Lecture 26

Monte Carlo Integration

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Logistics

Course Note: Final Exam Scheduled: Tues, Dec 10, 12:30pm - 02:30pm.

Course Note: Thurs, Dec 5th will be completely Q/A on the Final. No new material will be covered.

Motivation

Monte Carlo and Randomness

- Central to the PageRank (and many many other applications in finance, science, informatics, etc) is that we randomly process something
- What we want to know is “on average” what is likely to happen
- What would happen if we have an infinite number of samples/trials?
- Let’s take a look at an integral computation
  This is looking at something “in the limit”, say as h goes to zero

Integration

some slides from f. pellanccini

- Integral of a function over a domain D

$$\int_{x \in D} f(x)\, dx$$

- The size of a domain

$$A_D = \int_{x \in D} dx$$

- Average of a function over some domain

$$\frac{\int_{x \in D} f(x) dx}{A_D}$$

Integral example 1

The average “daily” snowfall in Albuquerque last year

- Function $s(day)$: snowfall on a particular day
- Domain size: year (1D time interval)
- Integration variable: day

$$average = \frac{\int_{day \in year} s(day)\ d_{day}}{length\ of\ year}$$

Integral example 2

The average snowfall in NM

- Function $s(location)$: snowfall depending on (x, y) location
- Domain: NM (2D surface)
- Integration variable: (x, y) location

$$average = \frac{\int_{location \in NM} \; s(location) \; d_{location}}{area \; of \; NM}$$

Integral example 3

The average snowfall in NM for any arbitrary day

- Function $s(location,\ day)$: snowfall depending on location and day
- Domain: NM $\times$ year (2D space $\times$ time, or 3D)
- Integration variable: location and day

$$average = \frac{\int_{day \in year} \int_{location \in NM} s(location,\ day)\ d_{location,day}}{area\ of\ NM \cdot length\ of\ year}$$

Discrete random variables

- Random variable x
- Values: $x_0, x_1, \ldots, x_n$
- Probabilities $p_0, p_1, \ldots, p_n$ with $\sum_{i=0}^{n} p_i = 1$

Throwing a die (1-based index)

- Values: $x_1 = 1, x_2 = 2, \ldots, x_6 = 6$
- Probabilities $p_i = 1/6$

Expected value and variance

- Expected value: average value of the variable

$$E[x] = \sum_{j=1}^{n} x_j p_j$$

- Average of some function of the variable

$$E[g(x)] = \sum_{j=1}^{n} g(x_j) p_j$$

- Variance: variation from the average

$$\sigma^2[x] = E[(x - E[x])^2]$$

Throwing a die

- Expected value: $E[x] = (1 + 2 + \cdots + 6)/6 = 3.5$
- Variance: $\sigma^2[x] = 2.916$

Estimated $E[x]$

- To estimate the expected value, draw a collection of random values (according to their probability) and average the results

$$E[x] \approx \frac{1}{N} \sum_{j=1}^{N} x_i$$

- Bigger N gives better estimates

Throwing a die

- 3 rolls: $3, 1, 6 \rightarrow E[x] \approx (3 + 1 + 6)/3 = 3.33$
- 9 rolls:
  $3, 1, 6, 2, 5, 3, 4, 6, 2 \rightarrow E[x] \approx (3 + 1 + 6 + 2 + 5 + 3 + 4 + 6 + 2)/9 = 3.51$

Law of large numbers

- By taking N to ∞, the error between the estimate and the true expected value is statistically zero.
- That is, the estimate will converge to the correct value.
- The probability $P(\cdot)$ is

$$P\left(E[x] = \lim_{N\to\infty} \frac{1}{N}\sum_{i=1}^{N} x_i\right) = 1$$

Continuous random variable

- Random variable: x
- Values: $x \in [a, b]$ (any real number between a and b!)
- Probability: density function $\rho(x)$ with $\int_a^b \rho(x)\,dx = 1$
- Probability (technically "probability density") that the variable has a specific value x_i: $\rho(x_i)$

Uniformly distributed random variable

- In this case, the probability of any particular value being chosen is equal.
- Thus, $\rho(x)$ is constant
- Also, since $\int_a^b \rho(x)\,dx = 1$, this implies $\rho(x) = 1/(b-a)$
  - In discrete case, probability of any outcome depended on number of possible outcomes: 6 outcomes, probability $1/6$.
  - In continuous case, probably density also depends on number of possible outcomes: between 5 and 8, probability density $1/3$.

