# Computational Physics Exercise 3: Random Numbers and Monte Carlo

Paul Hayes
*Level 6 Computational Physics, School of Physics, University of Bristol.*
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## MONTE-CARLO METHODS

Monte-Carlo methods are a form of computational algorithm that can give approximate numerical solutions to a range of problems, through the application of repeated, randomised experiments. Using Monte-Carlo methods, over a large enough set of randomly generated samples, the average result will tend to the expected value, with increasing accuracy [1].

## I. RANDOM NUMBERS IN A DISTRIBUTION

A coordinate transform may be used to convert generated random numbers in a normalised uniform distribution, $P(x)$, between $x_o$ and $x_{gen}$, to a non-uniform one, $P'(x')$, between $x'_o$ and $x'_{req}$. If the cumulative distributions over the limits are equal, this may be written as,

$$\int_{x'_0}^{x'_{req}} P'(x)dx' = \int_{x_o}^{x_{gen}} P(x)dx. \tag{1}$$

If $P(x)$ has limits between 0 and 1, the integral on the right hand side is simply $x_{gen}$. Let the left hand integral be,

$$\int_{x'_0}^{x'_{req}} P'(x)dx' = Q(x'_{req}), \tag{2}$$

then using these in Eq.1 and inverting gives,

$$x'_{req} = Q^{-1}(x_{gen}). \tag{3}$$

If finding and inverting the definite integral Q is difficult, a ”reject-accept” method may be used. First, a random number $x'$ is generated in a required range. A second random number $y'$ is then generated within a uniform distribution between 0 and $y_{max}$, where $y_{max}$ is a any value equal to or larger than the maximum value of $P'$. If $y' < P'(x')$ then the generated $x'$ is accepted. Anything outside this condition is rejected.

### A. Method

These two methods are used to generate random angles, $0 < \theta < \pi$, in a distribution proportional to sin$\theta$.

Using the analytical method, in Eq.2, the probability density function $P'(x')$ is set to be sin$\theta$, where $\theta$ is over the required range. Following the steps of integrating and inverting this function, gives,

$$\theta_{req} = arccos(x_{gen}). \tag{4}$$

Thus, generating random values in a uniform distribution, where $-1 < x_{gen} < 1$, gives values of $\theta$ in the required range of $0 < \theta < \pi$.

In the ”reject-accept” method, random values of $\theta$ are generated in the required range in a uniform distribution. The value, $y'_{max}$, is calculated from the maximum value of the probability density function, sin$\theta$. A further uniformly distributed set of values in the range $0 < y' < y'_{max}$ is generated. All $\theta$ such that, $y' < sin(\theta)$, are accepted and are therefore in a sin$\theta$ distribution, where $0 < \theta < \pi$.

### B. Results and Discussion

#### Comparison of the Analytical and Reject-Accept methods

Using a high sample size of 1x$10^7$, the distribution of angles seen in FIG.1 and FIG.2 show that both the Analytical and Reject-Accept methods closely approximate a sine distribution, as required. Indeed, P-values at this sample size from a Chi-Squared test are $P = 4.24$x$10^{-113}$ and $P = 4.21$x$10^{-112}$ for the Analytical and Reject-Accept methods respectively, showing no significant different between expect and observed values.

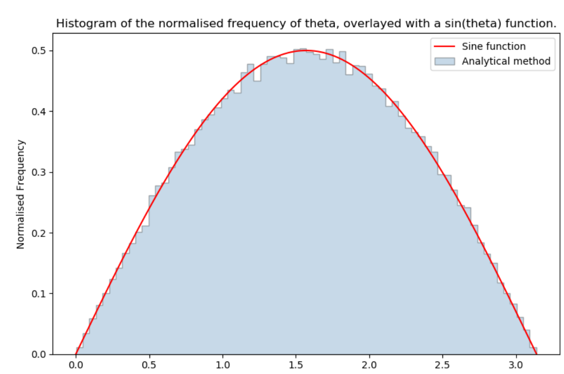


FIG. 1. Histogram of the normalised frequency of theta using the Analytical method, with a sine function overlayed.

