Nonuniform random numbers

All the Python random number functions we have described generate uniformly distributed random numbers. In physics, however, there are many processes that happen with nonuniform probability. Consider again, for instance, the example about radioactive decay, where we have N atoms of a radioisotope with half-life tau. The probability that a particular atom decays in time t is $1 - 2^{-t/\tau}$ and hence the probability that it decays in a small time interval dt is:

$$1 - 2^{dt/\tau} = 1 - exp(-\frac{dt}{\tau}ln2) = \frac{ln2}{\tau}dt$$

where we have dropped terms in $(dt)^2$ or smaller. Now we can ask what the probability is that a particular atom decays between times t and t + dt. In order to undergo such a decay, an atom must survive without decay until time t, which happens with probability $2^{t/\tau}$, then decay in the following interval dt, which happens with probability $\frac{ln2}{\tau}dt$. Thus, the total probability P(t)dt of decay between times t and t + dt is:

$$P(t)dt = 2^{t/\tau}\frac{ln2}{\tau}dt \qquad (1)$$

This is an example of a non-uniform distribution. The decay times t are distributed in proportion to $2^{t/\tau}$, so that earlier decay times are more probable than late ones, although all possible times can occur with some probability.

One way to calculate the decay of a sample of N atoms, which is significantly more efficient than the method we used in the previous example, would be to generate N random numbers drawn from this nonuniform probability distribution, to represent the time at which each of the atoms decay. The catch is that in order to do so, we have to be able to generate nonuniform random numbers drawn from equation 1.

How can we do that? **If you have a source of uniform random numbers, then you can turn them into nonuniform ones using any of several techniques, the most commom one is the transformation method.**

TRANSFORMATION METHOD

Suppose you have a source of random floating-point numbers z drawn from a distribution with probability density q(z), meaning that the probability of generating a number in the interval z to z + dz is q(z)dz. And suppose you have a function x = x(z). Then, when z is one of our random numbers, x(z) is also a random number, but in general it will have some other distribution p(x), different from q(z). Our goal is to choose the function x(z) so that x has the distribution we want.

The probability of generating a value of x between x and x + dx is by definition equal to the probability of generating a value of z in the corresponding z interval. That is:

$$p(x)dx = q(z)dz$$

The common situation is that we have a source of random numbers that are uniform on the interval from zero to one. In that case q(z) = 1 between zero and one, and zero everywhere else. Then, integrating the above equation on both sides:

$\int_{-\infty}^{x(z)} p(x')dx' = \int_0^z dz' = z$ (2)

If we can do the integral on the left, we end up with an equation that must be satisfied by the value x(z), then we have our function x(z). There are two catches though: first, we cannot always do the integral, and if so, we cannot always solve the equation. Nevertheless, when we can do both, this method gives us what we want.

As an example, suppose we want to generate random real numbers x in the interval from zero to infinity with the exponential probability distribution shown as follows:

$p(x) = \mu e^{-\mu x}$

This distribution is propertly normalized. Using equation 2:

$\mu \int_0^{x(z)} e^{-\mu x'} dx' = z$

$\mu \left(\frac{-1}{\mu}\right) \left[e^{-\mu x'}\right]_0^{x(z)} = z$

$1 - e^{-\mu x(z)} = z$

Then, solving for x:

$x = -\frac{1}{\mu} ln(1 - z)$ (3)

All we need to do is generate uniform random numbers z in the interval from zero to one and feed them into this equation to get exponentially distributed x values. Let's try the radioactive decay example with new method.

Example:

Using the transformation method, generate 1000 random numbers from the nonuniform distribution of equation 3 to represent the times of decay of 1000 atoms of ^{208}Tl (which has half-life 3.053 minutes). Then, make a plot showing the number of atoms that have not decayed as a function of time. Hint: look for the **numpy.sort** function.

Gaussian random numbers

A common problem in physics calculations is the generation of random numbers drawn from a Gaussian distributions:

$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} exp(-\frac{x^2}{2\sigma^2})$

Where σ is the width, or standard deviation, of the distribution and the factor in front of the exponential is for normalization. Applying the transformation method we get:

$\frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{x} exp(-\frac{x^2}{2\sigma^2})dx = z$

Unfortunately it is not known how to perform this integral, so the transformation method is not useful here. Let's use a different trick.

