University of Cape Town - Department of Physics
Honours Computational Physics

TOPIC 1 - BASIC MONTE CARLO : SAMPLING - METROPOLIS METHOD

This worksheet accompanies the EJS simulation `BasicMC_No7_SamplingMetropolis.jar`

The challenge: We need to sample according to a distribution $p(x)$ with $x \in [a, b]$ but have access just to a uniform random generator.

As already seen, the rejection, transformation and combination analytic-rejection methods provide three possibilities. Another option is the Metropolis method that produces a random walk of points $\{x_0, x_1, x_2, \dots\}$ that asymptotically approaches the distribution $p(x)$ after many steps. The random walk is defined by a transition probability $T(x_i \to x_j)$ from one value x_i to another x_j. It is sufficient (but not necessary) for the transition probability to satisfy the 'detailed balance' condition:

$$p(x_i)\, T(x_i \to x_j) = p(x_j)\, T(x_j \to x_i).$$

Many transition probabilities can be constructed that satisfy this condition, but the choice made in the Metropolis method is,

$$T(x_i \to x_j) = \min\left[1, \frac{p(x_j)}{p(x_i)}\right].$$

We use the **'Metropolis method'** to generate x_{i+1} from x_i in the following manner:

- Choose a trial position $x_{\text{trial}} = x_i + \delta_i$, where δ_i is drawn uniformly from the interval $[-\Delta, +\Delta]$
- Calculate $w = p(x_{\text{trial}})/p(x_i)$
- If $w \geq 1$, accept the change and let $x_{i+1} = x_{\text{trial}}$
- If $w < 1$, generate a random r uniformly drawn from the interval $[0, 1)$
- If $r \leq w$, accept the change and let $x_{i+1} = x_{\text{trial}}$
- If the trial position is not accepted, then let $x_{i+1} = x_i$

The best choice of starting point for the walk is at the maximum of $p(x)$. Special care needs to be taken when choosing the parameter Δ. If Δ is too large, only a small percentage of trial steps is accepted. If it is too small, a large percentage is accepted, but it takes a great deal of time (possibly infinite time) for the entire domain to be sampled. An ideal choice leads to between $\frac{1}{3}$ and $\frac{1}{2}$ of the trial steps being accepted.

One downside of this method is that nearby points are often highly correlated. One should therefore not use every generated point, but rather select points separated by some constant l. Furthermore, the first m steps should be ignored to remove the dependence on initial conditions. Obviously, l and m depend on the probability distribution $p(x)$, the parameter Δ and the starting point.

Questions:

1. To investigate correlations, one can calculate the auto-correlation function $C(k)$ defined by

$$C(k) = \frac{\langle x_{i+k} x_i \rangle - \langle x_i \rangle^2}{\langle x_i^2 \rangle - \langle x_i \rangle^2},$$

where $\langle \cdots \rangle$ denotes an average over the sample.

   (a) What is the value of $C(k = 0)$?

   (b) If x_i were completely random (i.e. uncorrelated), what value would you expect for $C(k \neq 0)$?

2. Use the associated EJS simulation to investigate the use of the Metropolis sampling method to generate x according to:

   i) $p(x) = A \exp(3 \cos x)$, with $x \in [-\pi, \pi]$, and

   ii) $p(x) = B \left\{ \exp\left[-(x-5)^2\right] + 2 \exp\left[-\frac{1}{2}(x-12)^2\right] \right\}$, with $x \in [0, +\infty)$.

   - Consider the effect of your choice of starting position and parameter Δ.
   - Determine the qualitative dependence of the acceptance rate and the equilibration time on Δ (one possible criterion for equilibrium is to check that the sample's $\langle x \rangle$ and σ, the square-root of the variance, match those of the distribution).
   - Investigate the correlation between near neighbours and suggest an optimal choice of l.