Lorenzo Vergari - Homework 5 - NE 255

1. **(30 points)**

(a) (10 points) Consider the PDF:

$$\mathbf{p(x) = 3x^2 + x}$$

on the interval 0 < x < a. What value of a will make p(x) a valid PDF?

In order for p(x) to be a valid PDF, it must be non-negative in its domain and its integral must be unitary. Therefore:

$$p(x) > 0 \rightarrow x > 0 \; OR \; x < -\frac{1}{3}$$

$$\int_0^a p(x)dx = \left[x^3 + \frac{x^2}{2}\right]_0^a = a^3 + \frac{a^2}{2} == 1 \rightarrow a = 0.85809433$$

(b) (10 points) Consider the bounding function:

–

$$\mathbf{g(x) = 5\sqrt{x}.}$$

What is the efficiency of rejection sampling using this bounding function for the above PDF? Use limits of 0 < x < a, where a is the value calculated above.

The efficiency of rejection sampling is defined as:

$$Efficiency = \frac{\int_0^a p(x)dx}{\int_0^a g(x)dx}$$

Therefore, in our case, the numerator is equal to 1 and the denominator is:

$$\int_0^a g(x)dx = \left[5 * \frac{2}{3} * x^{\frac{3}{2}}\right]_0^a = \frac{10}{3}a^{\frac{3}{2}} = 2.64960597$$

Hence, the efficiency is equal to $\frac{1}{2.64960597} = 0.37741461 \approx 37.7\%$

(c) (10 points) When would we use rejection sampling? Give an example of a PDF and corresponding CDF that would require the use of rejection sampling.

Rejection sampling is an appropriate choice when we don't have a CDF that can be easily inverted (or inverted at all), preventing us from sampling from its ordinate [0,1] interval and retrieving the abscissa from that.
An example is the following:

$$p(x) = Ae^{-x^4}\ in\ (0,1)$$
$$(A = 1.18366\ for\ normalization)$$

In this case, we can define the CDF:

$$CDF(x) = \int_0^x p(t)dt = A\int_0^x e^{-\frac{t}{4}}\,dt$$

However, there is no easy way to have an analytical form of this CDF, so it is much simpler to just use rejection sampling.

2. (30 points)

(a) (15 points) When using analog Monte Carlo methods, how can we improve the accuracy of our answers? How can we improve the precision? For the latter, include mathematical reasoning (equations) in your response.

Accuracy is related to how well our result matches the true value of the quantity we are simulating. It is affected by the mathematical and physical model we are using to depict the phenomenon, as in the case of approximations and systematic errors included in our equations/ formula. It is also due to systematic errors of the instrument/ code and of the user. We can improve accuracy by developing a better mathematical and physical model and troubleshooting systematic errors of our computer. For example, if in one point of the MC code we approximate a very complex CDF describing a cross sections with a simplified version (e.g. a Taylor expansion), we will lose accuracy. Conversely, using the non-approximated CDF would then improve our accuracy.

Precision is related to degree to which repeated simulations of the same run give the same result. We can increase precision by reducing the *spread* of such results, by increasing the number of histories, enlarging the number of samples in each bin of our histograms, using variance reduction techniques. Indeed, we can relate to such *spread* by means of the relative error, defined as:

$$R = \frac{S_{\bar{x}}}{\bar{x}} = \frac{1}{\sqrt{N}}\frac{\mathrm{S_x}}{\bar{x}}$$

Here, $\bar{x}$ is the sample mean, S_x is the standard deviation and $S_{\bar{x}}$ is the standard deviation of the mean. Therefore, we reduce the spread around the sample mean by increasing the number of points N, i.e. by increasing the number of histories or including more points within the bin.

(b) (15 points) What is the purpose of using variance reduction in Monte Carlo calculations? What precautions should be taken when using variance reduction methods?

Variance reduction techniques are several methods aimed at increasing the precision of a MC method in distinct ways. Their main objective is to increase precision in some regions of the phase space we are interested by tracking only or mostly particles within these regions, altering the physical/ mathematical method but still maintaining a "fair game". The purpose of VR techniques is to increase precision more than just increasing runtime would do (as showed before, $R \sim 1/\sqrt{N} \sim 1/\sqrt{T}$). Therefore, the effectiveness is measured through a Figure Of Merit that accounts for both precision and run time ($FOM = 1/R^2T$).

By altering the "analog" physical model governing the simulation, VR methods can lead to incorrect answer without us noticing. Therefore, a few precautions must be taken.
We need to make sure that we are preserving the "fair game" and we are not over-weighting or double counting some of the contributions, thus inserting a bias towards certain phenomena.
At the same time, when we use truncation methods, we need to be sure that the parts of the problem we are neglecting do not actually count towards the result

3. **(40 points) Write a Monte Carlo code to track particles and tally behavior of interest. Use the following parameters:**
   - **(b) 1-D space, from x = 0cm to x = 10cm**
   - **(c) Particles born uniformly randomly anywhere in region 1 (see below table)**
   - **(d) Isotropic scattering, either in the positive or negative direction**
   - **(e) Monoenergetic particles**
   - **(f) All particles are born with a weight of 1; this is not changed**
   - **(g) 100,000 histories**

	Region 1	**Region 2**
Boundaries [cm]	**[0,5)**	**[5,10]**
$\Sigma s[cm^{-1}]$	**45**	**8**
$\Sigma \gamma[cm^{-1}]$	**4**	**50**

How many particles undergo capture reactions in region 2? How many forward scattering events occur in region 1? Values can be reported without error or variance here since the requested values are exact counts.

See attached matlab code. Note: Void Boundary Conditions are assumed at the boundaries

- Capture reactions in region 2:

```
>> Tally_capture

Tally_capture = 1134
```

- Forward scattering in region 1:

```
>> Tally_FWS

Tally_FWS =

    546859
```