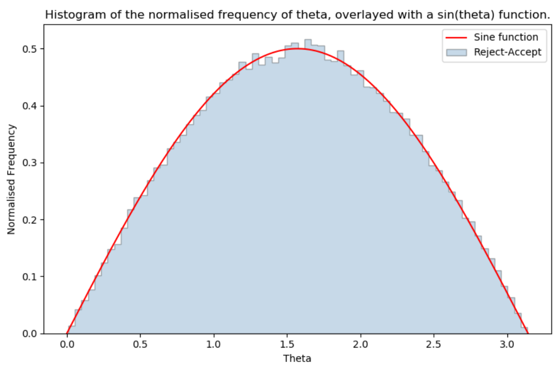


FIG. 2. Histogram of the normalised frequency of theta using the Reject-accept method, with a sine function overlayed.

The variation in absolute error between the sine function and the distributions, as a function of sample size is seen in FIG.3. The absolute error follows a $\frac{1}{\sqrt{N}}$ trend, which is in agreement with the expected value [2]. There is no difference seen between the absolute error in either method.

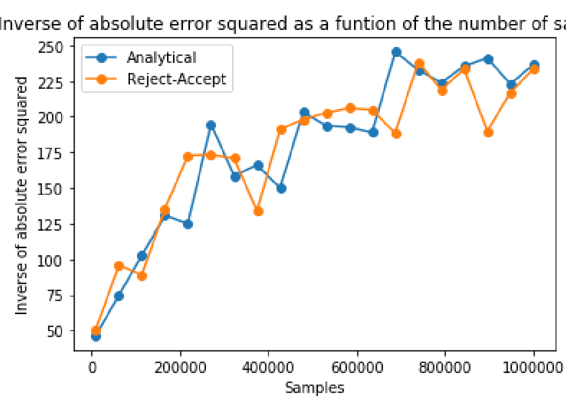


FIG. 3. Inverse of the absolute error squared as a function of the number of samples for the two methods.

The computational time to produce the sine distribution for each method, over a range of sample sizes is seen in FIG.4. There is a clear linear relationship. This is expected as N only has $\mathcal{O}(N)$ errors in the code. The reject-accept method is on average 126% slower than the analytical method. This is to be expected as the reject-accept method, as suggested by its name, has to reject a large proportion of its samples that do not fit a sine distribution. Whereas the analytical method uses the total range of random samples.

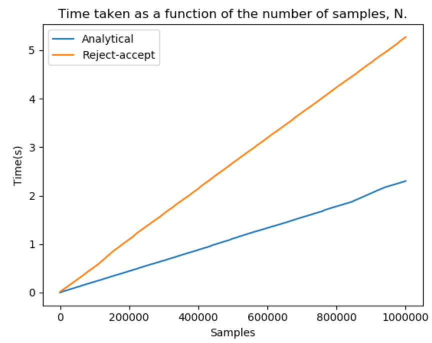


FIG. 4. Time to compute the distribution as a function of the number of samples, N.

## II. SIMULATIONS

Radioactivity is an inherently random process [3]. As such, experimental data can be simulated well using Monte-Carlo methods.

A beam of unstable nuclei, with mean lifetime of 520 $\mu$s, is injected at 2000m/s travelling in the z-axis. The decay product is a gamma ray which will be emitted isotropically. At a distance of 2m from the injection point, a detector array is set up with x and y resolutions of 0.1m and 0.3m respectively.

### A. Method

The activity of the nuclei as a function of time obeys,

$$\frac{A}{A_o} = e^{\frac{-t}{\tau}}. \tag{5}$$

By setting the initial activity, $A_o$ to be 1 and the time $t = v\mathrm{x}z$, where v is the velocity of the nuclei and z is the distance from the source to decay point, this can be written as a probability density function, with $\tau$=520$\mu$m$s^{-1}$:

$$P(z) = e^{-1.04z}. \tag{6}$$

To model the isotropic emission of the gamma ray, random number generators are used to give the angles $\theta$ and $\phi$ of emission, 0< $\theta < \pi$ and 0< $\phi < 2\pi$. These angles are used in spherical polar coordinates, with the radius of the sphere set to be r=(2-z)/cos($\theta$). The coordinates (x,y) may then be calculated for a given emission point from:

$$x = rsin(\theta)cos(\phi), y = rsin(\theta)sin(\phi). \tag{7}$$

The probability density function in EQ.6 is used in the reject-accept method with the range 0 < z < 2. This gives a distribution of decay points of the nuclei.

Care needs to be taken when generating the random angles $\theta$ and $\phi$. A uniformly distributed set of angles for $\theta$ will not give an evenly distributed set of coordinates on a given sphere.

This is because there will be a greater separation of points on the circumference at z=0, due to the nature of a sphere. Therefore, the Analytical method from task 1 is used to distribute the values evenly over the sphere. This is seen in FIG.5.

