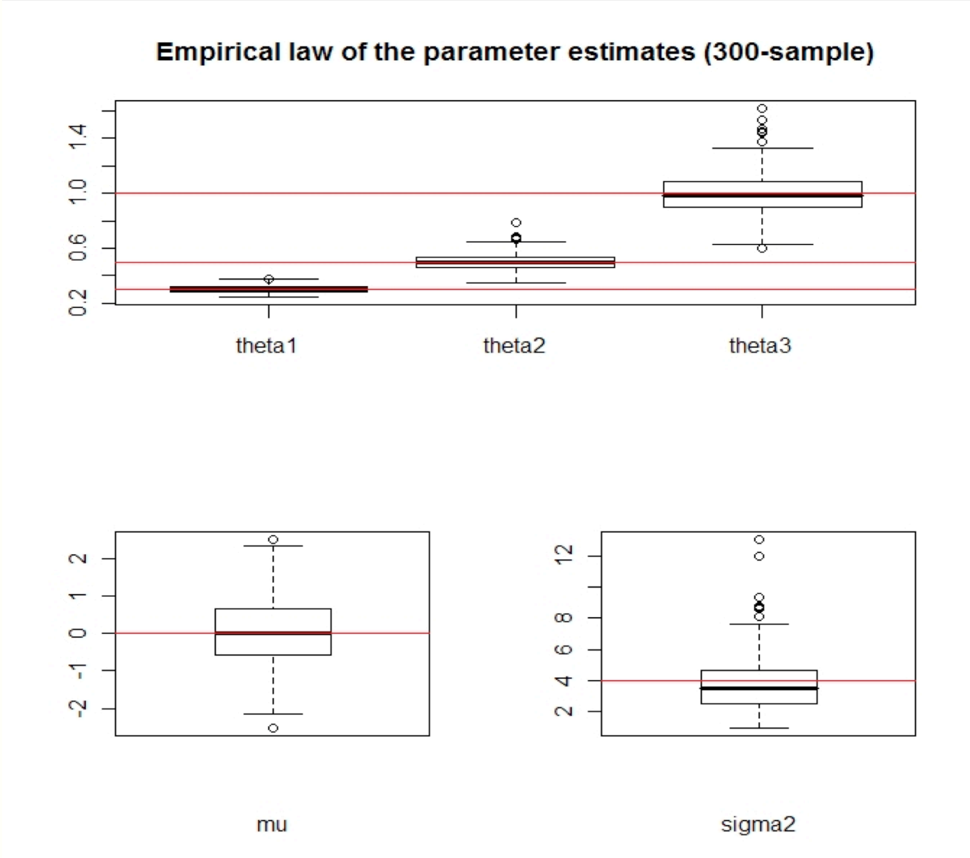
  -> not a Bayesian point of view

  -> also suited for stochastic simulators
- Prediction: simple & universal kriging formulae (mean, variance)
- Validation: leave-one-out, k-fold cross validation (in DiceEval)
- Covariance functions: (at now) Gaussian, Power-Exponential, Matern 3/2, 5/2 and Exponential

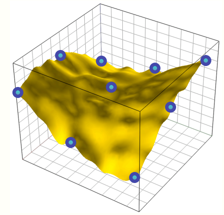
Trustworthy software ?