Imagine we have two independent random numbers x and y, both drawn from a Gaussian distribution with the same standard deviation σ. The probability that the point with position vector (x,y) falls in some small element dxdy of the xy plane is then:

$$p(x)dx\ p(y)dy = \frac{1}{\sqrt{2\pi\sigma^2}}exp(-\frac{x^2}{2\sigma^2})dx\ \frac{1}{\sqrt{2\pi\sigma^2}}exp(-\frac{y^2}{2\sigma^2})dy$$

$$p(x)dx\ p(y)dy = \frac{1}{\sqrt{2\pi\sigma^2}}exp(-\frac{x^2+y^2}{2\sigma^2})dxdy$$

We could alternatively express this in polar coordiantes as the probability that the point falls in the elemental area $rdrd\theta$ with radial coordinate between r and r + dr and angular coordiante between θ and θ + $d\theta$. Making the appropriate substitutions $x^2 + y^2 \to r^2$ and $dxdy \to rdrd\theta$ we get:

$$p(r,\theta)drd\theta = \frac{1}{2\pi\sigma^2}exp(-\frac{r^2}{2\sigma^2})rdrd\theta$$

$$p(r,\theta)drd\theta = \frac{r}{\sigma^2}exp(-\frac{r^2}{2\sigma^2})dr\ \frac{d\theta}{2\pi}$$

$$p(r,\theta)drd\theta = p(r)dr\ p(\theta)d\theta$$

The distributions $p(r)$ and $p(\theta)$ are correctly normalized to unity. If we generate random values of r and θ according to these two distribuitons and regard them as the polar coordinates of a point in 2D space, then that point will have the same probability distribution as our original point (x,y).

Generating the θ variable is trivial, the distribution $p(\theta) = 1/(2\pi)$ is just a uniform distribution, so all we need to do is produce a uniformly distributed real number between 0 and 2π, which we do by generating a number between zero and one and multiplying it by 2π. The radial coordiante r can be generated using the transformation method:

$$p(r) = \frac{r}{\sigma^2}exp(-\frac{r^2}{2\sigma^2})dr$$

Putting this distribution in place of p(x) in equation 2, we obtain:

$$\frac{1}{\sigma^2}\int_0^{r(z)} exp(-\frac{r^2}{2\sigma^2})rdr = z$$

$$1 - exp(-\frac{r^2}{2\sigma^2}) = z$$

$$r = \sqrt{-2\sigma^2 ln(1-z)}$$

With this value for r and our random value for θ, our 2 Gaussian random numbers are given by converting back to Cartesian coordinates:

$$x = rcos\theta$$

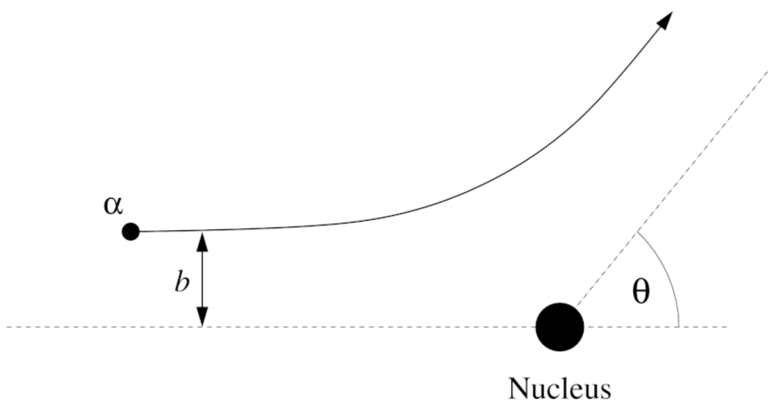
$$y = rsin\theta$$

Example: Rutherford scattering

At the beginning of the 20th century, Ernest Rutherford and his collaborators showed that when an alpha particle (i.e. a helium nucleus of two protons and two neutros) passes close to an atom, it is scattered, primarily by electric repulsion from the positively charged nucleus of the atom, and that the angle θ through which it is scattered obeys:

$$tan(\frac{\theta}{2}) = \frac{Ze^2}{2\pi\epsilon_0 Eb}$$

where Z is the atomic number of the nucleus, e is the electron charge, ϵ_0 is the permittivity of free space, E is the kinetic energy of the incident alpha particle, and b is the impact parameter, i.e. the perpendicular distance between the particle's initial trajectory and the axis running through the nucleus.



Consider a beam of alpha particles with anergy 7.7 MeV that has a Gaussian profile in both its x and y axes with standard deviation $\sigma = a_0/100$, where a_0 is the Bohr radius. The beam is fired directly at a gold atom. Simulate the scattering process for one million alpha particles and calculate the fraction of particles that bounce back on scattering, i.e. that scatter through angles greater than 90°.

Solution:

The threshold value of the impact parameter for which this happens can be calculated from the equation above with $\theta = 90^\circ$:

$$b = \frac{Ze^2}{2\pi\epsilon_0 E}$$

If b is less than this value, then the particle bounces back.

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