Analytical results for tests

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Abstract

We summarise the analytical results used in the tests for scikit-monaco.

Following Numerical Recipes, we calculate the standard error in the Monte-Carlo integration of the function f as:

$$\operatorname{Err}_{N}(f) = \Omega \sqrt{\frac{\langle f^{2} \rangle - \langle f \rangle^{2}}{N}}$$
 (1)

where N is the number of points and $\langle g \rangle = \int_{\Omega} g(x) dx$, where Ω is the volume being sampled during the integration and x denotes all the variables of integration.

1 Constant function

Let f(x) = 1. Then, $\langle f \rangle = \Omega$, where Ω is the volume of integration. $\langle f^2 \rangle = 1$, such that $\text{Err}_N = 0$ for all N > 0.

2 Product function

Let $f(x) = \prod_{i=1}^{d} x_i$, where d is the dimensionality of the integration. Thus, if d = 2, f(x,y) = xy. We consider the d-dimensional hypercube with upper and lower limit b and a, respectively, such that each $a \le x_i \le b$.

$$\langle f \rangle = \int \cdots \int_a^b \prod_i x_i dx_i = \left(\frac{b^2 - a^2}{2}\right)^d$$
 (2)

$$\langle f^2 \rangle = \int \cdots \int_a^b \prod_i x_i^2 dx_i = \left(\frac{b^3 - a^3}{3}\right)^d$$
 (3)

If a=0 and b=1, we have $\langle f \rangle = 1/2^d$ and $\langle f^2 \rangle = 1/3^d$. Then, $\mathrm{Err}_N(f) = \frac{\sqrt{1/3^d-1/4^d}}{N}$.

3 Gaussian

Let $f(x) = \prod_i^d \exp(-\beta^2 x_i^2)$. Again, we consider the hypercube such that $a \le x_i \le b$ for each i. Then:

$$\langle f \rangle = \frac{\sqrt{\pi}}{2\beta} (\operatorname{erf}(\beta b) - \operatorname{erf}(\beta a))$$
 (4)

$$\langle f \rangle = \frac{\sqrt{\pi}}{2\beta} (\operatorname{erf}(\beta b) - \operatorname{erf}(\beta a)$$

$$\langle f^2 \rangle = \frac{\sqrt{\pi/2}}{2\beta} (\operatorname{erf}(\sqrt{2}\beta b) - \operatorname{erf}(\sqrt{2}\beta a)$$
(5)