Bench based on analytical functions

Jean-Marc Martinez

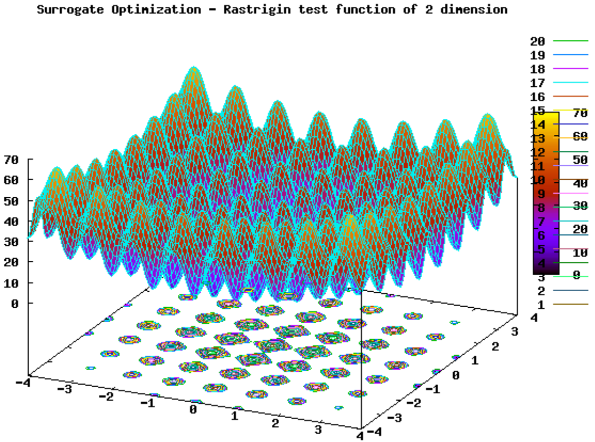
CEA DEN/DM2S Saclay

12-14/03/2008 CEA Cadarache

Introduction

- The goal is the approximation of a numerical model by a surrogate model (polynomial, neural networks, kernel functions, ...) built from a design of numerical experiment of minimal size to reduce the number of numerical evaluations.
- Analycal bench proposed here can be used to evaluate methods dealing with optimization or global sensitivity analysis problems.

Optimisation : Rastrigin test function

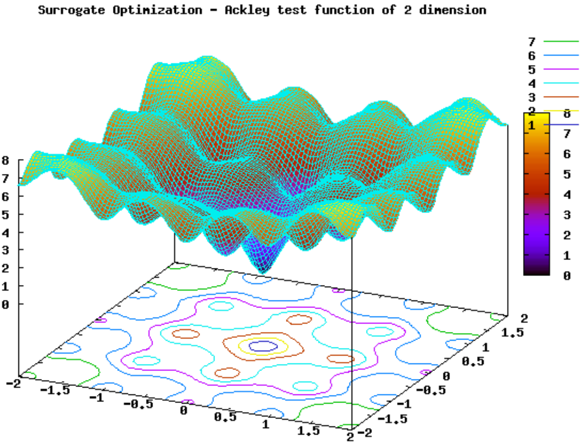


$$f(x) = 10n + \sum_{i=1}^{n}(x_i^2 - 10\cos(2\pi x_i))$$

$$f_{\min} = 0, \arg\min_{\mathbf{x}} f(\mathbf{x}) = \mathbf{0}$$

Réf. : H. Miihlenbein, M. Schomisch, and J. Born, "The parallel genetic algorithms as function optimizer", Parallel Computing, Vol 17, pp. 619-632, 1991.

Optimisation : Ackley test function



$$f(x) = 20 + e - 20e^{-0.2\sqrt{\frac{1}{n}\sum_{i=1}^{n} x_i^2}} - e^{\frac{1}{n}\sum_{i=1}^{n}\cos(2\pi x_i)}$$

$$f_{\min} = 0, \arg\min_{\mathbf{x}} f(\mathbf{x}) = \mathbf{0}$$

Réf. : T. Back, "Evolutionary algorithms in theory and practice", Oxford University Press, 1996.

Sensitivity analysis - Ishigami function

$$f(\mathbf{x}) = \sin(x_1) + a\sin^2(x_2) + bx_3^4\sin(x_1)$$

Random variables x_1, x_2, x_3 independent, uniform in $[-\pi, +\pi]$.

$$\texttt{Mean} = \frac{a}{2}, \quad \texttt{Variance} = \frac{a^2}{8} + b\frac{\pi^4}{5} + b^2\frac{\pi^8}{18} + \frac{1}{2}$$

The fraction of variance $\sigma^2_{i_1,i_2\ldots}$ due to the interaction of variables $i_1, i_2 \ldots$:

$$\sigma_1^2 = \frac{1}{2} + b\frac{\pi^4}{5} + b^2\frac{\pi^8}{50}$$

$$\sigma_2^2 = \frac{a^2}{8}$$

$$\sigma_{13}^2 = \frac{b^2\pi^8}{18} - \frac{b^2\pi^8}{50}$$

other terms are zero $\Rightarrow \texttt{Variance}(f) = \sigma_1^2 + \sigma_2^2 + \sigma_{13}^2$.