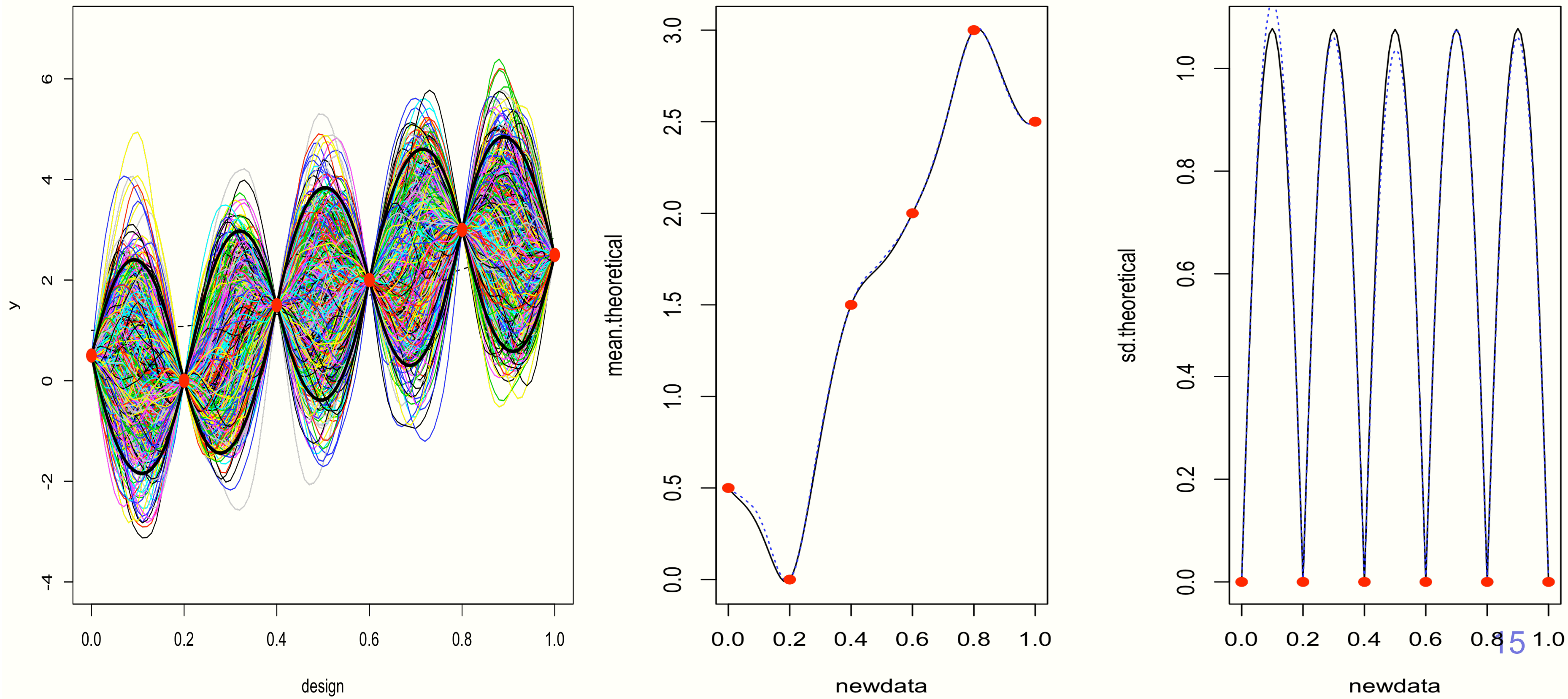
- Some tests we conducted
  - Simulate and re-estimate parameters



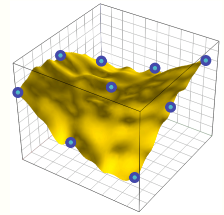
Trustworthy software ?

