Lecture Notes for PHYS 527 Fall 2007

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11 Lecture: Monte Carlo Methods

11.1 Summary of Simple Monte Carlo Integration

We have a set of N random points uniformally distributed in a multi-dimensional volume, V, $x_1, \ldots x_N$. The basic Monte Carlo theorem for the integration of a function, f, over the volume, V is given by

$$\int f dV \approx V\langle f\rangle \pm V\sqrt{\frac{\langle f^2\rangle - \langle f\rangle^2}{N}}\,.$$

The angle brackets are the arithmetic mean over the N sample of points

$$\langle f\rangle \equiv \frac{1}{N}\sum_1^N f(x_i)\ \langle f^2\rangle \equiv \frac{1}{N}\sum_1^N f^2(x_i)\,.$$

11.2 Random Numbers

No numerical algorithm can generate a truly random sequence of numbers, but they can generate repeating sequences of M integers which are fairly good representations of a randomly distributed range of integers from 0 to $M-1$. This type of sequences is called pseudo-random. For practical purposes, we want the program that produces the random number to be different from and statistically uncorrelated to the program that will use the random number. Any two different random number generators ought to produce statistically the same results when coupled to your programs.

The most well-know algorithm for generating random sequences of integers is the linear congruential method. In this method the nth integer is related to the nth+1 integer by

$$I_{n+1} = (AI_n + C)\ mod(M)$$

where A, C, and M are positive integer constants.

- The first number in the sequence is the "seed" values and is selected arbitrarily by the user.

- Each initializing value of seed will produce a different random number or sequence of random numbers.
- The same seed, however, will produce the same sequence.
- Example: $A = 7$, $C = 0$, and $M = 10$

$$I_{n+1} - AI_n = mod(10)$$

so $I = 3, 7, 1, 9, 3, 1, \ldots$.

- These are bad choices of our integers, but exhibits a problem of linear congruential methods, the recurrence will eventually repeat itself, with a period that is no greater than M,
- When A, C and M are properly chosen, the period will be of maximal length.
- All integers between 0 and m-1 will appear at some point so one initial seed is as good as another (a good thing).
- This method is very fast, but is not very good because it does tend to correlate.
- If using a supplied random number generator, check to make sure it is not linear congruential method before using it¡
- Matlab uses different algorithms depending on the version. Type help rand at the prompt to see which one you are using.

11.3 Distribution Functions

In the last section, we saw how to generate a random number, x, with a uniform probability density. Now we want take a function of it, $y(x)$.

- Let $P(x)dx$ represent the probability of finding the random variable x in the interval x to $x + dx$. $P(x)$ is the probability density. When $P = 0$, there is no chance that the variable is in the interval, and $P = 1$ means it is certain.
- Probability densities are subjected to the normalizing constraint

$$\int_{-\infty}^{+\infty} P(x)dx = 1\,.$$

- A random variable x, uniformally distributed in the range x_1 to x_2 has a probability density

$$P(x)dx = \{ \begin{array}{cc} 1/(x_2 - x_1) & \text{if } x_1 \leq x \leq x_2 \\ 0 & \text{otherwise} \end{array}$$

- We can construct the variable x to be a random number between x_1 and x_2 by: $x = x_1 + (x_2 - x_1)(random)/(M-1)$
- Let $y = f(x)$ where f is a known function and x is a random variable.
- The probability of x is $P_x(x)$. The probability of y will be given by $P_y(y)$. There is a fundamental transformation law of probabilities that just means that probability is conserved:
$$\mid P_x(x)dx \mid = \mid P_y(y)dy \mid \ .$$
This states that the probability of finding x in the interval x to $x + dx$ is the same as finding y in y to $y + dy$.
- It follows that
$$P_y(y) = \frac{P_x(x)}{\mid f'(x) \mid'}$$
where $f' = df/dx$.