Réf. : T. Ishigami, T. Homma, An importance qualification technique in uncertainty analysis for computer models. Proc. of the Isuma '90, First Int. Symp. on Uncertainty Modelling and Analysis, Univ. of Mariland.

Sensitivity analysis - gSobol test function

$$f(\mathbf{x}) = \prod_{i=1}^{d} g_i(x_i) \texttt{ avec } g_i(x_i) = \frac{|4x_i - 2| + a_i}{1 + a_i}, a_i \geq 0$$

Random variables x_i independent, uniforme in $[0, 1]$. And the variable x_i are all the more influential than its parameter a_i is small.

$$\texttt{Mean} = 1, \texttt{ Variance} = \prod_{i=1}^{d}[1 + \frac{1}{3(1 + a_i)^2}] - 1$$

The fraction of the variance $\sigma^2_{i_1, i_2 \ldots}$ due to the interaction of variables $i_1, i_2 \ldots$:

$$\sigma^2_{i_1, i_2, \ldots} = \prod_{i = i_1, i_2, \ldots} \frac{1}{3(1 + a_i)^2}$$

A choice of parameters a_i can be $a_i = (i - 1)/2$.

Réf. : A. Saltelli, I.M. Sobol, About the use of rank transformation in sensitivity analysis of model output. Reliab. Eng. Syst. Safety 1995 ;50(N3) :225-239.

Introduction of the new analytical bench

A generalisation of the gSobol bench $f : [0,1]^d \rightarrow R$ based on a set of basis functions $g_{i=1,\ldots,d} : [0,1] \rightarrow R$:

$$f(\mathbf{x}) = \prod_{i=1}^{d} [1 + \alpha_i g_i(x_i)]$$

with zero mean and unit variance of g_i :

$$\begin{aligned} < g_i > &= \int_0^1 g_i(x_i) dx_i = 0 \\ < g_i^2 > &= \int_0^1 g_i(x_i)^2 dx_i = 1 \end{aligned}$$

We deduce teh mean, the variance and the indices of sensitivity of $f(x_1, \ldots, x_d)$:

$$\begin{aligned} < f > &= 1 \\ < f^2 > &= \prod_{i=1}^{d} (1 + \alpha_i^2) \\ \sigma^2_{i_1, i_2 \ldots, i_r} &= \prod_{j=1}^{r} \alpha^2_{i_j} \end{aligned}$$

Basis function based on Dirichlet Kernel

The Dirichlet kernel of level n is :

$$D_n(x) = \frac{\sin((2n+1)\pi x)}{\sin(\pi x)}$$

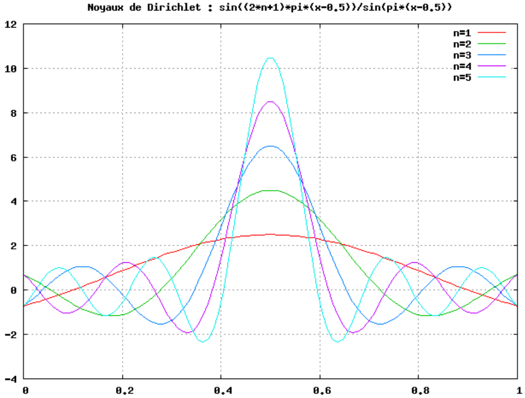
for $x \in [0, 1]$, periodic $T = 1$ with properties :

$$\begin{aligned} \int_0^1 D_n(x)dx &= 1 \\ \int_0^1 D_n^2(x)dx &= 2n+1 \end{aligned}$$

