

Lab 5: Random Processes

Due date: Wednesday October 2nd

Goals: We want to see how we can use Monte Carlo to solve a difficult problem in scientific computing, locating the global extrema of a function. We will only consider functions of one independent variable.

Using Monte Carlo for Optimization

We consider the 1D optimization problem of finding a point x in a given domain $D \subset \mathbb{R}^1$ where the function $f(x)$ attains its global minimum. If we can solve this problem, then we can also find its global maximum by finding the global minimum of $-f(x)$. The difficulty with optimization is that the function may have several local minima. Most minimization algorithms can be “trapped by a local minimum. We are going to see how we can develop an algorithm which uses Monte Carlo sampling to estimate the location of the global minimum.

It would be fair to ask why we bother randomizing this algorithm. Why not just divide up the region into say 500 equally spaced points; then you will guarantee that you sample all the space just as well (even better, because you know there cant be any large gaps). There are several reasons to use pseudorandom sequences to sample the domain. One of the reasons is that in two or three dimensions we may have a very complicated geometry. Another reason is that when we go to higher dimensions, i.e., a function of several variables, then our 500 points in one dimension becomes 500^d in d dimensions. It should be noted that there are much better sampling methods than Monte Carlo and those should be used in practice. Assume that we want to find the global minimum of $f(x)$ on $[a, b]$. We want to do this in as few function evaluations (i.e., evaluation of f at a point) as possible. Our first strategy will be to sample $[a, b]$ with n points $\{x_i^0\}_{i=1}^n$ using Monte Carlo and evaluate the function at each of those points. As we sample each point we keep track of which x value has the smallest function value. From all the sampling points we choose the location where $f(x)$ takes on its minimum value and that will be our answer. This algorithm will converge as $n \rightarrow \infty$. We will consider modifications to this algorithm in the exercises. We consider three functions, each more difficult than the previous for locating its minimum.

$$f_1(x) = |\cos \Pi x| \quad \text{on } [0, 1]$$

$$f_2(x) = \cos(x) + 5 \cos(1.6x) + 2 \cos(2.0x) + 5 \cos(4.5x) + 7 \cos(9.0x) \quad \text{on } [2, 7]$$

$$f_3(x) = -[\operatorname{sech}^2(10.0(x - 0.2)) + \operatorname{sech}^2(100.0(x - 0.4)) + \operatorname{sech}^2(1000.0(x - 0.6))] \quad \text{on } [0, 1]$$

To compare codes, please use a seed of 56789 for easier grading.

1. Plot the three functions $f_i(x)$, $i = 1, 3$ on their domains. From the graphs estimate the location of the global minimum and all local minimum of the functions.
2. Write a code to implement our sampling algorithm for locating a global minimum of a function. Your code should have the following structure:
 - Input: n the number of sampling points
 - x_l, x_r the endpoints of the interval where the function is defined (so you can map the random point to that interval)

- Output: the location and value of the minimum that the algorithm found.

Make sure your code is working properly by finding the local minimum of our “easy function” $f_1(x)$. For $f_1(x)$ we know the exact location of its global minimum. Make a table of n and the error in the location of the minimum as n increases. For example, $n = 25, 50, 100, 200, 400, 800, 1600$.

3. If we have a good approximation to the location of the global minimum, it probably doesn't make sense to keep sampling in the entire domain; you saw in #2 that sometimes doubling the number of points didn't improve the accuracy. A better strategy might be that once we have an approximation then we only sample around that approximation to zoom in on a more accurate approximation to the location of the minimum. Of course, if we have too few random points in our initial sweep and have an erroneous location, then zooming in is not going to help us; that is why this approach is not guaranteed to converge unlike the brute force approach in #2. After we have located our approximation, say x_1^* to the local minimum by generating n random points, then we will sample in the interval $[x_1^* - \delta, x_1^* + \delta]$ using say $n_1 = n/2$ points (of course you can change this) to get points $\{x_{1i}^*\}_{i=1}^{n_1}$ and we can determine our second approximation to the global minimum x by evaluating $f(x)$ at each of these random points. The procedure can be repeated. At the last step, we choose the location where $f(x)$ takes on its smallest value; this is our approximation to x^* . Remember that the algorithm is not guaranteed to converge to a global minimum but if our initial sampling is good enough, we should be able to capture the minimum for most functions. Modify your code to input n_{zoom} , the number of zooms we will use; if $n_{zoom} = 0$ you should have the algorithm from #2. We want to run the code for f_2, f_3 and compare the number of function evaluations required as a function of n_{zoom} to find the global minimum and its location to a desired accuracy. You should choose the calculations which best support your conclusion.
4. (Optional, extra credit) Can you think of a way to modify the algorithm (besides taking n larger) to ensure a better chance of your initial sweep capturing the location of the global minimum? If so, discuss this and implement and compare, if time allows. If you don't have time for this now, you could choose it as a final project (and expand it a bit using other sampling methods).