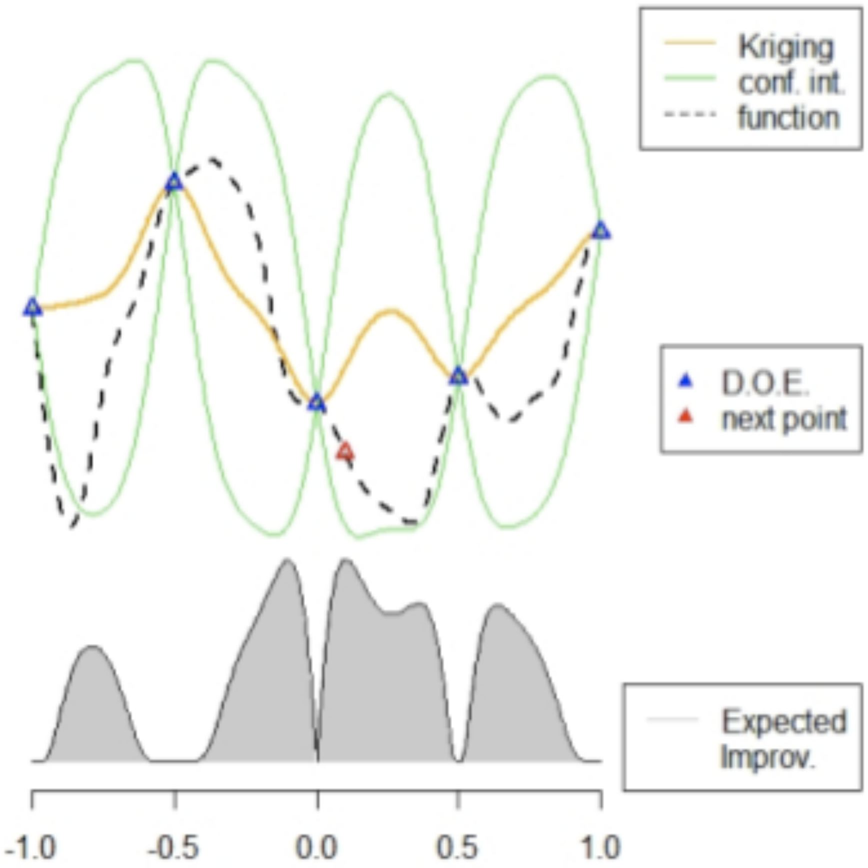


- Some tests we conducted
  - Check the simple kriging formulae by simulation



Kriging-aided optimization

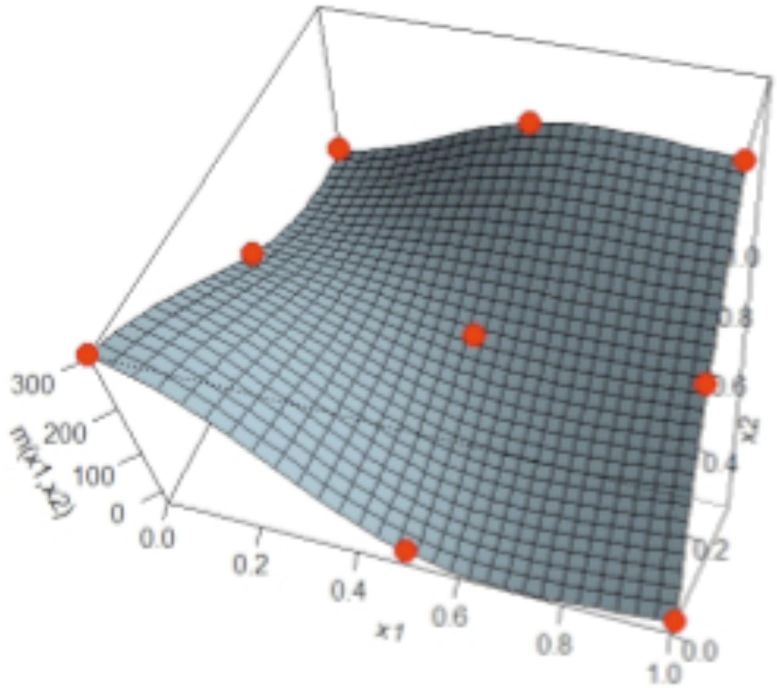


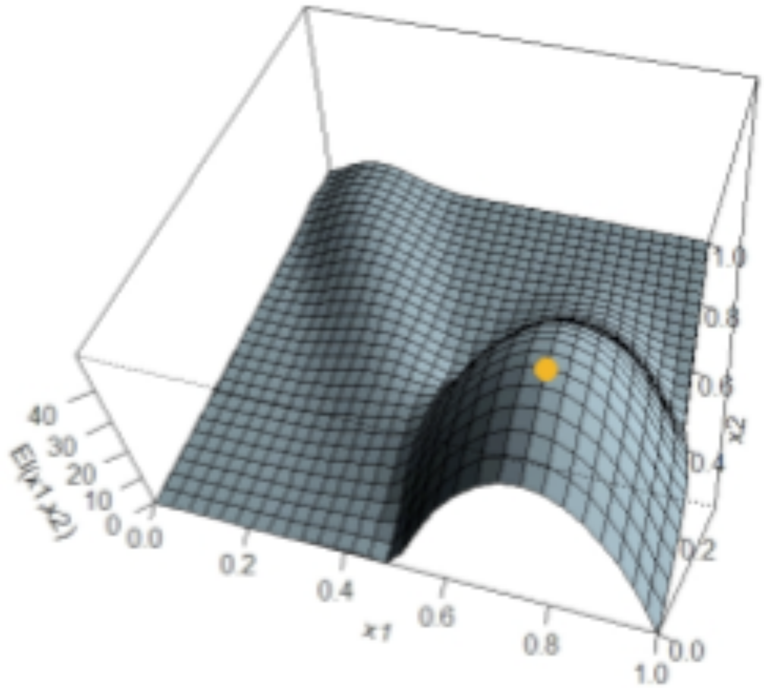


- The Expected Improvement criterion

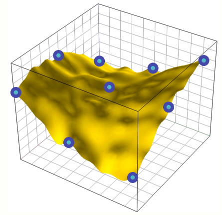
$EI(x) = E(\ [\min(Y(X)) - Y(x)]^{+} | Y(X)=\mathbf{Y})$

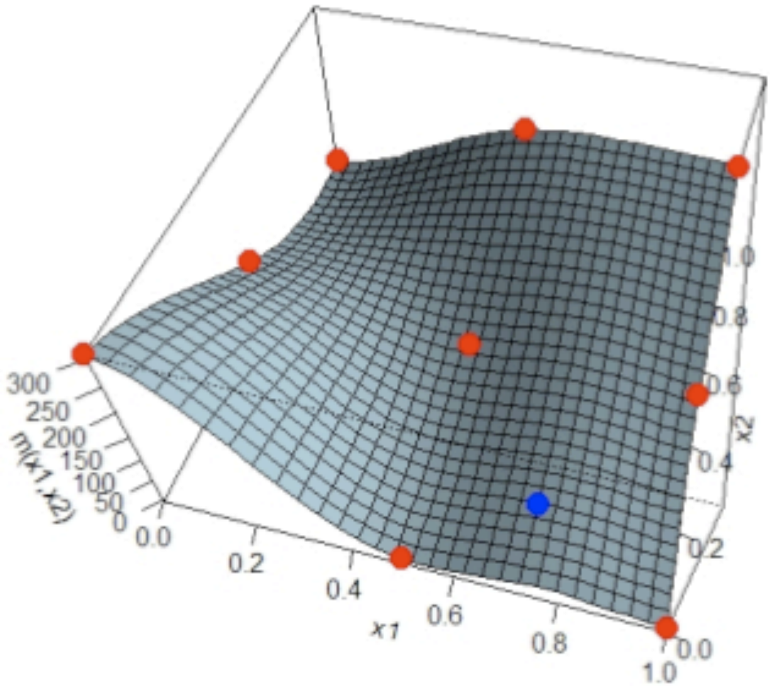
Kriging-aided optimization
Some illustrations

