# CALIBRATION WITH DIRECT OPTIMIZATION BAYESIAN CALIBRATION



# USE DIRECT OPTIMIZATION FOR CALIBRATION

• See Tutorial 12 for direct optimization

• See Tutorial 10 for calibration

#### A. Import DOE / Direct Optimization

- B. If outputs of chosen simulator are functional variables
  - 1. Define calibration / import exeprimental data
  - 2. Define Optimization problem to change possibly the inputs bounds
    - $\rightarrow$  define optimization problem formulation / change inputs info for optimization
  - 3. Define initial inputs values
  - 4. Launch initial values to run a first simulation
    - $\rightarrow$  objective functions are built with default weights (set to 1)
  - 5. Change possible the weights in Define calibration / define objective function
- C. Define Optimization problem
  - Define objective function to be minimized



# BAYESIAN CALIBRATION [1][2][3][4]

Solver = HubOpt Bayesian calibration
Set maximal number of simulations (maxeval)
Set the size of initial DoE (nx0)
Set the number of simulations per iteration see also advanced parameters for optimizer

Export iterates of optimization

Outputs of HubOpt solver in lagun/Saved\_Optimizations/yyyy-mm-dd\_\*\*h\*\*m\*\*s

PostSample\_X.txt : sample of the posterior inputs

PostSample.txt : sample of the posterior inputs and associated objective function values

Sample.RDS : R data structure containing kriging models, posterior samples, posterior quantiles, ...



A. Import DOE from file *PostSample.txt* (see Tutorial 2.2) Preliminary exploration / parallePlot with histograms to analyze the posterior distribution





B. Export iterates  $\rightarrow$  can be used in "import DOE" functionality

- 1. To build kriging model of objective function
- 2. Explore with surrogate model (see Tutorial 4)

# Refine sampling in reduced input domain



#### B. Export iterates $\rightarrow$ can be used in "import DOE" functionality

- 1. To build kriging model of objective function
- 2. Explore with surrogate model
- 3. Refine Sampling



- B. Export iterates  $\rightarrow$  can be used in "import DOE" functionality
  - 1. To build kriging model of objective function
  - 2. Explore with surrogate model





**Inverse sampling** 

of objective function

for small values

#### B. Export iterates $\rightarrow$ can be used in "import DOE" functionality

- 1. To build kriging model of objective function
- 2. Explore with surrogate model
- 3. Refine sampling
- 4. Inverse sampling

# → display sampling and export sampling



#### C. Export iterates $\rightarrow$ can be used in "import DOE" functionality

- 1. To build kriging model of objective function
- 2. Explore with surrogate model
- 3. UQ with surrogate model (see Tutorial 5)
- 4. Fit a model to posterior input laws
  - change uncertainty definition (marginals): set all to "estimated"
  - change uncertainty definition (dependence): groups unknown
  - distribution fitting (maginals) with file *PostSample\_X.txt* : try parametric and then non-parametric
  - select distributions (marginals)



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- 1. To build kriging model of objective function
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  - select distributions (marginals)
  - distribution fitting (dependence)







C. Export iterates  $\rightarrow$  can be used in "import DOE" functionality

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- 1. To build kriging model of objective function
- 2. Explore with surrogate model

- 3. UQ with surrogate model (see Tutorial 5)
- 4. Fit a model to posterior input laws
- Step 2: Uncertainty Propagation Probability Estimation Global Propagation Choose Output to Visualize Choose UQ propagation visualization 💾 Propagate Uncertaintie Probability Distribution Function Uncertainty Propagation for OFtotal Sample Size Estimated Probability 10000 0 Density Function 160µ Gaussian with same moment 🛓 Export UQ propagatio 140u 120µ 100µ 80µ 60µ 40µ 20µ 20k 25k 30k 35k 40k 15k OFtotal Download V OF1 OF2 OF3 OFtotal Mean 5542 170.9 625.4 6318 202.3 346.9 6815 Standard deviation 6697 Median 2684 99.73 732.9 3494 Ouantile 25% 725 35.13 333.2 1388

8033

220.4

864.6

8974







[1] Da Veiga, S., Sinoquet, D. and Gervais-Couplet, V., Tests et améliorations envisagées pour l'optimisation Bayésienne, implémentation dans Condor via la plateforme HubOpt, 2010, Note technique

[2] Da Veiga, S., Nouvelle formulation de l'optimisation Bayésienne, 2011, Note technique 56\_NT\_SDV\_07\_2011

[3] Kennedy, M.C., O'Hagan, A., Bayesian calibration of computer models», 2001, J Royal Stat Soc: Series B (Stat Methodol) 63:425–464

[4] Perrin, G., Adaptive calibration of a computer code with time-series output, 2020, Reliab Eng Syst Saf, 196

