

TD 5 - Exercises in R on kriging

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Required R packages: DiceKriging, DiceView

Before beginning, fix the random seed at the value: 12345

```
> set.seed(12345)
```

We consider the 1D analytical function on [0,1]:

$$f(x) = \sin(12(x - 0.7)^2) \cos(4(x - 0.8)) + (x - 0.1)^2/2$$

a. Function

Represent (plot) the function on [0,1] by evaluating f on 1000 equi-distributed points. This will be our test sample.

b. Simple kriging

With the $km()$ function of the "DiceKriging" package, build a simple kriging on f , with a design of experiments of 5 points equi-distributed on [0,1]. Use a Gaussian covariance with hyperparameters $\mu=0$ (mean), $\sigma^2=0.5$ (variance) and $\theta=0.2$ (range).

Follow the following steps: build the design, run the function on the design points, plot the function and the design points, define the kriging parameters, build the kriging, make the kriging predictions on the test sample, compute the predictivity coefficient Q^2 , plot the results (the mean and the confidence intervals at 95%) on [0,1] (use the option « SK » of function $predict()$).

Visualize the kriging results by using the function $sectionview()$ of the "DiceView" package.

c. Kriging with unknown hyperparameters

Using a design of N=7 equi-distributed points, build:

- a simple kriging with the same method than in 2),
- a simple kriging with a Matern 3/2 covariance by not fixing the hyperparameters (let the function $km()$ estimate these hyperparameters).

Compute the Q^2 coefficient and visualize the kriging results by using the function $sectionview()$ of the "DiceView" package.

d. Adaptive design

From the last result with N=7 points, find the point x where the MSE is maximal and add this point to the design (by running the function f on it). Plot the new kriging mean and confidence interval.

Add sequentially 4 new points (by making a loop) using this adaptive design procedure. Plot the convergence curve of Q^2 in function of the sample size.

e. Quantile estimation

First, estimate the reference values of the 0.95-quantile of the function output with the test sample.

Then, from the design of N=12 points, estimate the 0.95-quantile of the function output with:

- the true function outputs,
- the kriging predictor,
- conditional simulations (function `simulate()`). Make a lot of conditional simulations and compute the quantile for each one (remark: in the `simulate()` function, put the argument "nugget.sim=1e-5"). Visualize 10 conditional simulations by superposing them to the previous kriging graph. Then compute the mean (which will be the estimator) and a 90%-confidence interval of the quantile estimator.

Interpret the results.