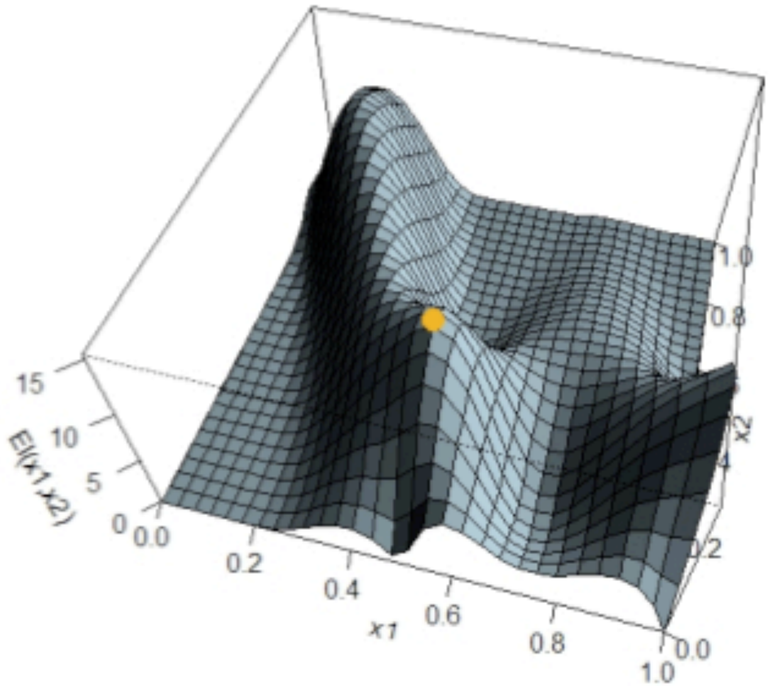




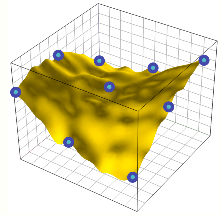
Kriging-aided optimization
Some illustrations