Continuous extensions

- Expected value

$$E[x] = \int_a^b x\rho(x)\,dx$$

$$E[g(x)] = \int_a^b g(x)\rho(x)\,dx$$

- Variance

$$\sigma^2[x] = \int_a^b (x - E[x])^2\rho(x)\,dx$$

$$\sigma^2[g(x)] = \int_a^b (g(x) - E[g(x)])^2\rho(x)\,dx$$

- Estimating the expected value

$$E[g(x)] \approx \frac{1}{N}\sum_{i=1}^{N} g(x_i)$$

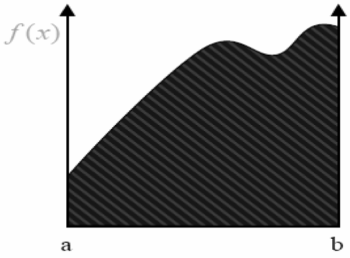
Multidementional extensions

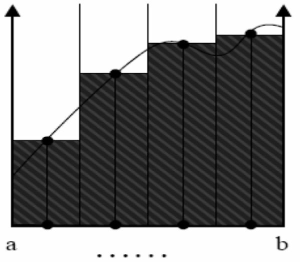
- Difficult domains (complex geometries)
- Expected value

$$E[g(x)] = \int_{x \in D} g(x)\rho(x)\, dx$$

(Deterministic) Numerical integration

- Split domain into set of fixed segments
- Sum function values, weighted by size of segments (Riemann!)
- Is this like an expected value? Perhaps $f(x_j)$ is the sampled value, and each value is “equally” likely to occur.





Notes

Algorithm

We have for a random sequence $x_1, \ldots, x_n$

$$\int_0^1 f(x)\,dx \approx \frac{1}{n}\sum_{i=1}^{n} f(x_i)$$

```
n=100;
x=rand(n,1);
e=f(x);
s=sum(e)/n;
```

Algorithm

We have for a random sequence $x_1, \ldots, x_n$

$$\int_a^b f(x)\,dx \approx \frac{1}{n}\sum_{i=1}^{n} f(x_i)$$

```
n=100;
x=(b-a)*rand(n,1) + a;  %This step will be important later
e=f(x);
s=sum(e)/n;
```

A great hammer!

Monte Carlo integration is VERY broadly applicable.

- **All** our previous integration techniques assumed (somewhere) that f(x) had some number of continuous derivatives. (polynomials, Taylor's theorem, etc)
- There are plenty of things that can be integrated which aren't even continuous!
- Also, a bunch of other problems can be re-written as an integral!

Computing pi!

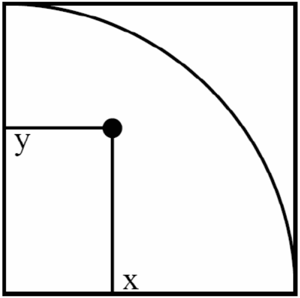
How do you compute pi in computer?