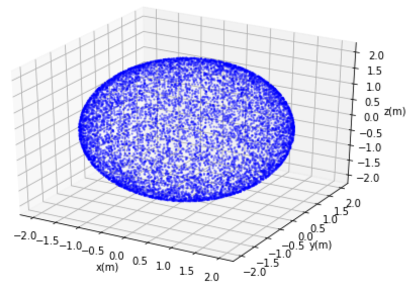


FIG. 5. Spherical distribution of points, with the analytical method used to find the set $\theta$.

### B. Results and Discussion

The distribution of 2D coordinates at which a sample of decayed gamma rays are detected is seen in FIG.6. Due to the nature of the exponential decay of the activity, seen in FIG.6, the distribution in the detection points will be centered at (x=0,y=0). and will fall off with distance from centre. This is what is seen in FIG.7.

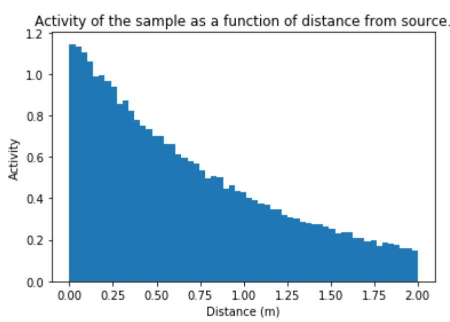


FIG. 6. Activity of the sample as a function of distance from source.

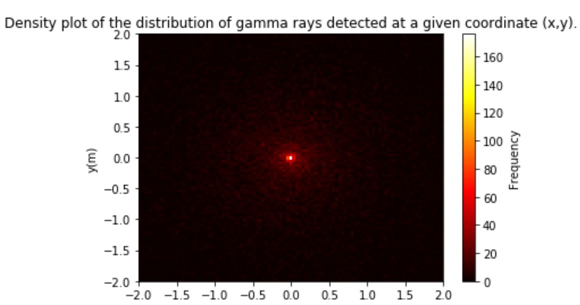


FIG. 7. 2D histogram of the frequency of detected gamma rays at given coordinate (x,y).

If the particle was stationary at z=0, the distribution of coordinates would follow an inverse square law, as a direct consequence of the isotropic emission of gamma rays. FIG.8 shows the inverse of the square root of the frequency of detection as a function of position for the moving nuclei. It is clear that at the central point it does not follow a straight line, but increases sharply. This is because the closer the gamma ray is to the detector, the higher the chance of it being detected nearer the centre.

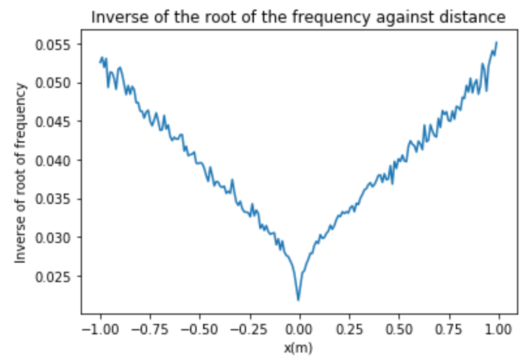


FIG. 8. Inverse of the root of the frequency against distance from centre.

The detector has a resolution of 0.1m in the x and 0.3 in the y directions. To account for this, normal distributions, with standard deviations of $\sigma = \frac{resolution}{3}$ are used, with a $3\sigma$ confidence limit and mean of the x and y coordinates. This smears each detected coordinate. This is seen in FIG.9. As expected, there is a broadening of detected coordinates around (x=0,y=0) in both axis, but greater in y.

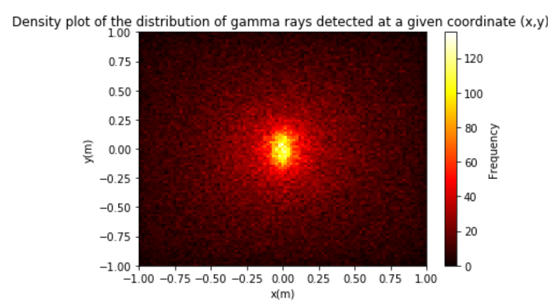


FIG. 9. Smeared distribution of x and y coordinates.

