Gaussian Process Regression – Lab 3

Mines Saint-Étienne, Data Science, 2016 - 2017

The aim of this lab session is to implement various methods for generating designs of experiments and to be able to asses the quality of a DoE. During the whole lab, we will assume that the DoE is over $[0,1]^d$, and we will denote by n the number of design points.

A reminder of *R* basic commands can be found on my webpage.

Latin Hypercube Samples

Q 1. Write a function with parameters n and d that returns a Latin hypercube design.

Q 2. Plot a few DoE for $d = 2$ or 3. Do they fill the space?

Q 3. What can you say about the distributions of the points on the marginals?

Centroidal Voronoi Tesselations

Q 4. Write a function with parameters n and d that returns a CVT design. Feel free to use either the McQueen or the k-means algorithm.

Q 5. Plot a few DoE for $d = 2$ or 3. Do they fill the space?

Q 6. What can you say about the distributions of the points on the marginals?

Low Discrepancy Sequence

The functions `sobol` and `halton` are already implemented in the package `randtoolbox`.

Q 7. Plot a few DoE for $d = 2$ or 3. Do they fill the space?

Q 8. What can you say about the distributions of the points on the marginals?

Assessing a design

Q 9. Write a function that takes a DoE as input and that returns the value of the maximin criterion.

Q 10. Write a function that takes a DoE as input and that returns the value of the minimax criterion.

Q 11. Write a function that takes a DoE as input and that returns the value of the minimax criterion.

Q 12. Write a function that takes a DoE as input and that returns the value of the discrepancy.

Q 13. Write a function that takes a DoE as input and that returns the IMSE criterion.

Q 14. According to these, which design is the best? You can also compare your DoE with n points sampled uniformly over $[0, 1]^d$.

Optimization of DoE

Q 15. Write an exchange algorithm that can optimize a LHS design.