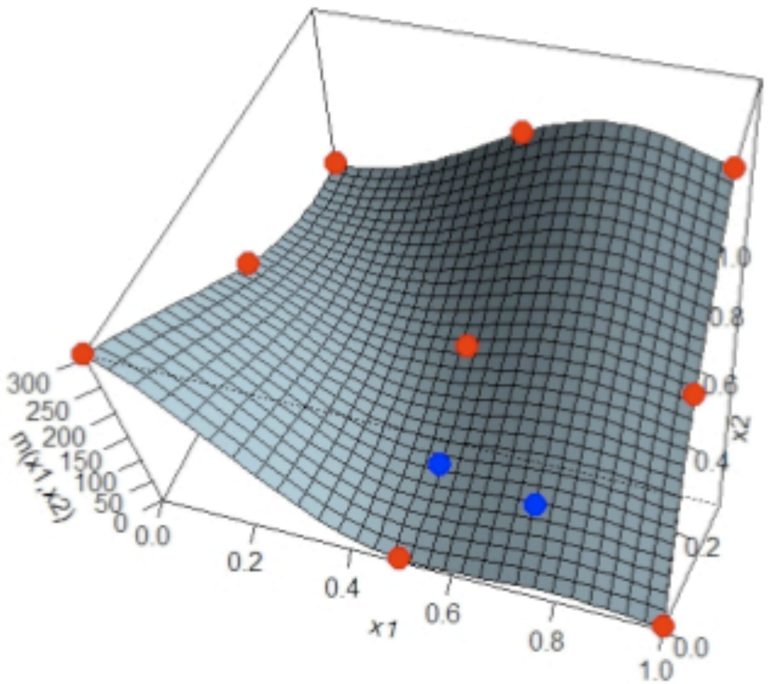


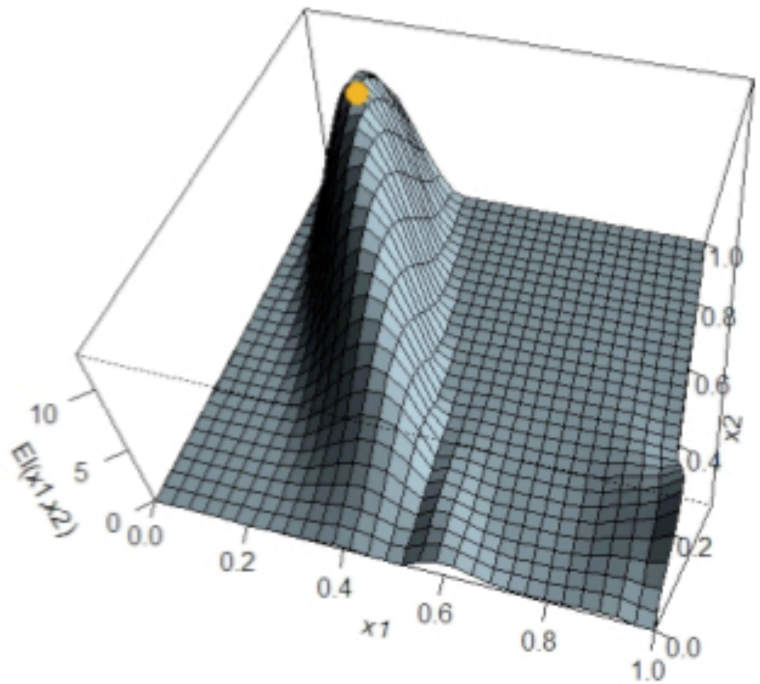




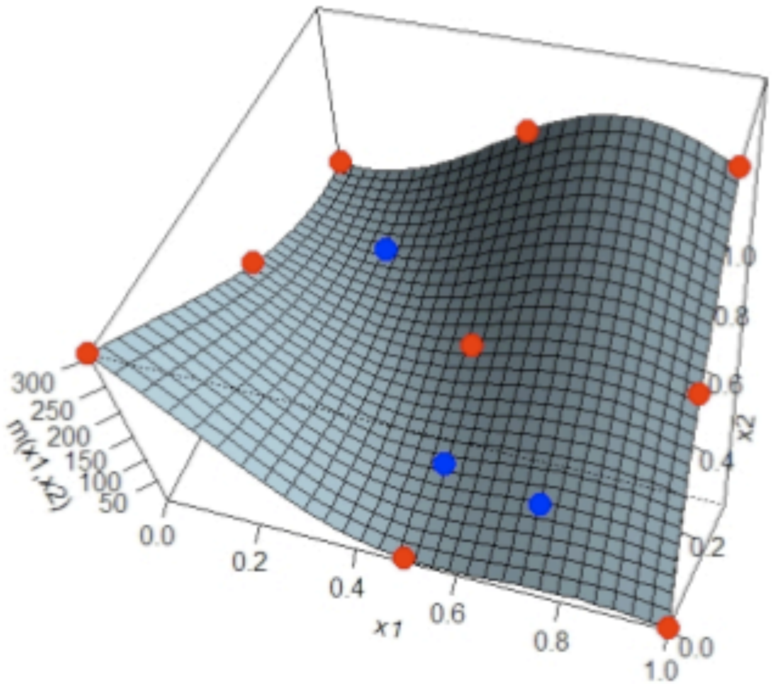
Kriging-aided optimization
Some illustrations

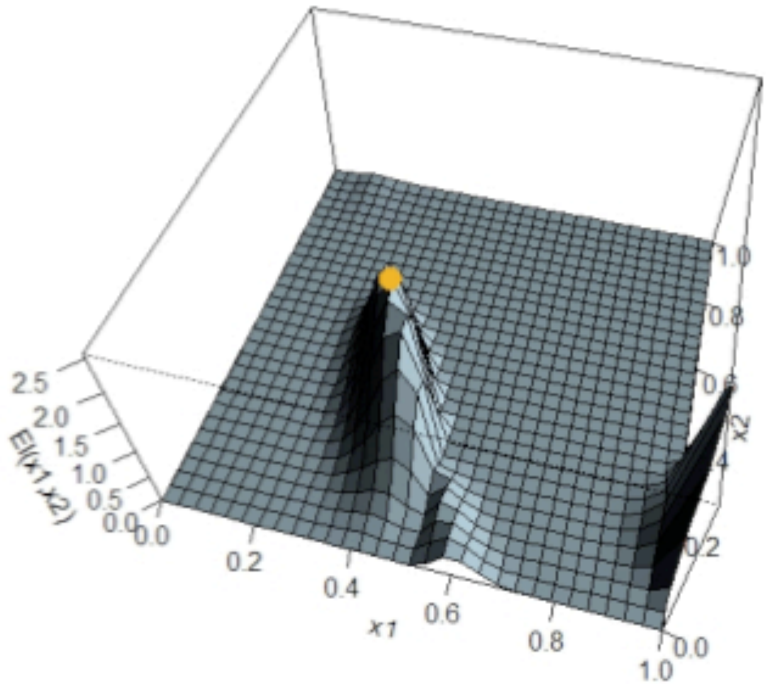




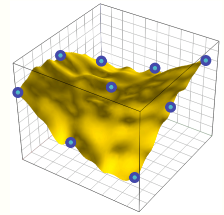


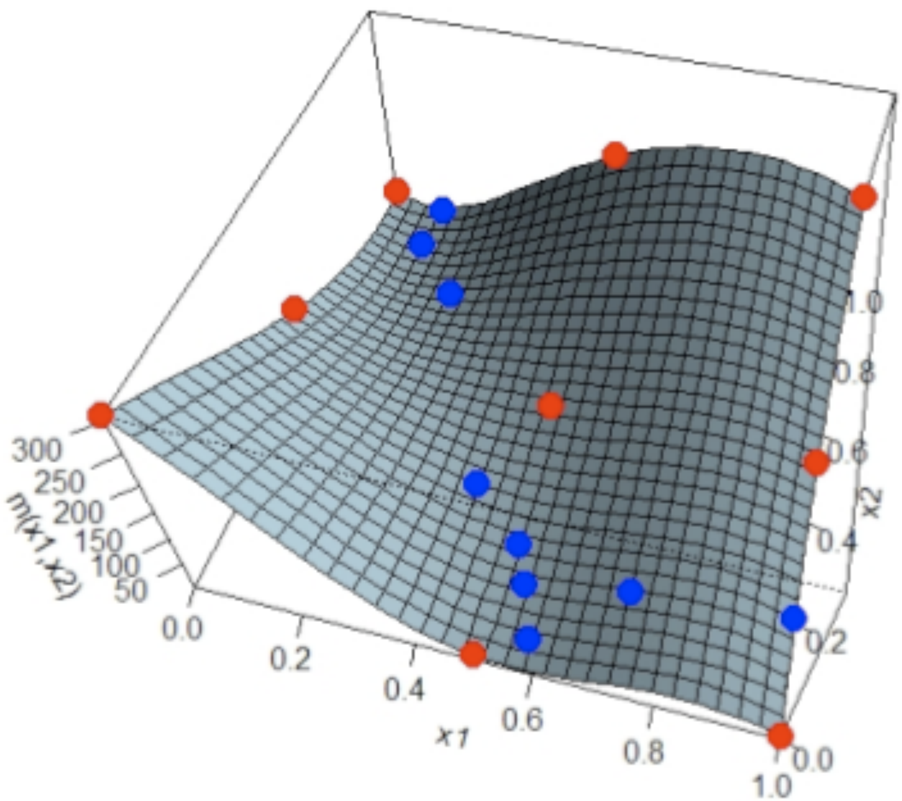
Kriging-aided optimization
Some illustrations



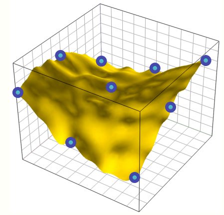


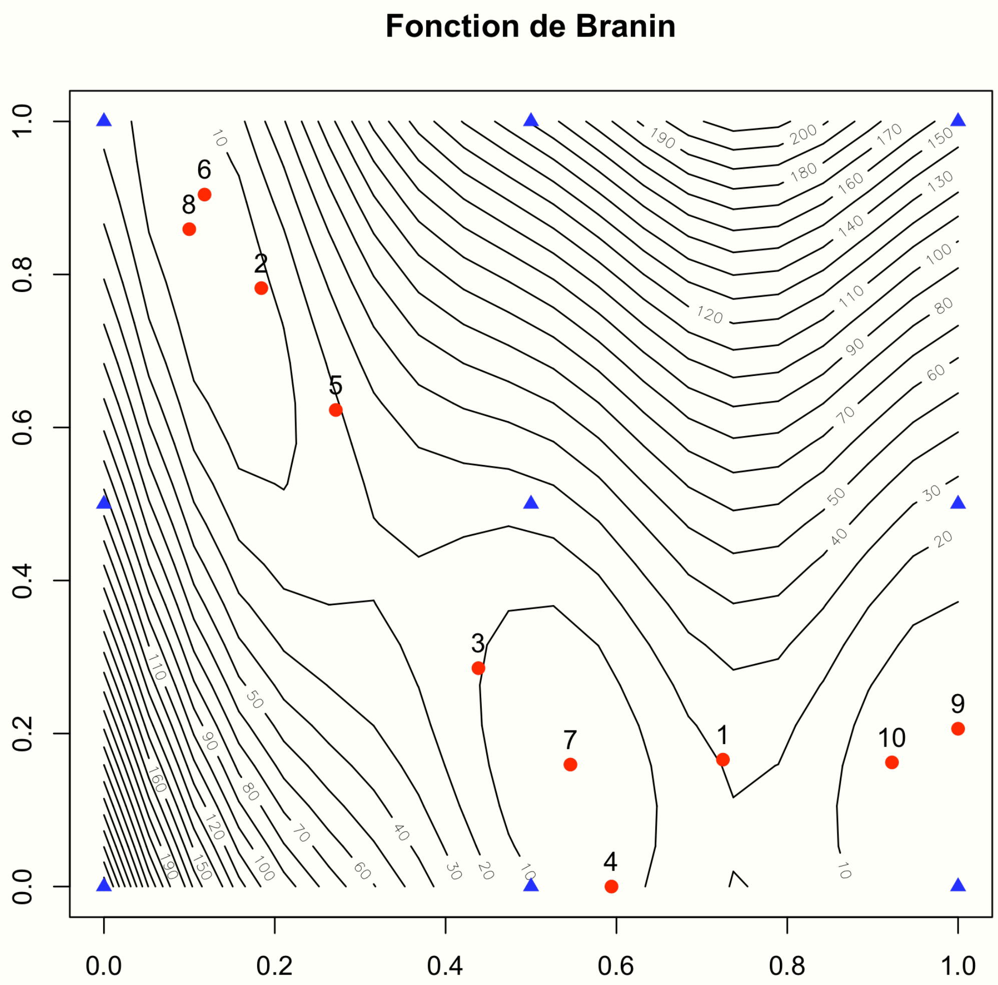
Kriging-aided optimization
Some illustrations





