

Computational Physics

Exercise 2 : Partial Differential Equations

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Abstract

1 Generating random numbers with non uniform distributions

1.1 Direct Sampling

For later purposes we want to use sequences of random numbers not necessarily following a uniform distribution (i.e. probabilities are not the same for each value. If our variable can only take a few finite values we can imagine that some probabilities will be non zero. However if we are dealing with a continuous variable $x \in [a, b]$ we can see that any probability will go to zero as there are in principle¹ an infinite amount of possible values x can take. In this case we need to consider the cumulative distribution function $F[1]$

$$F(x) = \int_a^x g(x)dx \quad (1.1)$$

Where $g(x) \geq 0$ is the probability distribution function. F represents the probability of getting a value between a and x and because of normalization we have $F(b) - F(a) = 1$. For $x \in [a, b]$ such that $F(x)$ is defined as in Equation 1.1, the fundamental theorem of sampling applies[2]

$$\int_0^1 e^{iFt} g_F(F) dF = \int_a^b e^{iF(x)t} g(x) dx \quad (1.2)$$

An by using the fact that $dF = g(x)dx$ we see that $g_F(F) = 1$ for any $g(x)$. In other words, for any PDF, the cumulative distribution function F will always be uniform and the integral is therefore giving us a link between a uniform distribution and a non-uniform one.

This is of great importance since we want to generate random numbers following non-uniform distributions $g(x)$ using uniform random generators.

1.2 Algebraical inversion

The first method to generate random numbers following a non-uniform distribution from a uniform one is to start again from Equation 1.1. As previously shown the values of F will follow a uniform distribution. Therefore we can

associate F to the values which are going to be returned by our uniform generator. Since x follows the distribution $g(x)$ we are interested in we want to find an expression relating x to F .

This can be done algebraically if F is invertible. Indeed if $F(x)$ is an invertible analytical function we have:

$$x(F) = F^{-1} \quad (1.3)$$

The values of x will follow the distribution $g(x)$ since this expression was derived from Equation 1.1. Hence if $F(x)$ can be expressed analytically from the integral we can find an expression of x as a function of F such that it follows the distribution $g(x)$.

1.3 Rejection Technique

The second method has the advantage it can be used when there is no algebraical inversion possible. The idea of rejection technique[3] is to consider a new function $f(x)$ such that $\forall x \in [a, b], f(x) > g(x)$ such as, for instance, the function with constant value g_{max} . Instead of choosing only one uniform random number, we choose two of them:

- x in the range $[a, b]$
- y in the range $[0, 1]$

These two values can be seen as the coordinates (x, y) of a point. If we plot the FDP we know it will always lie in the rectangle defined by $[a, b] \times [0, 1]$. We can choose to cut this rectangle in vertical bins. If we do so, each point (x, y) randomly chosen will lie in one of these bins. More importantly if we repeat the process many times, the points will fill the space under and above the curve defined by $g(x)$ in each bin. In particular this implies that the proportion of points under the curve will be related to the mean value of g in the bin. This is true for bins of any size and therefore it must be true in the limit of the size going to 0. In this case we have:

$$\frac{N_{under}}{N_{above}} = g(x) \quad (1.4)$$

¹This is true in the mathematical sense but technically wrong since computers will always be precise up to a certain digit

References

- [1] William R. Gibbs, 1994, Computation in Modern Physics, 29
- [2] William R. Gibbs, 1994, Computation in Modern Physics, 30
- [3] William R. Gibbs, 1994, Computation in Modern Physics, 38-39