The basis functions g_n are transformed to a set of basis function h_n with zero mean and unit variance :

$$h_n(x) = \frac{D_n(x) - 1}{\sqrt{2n}}$$

Dirichlet Kernel - Example $n = 1, \dots, 5$

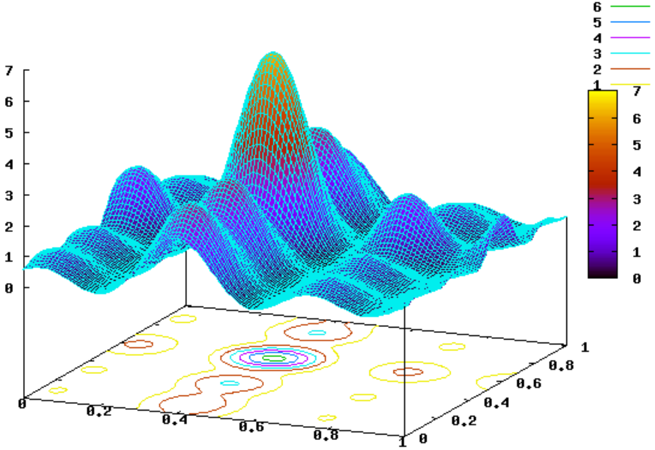


Remarque :

1. Oscillations and many extrema according to the dimension. So this bench can be used to evaluate the capability of optimization algorithms to deal with many local mimima.
2. The decomposition of ANOVA is known explicitly. So this bench is also adapted to evaluate global sensitivity analysis method.

Example - 1

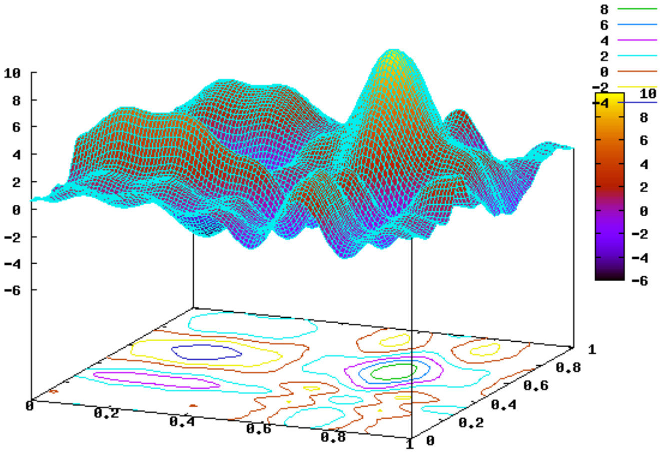
$$h_n(x) = [\frac{\sin((2n+1)\pi x)}{\sin(\pi x)} - 1]\frac{1}{\sqrt{2n}}$$
$$f(x_1, x_2) = [1 + 0.8h_3(x_1 - 0.4)][1. + 0.4h_4(x_2 - 0.6)]$$



$$\texttt{Mean}(f) = 1$$
$$\texttt{Var}(f) = (\sigma_1^2 = 0.8^2) + (\sigma_2^2 = 0.4^2) + (\sigma_{12}^2 = 0.8^2 \times 0.4^2) = 0.9024$$

Example - 2

$$f(x_1, x_2) = 1 + h_5(x_1 - 0.7) + 0.5h_8(x_2 - 0.3) + 2h_1(x_1 + 0.3)h_2(x_2 - 0.6)$$



$$\texttt{Mean}(f) = 1$$

$$\texttt{Var}(f) = (\sigma_1^2 = 1^2) + (\sigma_2^2 = 0.5^2) + (\sigma_{12}^2 = 2^2) = 5.25$$

Analytical bench based on Dirichlet Kernel

Function $f : [0,1]^d \rightarrow R$ for $d = 1, 2, \ldots$:

$$f(\mathbf{x}) = \prod_{k=1}^{d} [1. + \frac{(-1)^k}{k} h_k(x_k - \frac{2k-1}{2d})]$$

$$\texttt{with} \quad h_k(u) = \frac{1}{\sqrt{2k}} [\frac{\sin((2k+1)\pi u)}{\sin(\pi u)} - 1.]$$

Analytical formulae of the mean $= 1$, the variance $= \prod_{k=1}^{d}(1 + k^{-2}) - 1$ and the ANOVA functionnal decomposition from $\sigma^2_{i_1, i_2, \ldots} = \prod_{k=i_1, i_2, \ldots} k^{-2}$: