Experiment simulation with Monte-Carlo methods

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Both the transformation and accept-reject methods for generating random numbers with a chosen probability distribution are compared, and then used to model the production and detection of gamma rays. Monte-Carlo methods are then used to put a 95% confidence limit on the cross section of a new particle, calculated to be $\sigma = 0.41nb$.

I. INTRODUCTION

Monte-Carlo methods cover a wide base of algorithms used to simulate systems with inherently random processes or a large number of degrees of freedom. Such algorithms rely on generators which produce pseudo-random numbers, (as digital computers cannot generate truly random numbers) which are completely deterministic but *seem* to be drawn from some known distribution [1].

The production of gamma rays from a beam of nuclei, an inherently random process, can be simulated, and their energy deposition on a perpendicular detector plotted. This is an important tool for planning the safely and operation of a high energy beam experiment. The decay of a radioactive isotope can be written in terms of an exponential function,

$$A(t) = \frac{N_0}{\tau} e^{\frac{-t}{\tau}} \tag{1}$$

where *A(t)* is the activity of the sample at time t, N_0 is the initial number of nuclei and τ the mean lifetime of the sample [5]. To create an array of values for the time taken for a nucleus to decay, random numbers should therefore be drawn from an exponential distribution.

This report compares two different methods for using uniformly distributed numbers to generate those from another probability distribution. The first is the analytical transformation method, which generates a random deviate y from a known and invertible probability distribution *p(y)* [4]. A uniform distribution $x \sim U(0,1]$ is therefore transformed into one distributed as *f(y)* with

$$y(x) = F^{-1}(x) \quad \text{and} \quad F(y) = \int_0^y p(y)dy \tag{2}$$

[4].
However, this method may not always be possible if the inverse is not feasibly computed. Alternatively, the rejection method is a more general technique that can be used to generate a random deviate from a probability function *p(x)*, as long as it is less than some *f(x)* everywhere on the interval. Random co-ordinates are generated and then accepted if less than *p(x)*, or rejected otherwise [4]. This will need to be repeated to produce an array of the original size, but is applicable to a wider variety of distributions than the analytical method.

When modelling the decay of a radioactive isotope, the random times at which the samples decay can be produced using the transformation method, since Equation 1 is invertible, as can the angles at which the gamma rays are produced. The gamma rays are emitted isotropically, and their distributions generated from

$$\theta = cos^{-1}(1 - 2\xi_1) \quad , \quad \phi = 2\pi\xi_2 \tag{3}$$

where ξ denotes a random uniform distribution on the interval $(0, 1]$ and θ, ϕ spherical coordinates [2]. Additionally, random numbers with a normal distribution can be used to simulate the finite resolution of the detector, and those with a Poisson distribution to account for any background radiation.

Monte-Carlo methods can also be used for statistical analysis. In this report a confidence level is calculated for the cross section of a particle where the total number of candidate events is measured to be 5. Since the counts for both the background and collision events occur independently and at a constant rate, they are suitable to be modelled by a Poisson distribution. If the background rate is known with negligible uncertainty, then the total rate will be distributed as $T \sim Poisson(s + b)$, where *s, b* are the mean signal and background rates respectively [3]. In this case the mean signal rate is $L\sigma$ where the integrated luminosity, $L = 12 \pm 1(nb)^{-1}$ and the mean background, $b = 5.7 \pm 0.4$. Clearly the uncertainly on the background rate is not negligible, but using the Poisson distribution as an approximation, if $T \sim Poisson(10.5)$ then $P(T \leq 5) = 0.05$, giving an estimate of $\sigma \leq 0.4$ at a 95% confidence level. The Monte-Carlo method will take into account the larger error on the background rate and luminosity value, giving a more accurate bound on σ.

II. METHOD

Initially, two routines for generating random numbers from a chosen probability distribution are created. Both the transformation and rejection methods are compared in creating a random distribution of angles from

$0 < \theta < \pi$ in a distribution proportional to $sin(\theta)$, using the methods described above. The *scipy Mersenne Twister* function is used to produce uniformly distributed numbers, which has a long period of $2^{19937} - 1$ and very good distributional properties [1].

To test the produced distributions, normalised histograms are plotted of each array, and a sine curve, $y = asin(bx) + c$ fitted, using *scipy's curve_fit* function. The observed and expected heights of each histogram bin are compared and a χ^2 value for each produced, as well as a corresponding p-value, denoting the probability that the correct distribution will produce a larger χ^2 than calculated. The behaviour of these p-values with increasing array length will also be compared. Additionally, tests are carried out of the fitted parameters to each histogram, and compared to the values of the intended normalised distribution ($a = 0.5, b = 1, c = 0$). For each fit parameter and standard deviation, z values are computed,

$$z = \frac{|X - \mu| \pm \Delta}{\sigma} \tag{4}$$

where X is the intended fit parameter, μ is the measured fit parameter, σ its standard deviation, and Δ the equivalence bound. This z value is used to test for equivalence using a two-one-sided t-test (TOST) procedure. Two null hypotheses are tested: H01: $X - \mu \leq -\Delta$ and H02: $X - \mu \geq \Delta$. If both of these can be statistically rejected, we can conclude that the observed deviation falls within the equivalence bounds [6]. Again, the p-values for this test are compared for each method, using a value of $\Delta = 0.01$, as a function of the length of the array.

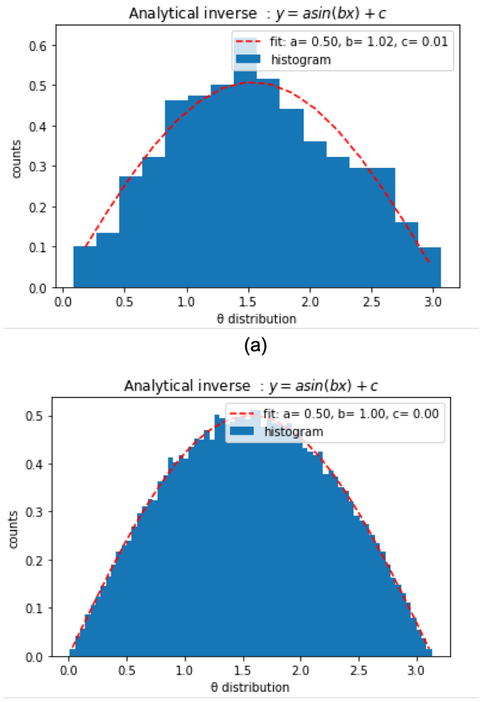
To model the decay of the radioactive isotope, inbuilt *scipy* functions were used to to create random numbers from exponential, uniform and normal distributions. The sinusoidal distribution of θ angles in Equation 3 was created using the transformation function from the previous part. Each distribution is tested by computing a χ^2 value between the observed and expected bin heights from their respective histograms, any corresponding p-value less than 0.95 will return an error, unless the number of nuclei modelled is less than 100.

To plot the distribution of gamma rays hitting the flat detector, the spherical co-ordinates of the angles and position of radiation produced must be transformed into Cartesian coordinates and projected onto the screen. Since only rays emitted between $0 < \phi < \pi$ will be picked up by the detector, the random uniform distribution of ϕ is only produced within this range. This will give twice the amount of events hitting the detector, however the overall distribution will be the same. To account for the finite resolution of the detector, normally distributed arrays of random variables, x *resolution* $\sim N(0, 0.1)$ and y *resolution* $\sim N(0, 0.3)$, are added on to the calculated x and y points. The final distributed is then represented in a two dimensional histogram, using a logarithmic scale and the screen size modelled as 12×12m.

The routine for statistical analysis makes use of normally distributed random values to generate mean background values, $b \sim N(5.7, 0.4)$, and integrated luminosity values $L \sim N(12, 1)$. For each value in these arrays, a pseudo experiment is modelled, with the signal and background events having Poisson distributions, with normally distributed mean values. Again, each of these distributions is tested by calculating χ^2 values between the observed and expected values. The total signal distribution can then be taken as the combination of the signal and background values, and is plotted as a histogram. To obtain the value of σ at a 95% confidence level, a *scipy bisection* optimisation routine is applied, looping through the above procedure until 95% of the expected values are above 5.

To test how many pseudo-experiments are required for stable values of sigma (which do not vary significantly by changing the seed), an array of 10 σ values are calculated for each N, the number of experiments. The variance of this array is then computed and plotted against N.