Example: **Poisson Distribution:** Consider
$$P_y(y) = \{ \begin{array}{cc} e^{-y} & \text{if } 0 \leq y \leq \infty \\ 0 & \text{otherwise} \end{array}$$
Let $y = f(x) = -ln(x)$ so that $|f'| = 1/x$. Suppose that
$$P_x(x) = \{ \begin{array}{cc} 1 & \text{if } 0 \leq x \leq 1 \\ 0 & \text{otherwise} \end{array}$$
then it follows that $P_y(y) = \frac{1}{|f'|} = x = e^{-y}$with $x = 0$ corresponding to $y = \infty$ and $x = 1$ to $y = 0$.

11.4 Rejection Methods

The task we began in the last section with the transformation method was to find a random variable with arbitrary distributions. The transformation method can be summarized in the following figure

The transformation method for generating a random deviate, y, from a known distribution p(y). The $\int p(y)dy$ must be known and invertible. A uniform deviate, x (equal to $\mathcal{R}$), is chosen between 0 and 1. Let $y = f(x) = -ln(x)$ so that $|f'| = 1/x$. Suppose that

$$P(x) = \{ \begin{array}{cc} 1 & \text{if } 0 \le x \le 1 \\ 0 & \text{otherwise} \end{array}$$

then it follows that $P(y) = \frac{1}{|f'|} = x = e^{-y}$with $x = 0$ corresponding to $y = \infty$ and $x = 1$ to $y = 0$.

$$P(y) = \{ \begin{array}{cc} e^{-y} & \text{if } 0 \le y \le \infty \\ 0 & \text{otherwise} \end{array}$$

The rejection method

- a powerful, general technique for generating random deviates with a known distribution function,
- does not require the computational of the indefinite integral of p(x),
- nor does it require the inverse of p(x).

The rejection method is based on a simple geometrical argument.

1. Draw a graph of the probability distribution, w(x) from a to b that you wish to generate.

2. If we could choose a random point in 2d with a uniform probability in the area under the curve, then x would have the desired distribution.

3. Draw a second function, q(x), known as the comparison function in which $\int q(x)dx$ is easily computable and $q(x) \ge w(x)$ for all x.

4. Imagine a method for choosing a random point in 2d that is uniform in the area under the comparison function, q(x), (x_{try}, y_{try}).

5. Whenever that point, (x_{try}, y_{try}), lies outside of the area under $w(x)$, we *reject* it and choice another random point. If it lies within the area under $w(x)$, we *accept* it.

6. The accepted points are uniform in the area under the curve.

7. The fraction of rejected points just depends on the ratio of the area of q(x) to the area of w(x).

Now we need to find a way to choose a uniform point in 2d under q(x).

1. Choose a q(x) in which $\int q(x)dx$ is known analytically and that is analytically invertible (i.e. transformation method).

2. Pick a uniform deviate ($\mathcal{R}_1$) between 0 and A, where A is the total area under q(x), $y(a) \leq y \leq y(b)$.

3. Use the transformation method to get x

$$y(x) = \int_a^x q(\hat{x})d\hat{x} + y(a)$$

4. Pick a uniform deviate ($\mathcal{R}_2$), between 0 and q(x)

$$0 \leq r \leq q(x)$$

5. Reject x if $r > w(x)$ or accept x of $r \leq w(x)$

6. The point (x, r) is uniformally distributed under $q(x)$.

Note there is an alternate method in Garcia:

1. pick the second deviate, $\mathcal{R}_2$, between 0 and 1.

2. Accept or reject according to whether it is less than or greater to $w(x)/q(x)$.

11.5 Application: Relativistic Maxwell-Boltzmann Distribution

We are going to investigate a program that constructs a random variable, γ with a probability distribution given by a Relativistic Maxwell-Boltzmann Distribution

$$w(\gamma) = \frac{\alpha}{K_2(\alpha)}\gamma(\gamma 62 - 1)^{1/2}e^{-\alpha\gamma}$$

where K_2 is the modified Bessel function and $\alpha = mc^2/kT$. This distribution is used quite frequently, for example in the kinetic theory of gases. When studying something with such a large number of particles, it is more useful to use statistical mechanics to understand the mean behavior instead of the instantaneous state of a single particle.

Set up the comparison function as $q(\gamma) = w_{max}$ then

$$y(\gamma) = \int_1^{\gamma} w_{max} d\gamma' = w_{max}(\gamma - 1)$$