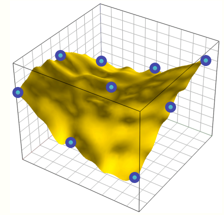
Kriging-aided optimization
Some illustrations

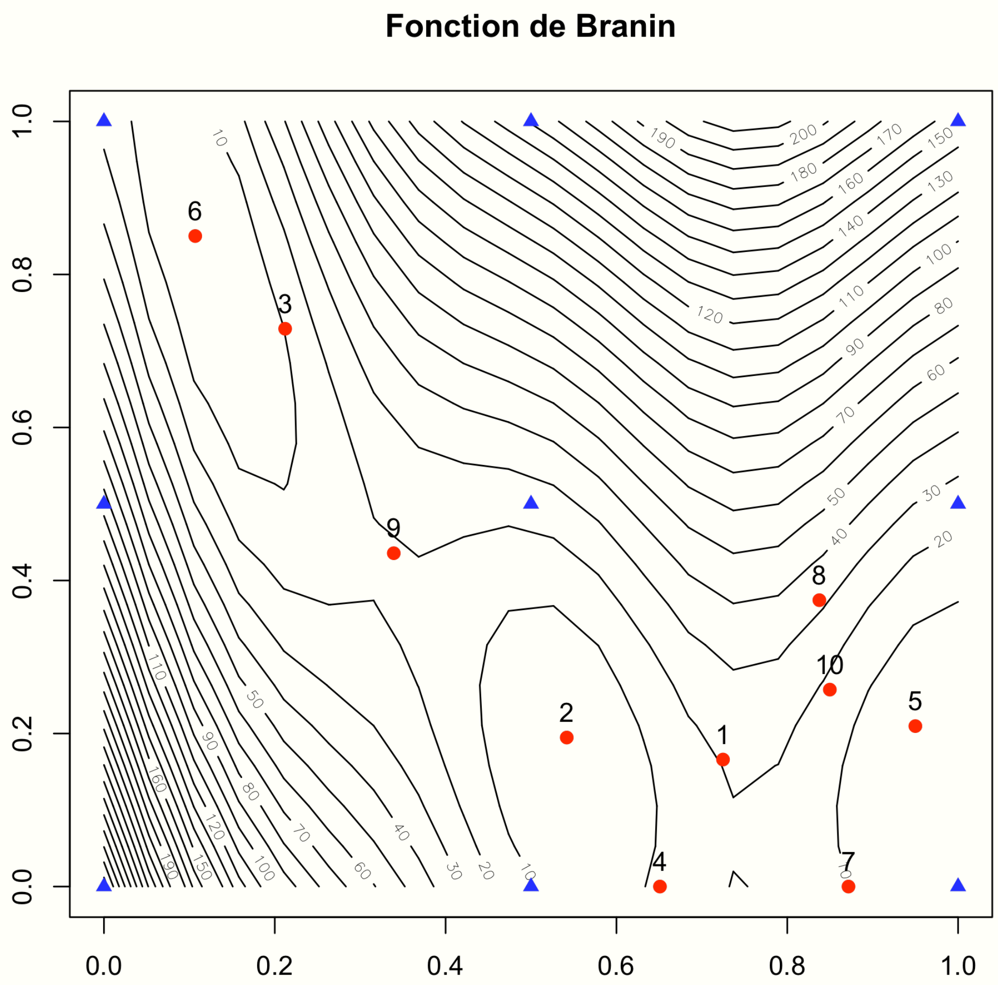




10 steps of EGO with a Gaussian kernel

Kriging-aided optimization
Some illustrations



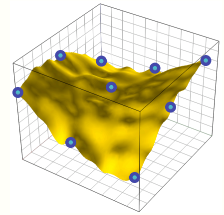


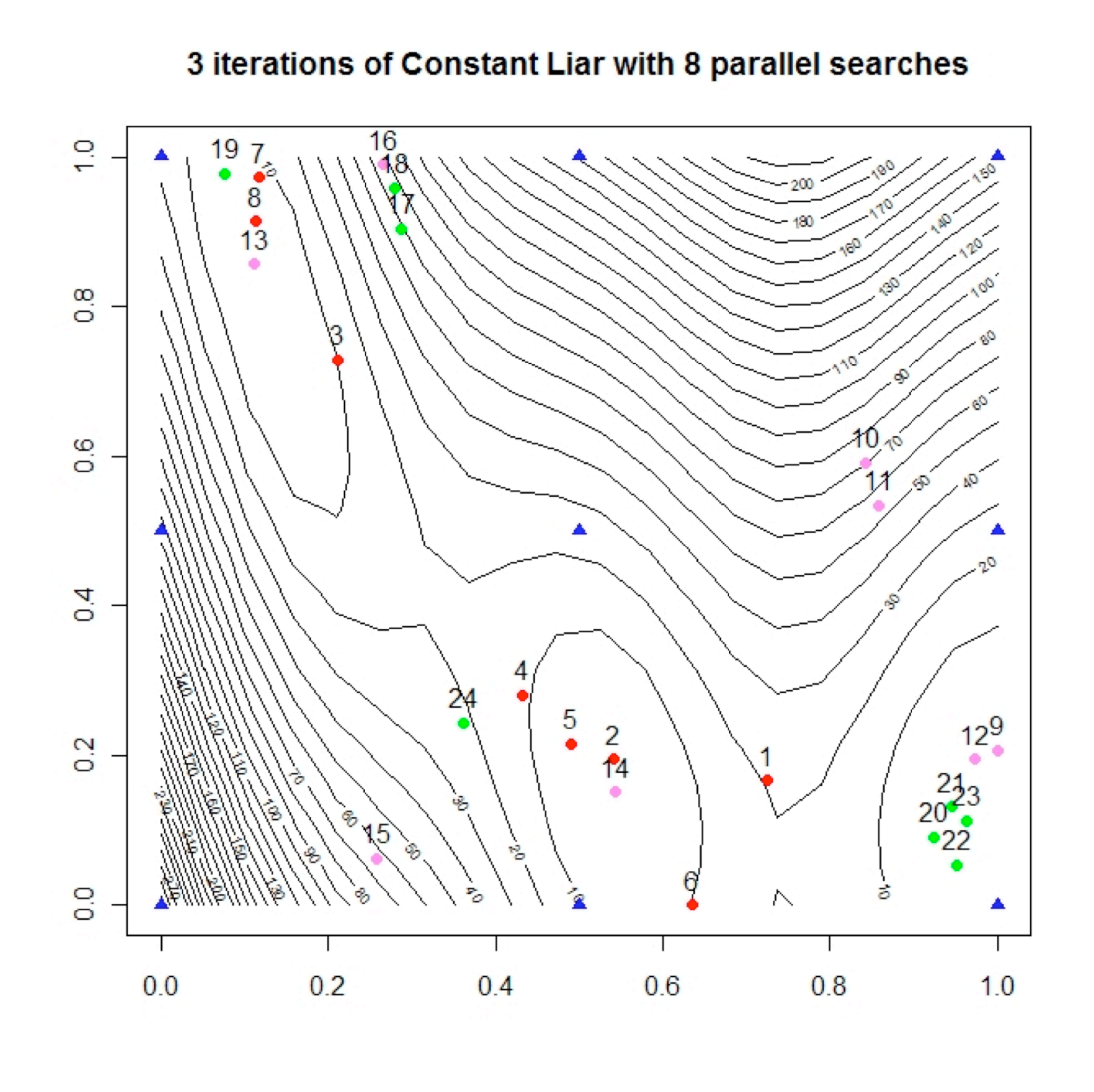
Parallel EGO:

for i in 1:10 do
- compute a new point with EGO step
- instead of running the simulator at this point, give the current minimum value

The 10 points can be given to 10 different computers

Kriging-aided optimization
Some illustrations



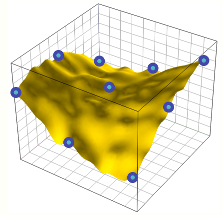


EGO.parallel.CL.nsteps

At each step
- Parallel EGO
- Evaluate the simulator at the new points (using different computers)
- Re-estimate the kriging model

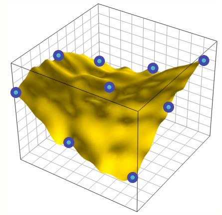
Step 1 -> red points
Step 2 -> violet points
Step 3 -> green points

Kriging-based optimization: what is implemented ?



– EI maximization with genetic algorithm `genoud` (package `rgenoud`), and analytical gradient (cst trend)
– Sequential EI maximization (EGO method)
  • The simulator runs must be done sequentially
– Multipoints EI maximization (EGO for parallel computing)
  • The simulator runs can be done with ≠ computers

Acknowledgements



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- Gregory Six, Gilles Pujol (Ecole des Mines de Saint-Etienne) for their help in R and C development.
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- Anestis Antoniadis (Université Joseph Fourier), Raphaël T. Haftka (University of Florida), Bertrand Iooss (Commissariat à l'Energie Atomique), André Journel (Stanford University), Rodolphe Le Riche (CNRS), Yann Richet (Institut de Radio-protection et Sûreté Nucléaire) for their relevant advices.