III. RESULTS



(a)

(b)

FIG. 1. Distribution of angles $0 < \theta < \pi$ proportional to $sin(\theta)$ (a) normalised histogram of array with 10^3 values (b) with 10^5 values, both fitted with a sinusoidal curve.

Figure 1 shows two different normalised histograms of randomly generated numbers in a sine distribution. As the number of values in the array increases in (b), the histogram displays more obviously sinusoidal behaviour. More quantitatively, from Figure 2 it is clear that there is a steep decline in the χ^2 value up to array lengths of about 30000, when the rate of change then starts to decrease. There is no clear difference in the distribution of the analytical and reject methods. When looking at the p-values of the χ^2 test, these very quickly tend to $p = 1$ at array lengths of ~ 25 for both methods.

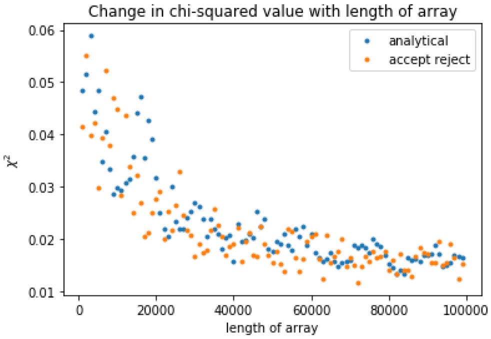


FIG. 2. Change in the χ^2 value between the observed histogram and one that you would expect for a $sin(\theta)$ distribution, both the analytical and reject methods shown.

The p-values of the equivalence tests on the fitting values are also analysed. These signify the probability that the difference between the actual and measured fit parameters lies outside the equivalence bounds of $\Delta = 0.01$. This p-value can be measured for each of the different fit parameters, *a, b, c*, and its average is plotted in Figure 3, as a function of the length of the array. Figure 3 shows an almost oscillatory relationship between the average p-value of the fit parameters and the length of array, particularly for the analytical routine. On average it appears that the accept-reject method produces more accurate values for the fit parameters than the analytical. Furthermore, the time taken to implement the analytical and rejection routines has been compared in Figure 4. Both methods have implementation times that scale linearly with the length of the array required, however the accept-reject method has a significantly steeper slope.

The overall outcome of the first physics example is shown in Figure 5. The majority of the counts are clustered in the center of the distribution, plotted on a logarithmic scale. The difference in the x and y resolutions is clearly seen, with more 'smudging' in the y direction.

The final histogram to find a 95% confidence level on σ is shown in Figure 6, the corresponding limit on the cross section of the new particle is $\sigma = 0.41nb$. A test done on the number of pseudo-experiments required to achieve a stable limit on σ is shown in Figure 7. There is a steep decline in the variance of the limits put on σ up to about 4000 pseudo-experiments, where the rate of change then decreases. Furthermore, the expected Poisson distribution of the total number of candidate events, $T \sim Poisson(s+b)$, was tested. The *scipy curve_fit* function found a Poisson distribution with a mean value of $\lambda = 10.6 \pm 0.4$ to Figure 6. This was compared to the ex-

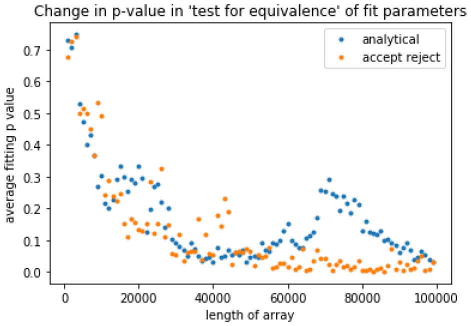


FIG. 3. Change in the average p-value value comparing the measured fit parameters to those you would expect for a normalised $sin(\theta)$ distribution, both the analytical and reject methods shown.

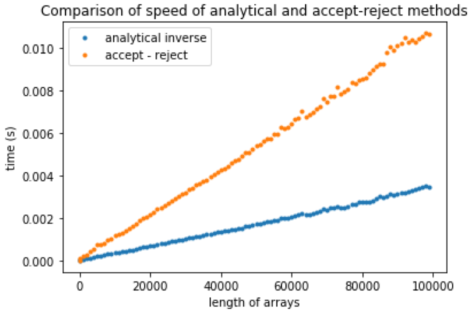


FIG. 4. Change in the average p-value value comparing the measured fit parameters to those you would expect for a normalised $sin(\theta)$ distribution, both the analytical and reject methods shown.