2D: example computing π

Use the unit square $[0,1]^2$ with a quarter-circle

$$f(x,y) = \begin{cases} 1 & (x,y) \in \textit{circle} \\ 0 & \textit{else} \end{cases}$$

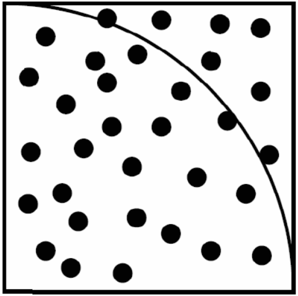
$$A_{\textit{quarter circle}} = \int_0^1 \int_0^1 f(x,y)\, dxdy = \frac{\pi}{4}$$



2D: example computing π

Estimate the area of the circle by randomly evaluating $f(x, y)$

$$A_{\text{quarter circle}} \approx \frac{1}{N} \sum_{i=1}^{N} f(x_i, y_i)$$



2D: example computing π

By definition, the unit circle has area $\pi r^2 = \pi$, so here

$$A_{quarter\ circle} = \pi/4$$

so

$$\pi \approx \frac{4}{N}\sum_{i=1}^{N} f(x_i, y_i)$$

2D: example computing π

```
Input: N
call rand in 2D to generate (x_i, y_i)
for i=1:N
   sum = sum + f(x_i, y_i)
end
sum = 4 * sum/N
```

monte_pi.c vs. monte_pi.m

Listing 1: C

```
 Usage: $ ./monte_pi  <niter>   <seed>
$./monte_pi 1000 2
... estimate of pi is 3.15516...
$./monte_pi 1000 0
... estimate of pi is 3.17918...
```

Listing 2: Matlab

```
Usage: monte_pi( niter )
>>> monte_pi( 1000 )
... estimate of pi is 3.12400...
>>> monte_pi( 10000000 )
... estimate of pi is 3.14131...
```

- With enough iterations, we can get a few digits of accuracy, finally
- The random number generator and seed can have a big impact

Error in Monte Carlo

Can we quantify the error?

Definition Reminders

- Expected value

$$\mathbb{E}[x] = \int_a^b x\rho(x)\,dx$$

- Variance

$$\sigma^2[x] = \int_a^b (x - E[x])^2 \rho(x)\,dx$$

- Facts: Expected Value is Linear, Variance is not (unless things are independent)

$$\mathbb{E}[5x + y] = 5\mathbb{E}[x] + \mathbb{E}[y].$$

$$\sigma^2[x + y] = \sigma^2[x] + \sigma^2[y] \quad .\ \text{IF } x \text{ and } y \text{ are independent.}$$

Notes

To the Board

2D: example computing π, algorithm

The expected value of the *error* is $\mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$

- We are guaranteed this error by the central limit theorem (CLT)
- Convergence does not depend on dimension
- Deterministic integration is very hard in higher dimensions
- Deterministic integration is very hard for complicated domains

Convgergence $\mathcal{O}(1/\sqrt{N})$?

$$
\begin{aligned}
\mathbb{E}[F_n] &= \mathbb{E}\left[S(D)\frac{1}{N}\sum_{i=1}^{N} f(X_i)\right] \\
&= \frac{1}{N}\sum_{i=1}^{N} \mathbb{E}\left[S(D)f(X_i)\right] \\
&= \frac{1}{N}\sum_{i=1}^{N} \int_{x\in D} f(x)\,dx \\
&= \int_{x\in D} f(x)\,dx
\end{aligned}
$$

So if we do this “averaging” process, we “expect” to get the integral we are trying to calculate.

Convgergence $\mathcal{O}(1/\sqrt{N})$?

But how far away from the "expected" value are we?

$$
\begin{aligned}
\sigma^2[F_n] &= \sigma^2\left[S(D)\frac{1}{N}\sum_{i=1}^{N} f(X_i)\right] \\
&= \frac{1}{N^2}\sum_{i=1}^{N}\sigma^2\left[S(D)f(X_i)\right] \quad (X_i\text{'s are independent}) \\
&= \frac{1}{N^2}\sum_{i=1}^{N}\sigma^2\left[Y\right] \\
&= \frac{N}{N^2}\sigma^2\left[Y\right]
\end{aligned}
$$

Therefore the standard deviation is

$$
\sigma[F_n] = \sqrt{\frac{1}{N}\sigma^2[Y]} = \frac{1}{\sqrt{N}}\sigma[Y].
$$