

Analytical results for tests

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Abstract

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

1 Uniform Sampling MC

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

$$\text{Err}_N(f) = \Omega \sqrt{\frac{\langle f^2 \rangle - \langle f \rangle^2}{N}} \quad (1)$$

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.

1.1 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 $N > 0$.

1.2 Product function

Let $f(x) = \prod_i^d x_i$, 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 $a \leq x_i \leq b$.

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

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

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

1.3 Gaussian

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

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

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

2 MISER Monte-Carlo

Testing that the MISER algorithm returns the correct value (within error bars) is trivial, provided the integral can be calculated by some “trusted” means.

Testing that the MISER algorithm returns the correct error is more difficult. Unlike for simple uniform sampling case, there is no easy formula for the calculation of the error. What we can do, though, is make sure that the error predicted is correct, *on average*.

Let’s assume that we are estimating an integral I . Let I^* denote the correct, analytical value of I .

Pre test

$\langle I \rangle$ is the average of all the MC calls.

$\langle \sigma \rangle$ is the average of the errors.

S_I is the standard error in $I - I^*$.

$$\langle I \rangle = I^* \pm \langle \sigma \rangle / \sqrt{N} \quad (6)$$

$$\langle \sigma \rangle = S_I \pm S_I / \sqrt{2(N-1)} \quad (7)$$

Then, if those tests pass, extract:

$\langle \sigma \rangle$: allowable error.

$\langle S_\sigma \rangle$: allowable error in error.