It is necessary to take into consideration special relativity. At a velocity of 2000m/s, the nuclei will have a gamma factor of $\gamma$=1.0000033. Using relativistic aberration, the angle in the lab frame of reference, $\theta'$, is related to the angle in rest frame of the nuclei, $\theta$ by[4],

$$tan(\frac{\theta'}{2}) = \frac{tan(\frac{\theta}{2})}{\gamma(1-\frac{v}{c})}. \tag{8}$$

As such, a given angle in the lab frame, $\theta'$, will be 0.0003% different from the rest frame angle, $\theta$. This has been incorporated into the distributions of the coordinates in FIG.7 and FIG.9, but the effect it too negligible to observe any significant change.

## STATISTICAL SOLUTIONS

A hypothetical experiment is looking for evidence for a new particle X. If a certain quantity of particles observed in an experiment meets a specific criteria, this can be used to give a confidence level that particle X was indeed discovered.

### A. Method

The quantity of X particles that are expected to be produced in this case are $signal = L\sigma$, where L is the luminosity of 10/nb and $\sigma$ is the currently unknown product cross-section. There are expected to be $5.8 \pm 0.4$ background events that satisfy the given criteria. One experiment found a total number of candidate events observed of 5. Therefore,

$$Totalcount = L\sigma + Background. \tag{9}$$

The signal can be found by carrying out Pseudo-experiments over a range of $\sigma$, and modelling the signal as the mean of a Poisson distribution. The background 'true' mean will follow a Normal distribution of standard deviation of 0.4. This mean is then also modelled as a Poisson distribution. By summing over these two Poisson distributions, the value of $\sigma$ at which $95\%$ of Pseudo-experiments are above the observed 5 can be found.

### B. Results and Discussion

For each Pseudo-experiment, a new value of $\sigma$ was trialed, and the percentage of the total count, from EQ.9, above 5 calculated. The results are seen in FIG.10, with the histogram of the total counts at this value of sigma in FIG.11. The value of the cross section at which $95\%$ of Pseudo experiments gives total counts above 5 is $\sigma = (0.46 \pm 0.05)$nb. Where the error is from repeated experiments.

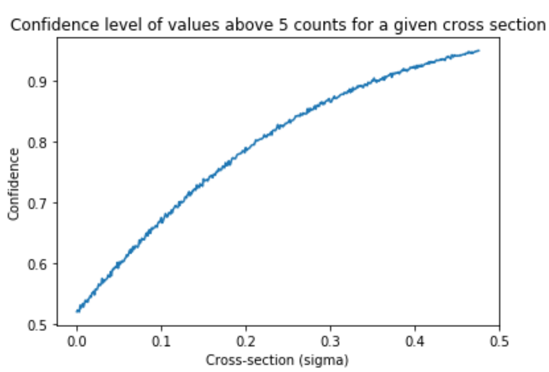


FIG. 10. Confidence level of total count above 5 for a given sigma.

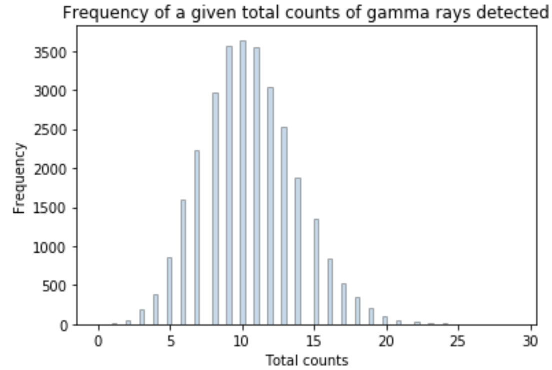


FIG. 11. Histogram of the total counts at which sigma gives a confidence of 0.95.

The curve seen in FIG.10 can be explained by the distributions used. The Background distribution remains fixed at around a mean of 5.8. As the value of the cross section, $\sigma$, is increased, the mean of signal Poisson distribution will increase and move away from the background. As the background Poisson distribution tails off for higher counts, the sum of the two distributions will not have as large an impact on the total at higher cross-sections. This is seen by the asymptotic curve.

## III. CONCLUSIONS

In producing a sine distribution in the given range, the analytical method gave a result with the same error as the reject-accept method, in less time. This was no surprise, due to the nature of the later method. The reject-accept method is however primarily used for modeling the the decay of the radioactive nuclei. These methods gave distributions of detected coordinates with the expected relationship, while confirming what was expected when the detector of the resolution was incorporated. In using Pseudo-experiments to find a value of a cross section of an unknown particle, it displayed the power of computational physics in being able to put a bound on the cross section.

## REFERENCES

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