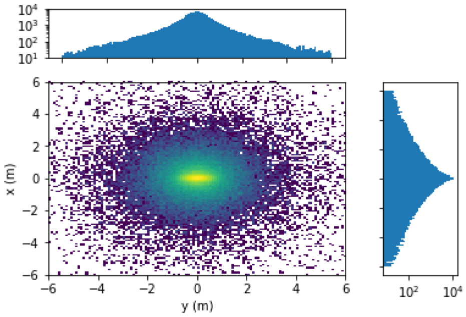


FIG. 5. 2D Histogram showing the gamma ray counts on a 12 × 12m screen, minor plots show the equivalent 1D histograms in the x and y directions. Logarithmic scales have been used.

pected Poisson distribution described above using a mean value of $\lambda = 5.7 + 12\sigma$, the χ^2 value for this comparison was 1.3.

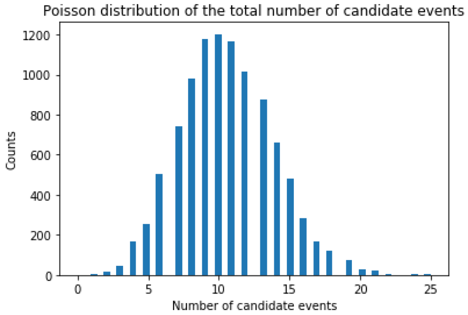


FIG. 6. Histogram showing the distribution of the total number of candidate events for 10^5 pseudo-experiments. 95% of the values occur above 5.

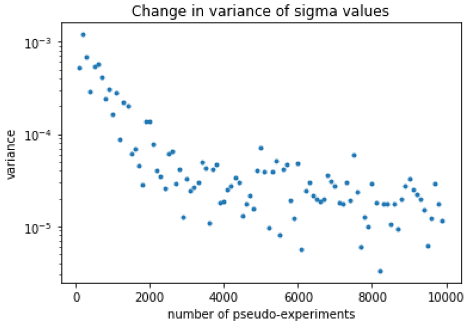


FIG. 7. Plot of the variance of sigma across 10 produced values for each set of pseudo-experiments. Plotted on a logarithmic scale.

IV. DISCUSSION

The first section of the results obtained clearly show that both the analytical and rejection methods are successful in generating random numbers from a given probability distribution. In both cases the χ^2 values between the observed and expected distributions drop very quickly, to values of the order of 10^{-2} within array lengths of 1000. Figure 3 shows that the rejection method on average slightly outperforms the analytical when comparing the p-values in testing for equivalence in the fit parameters. Further research could be conducted into why the analytical method in particular seems to produce oscillating p-values, which appears to be a more stringent test of the distribution of the random numbers generated. Despite this, the analytical method would still be preferable where possible, as the computational time is significantly less, and it only performs slightly less well in the other tests. The rejection method is still, however, a very useful tool if the desired probability distribution is not practically invertible.

Figure 5 shows that the distribution of the gamma rays is heavily centered in the middle of the screen, as you might expect from the sine distribution of the *theta* angles at which the gamma rays are produced. As the particles decay closer to the screen, this distribution will focus the gamma rays more and more in the center. To improve this pseudo-experiment the natural background radiation could be considered, which might ionise the detector, and a confidence level calculated for where this background could be distinguished from the experimental gamma rays. In another extension the material composing the detector could itself become radioactive after exposure to gamma rays, which could be modelled in the experiment. Finally, the size of the detector was chosen somewhat arbitrarily, however this could be improved by varying the size of the detector instead with the number of pseudo-experiments, so that the distribution of the gamma rays is always clearly visible.

A 95% confidence level puts a limit on the cross section of the new particle of $\sigma = 0.41nb$, close to the estimate of 0.4 made in the introduction. The Poisson fit on the final histogram confirms that $T \sim Poisson(s + b)$ is a reasonable approximation to the problem, although the χ^2 value of 1.3 is large for 5000 pseudo-experiments, reflecting the extra complexity that the uncertainty on the background adds. It was found that the obtained limits on the cross section became less dependant on the seed (on the actual random numbers generated) as the number of pseudo-experiments increased. After approximately 4000 experiments the rate of decrease in the variance of σ reduces.

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