LECTURE 19: MONTE CARLO METHODS

STAT 598z: Introduction to computing for statistics

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We want to calculate integrals/summations

- often expectations w.r.t. some probability distribution $p(x)$

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What is the prob. a game of patience (solitaire) is solvable?

$$P(\text{Solvable}) = \frac{1}{|\Pi|}\sum_{\Pi} \mathbb{1}(\Pi \textit{ is solvable})$$

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If we drop 3 points on the plane, each Gaussian distributed, what is average the area of the resulting triangle?

$$\mathbb{E}[A] = \int A(x_1, x_2, x_3)p(x_1)p(x_2)p(x_3)\mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_3$$

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For dataset (X, y), what is is average loss if you randomly choose a weight-vector according to some distribution (e.g. `rnorm`)?

$$\mathbb{E}_w[\mathcal{L}(X, y)] = \int (y - w^T X)^2 p(w)\mathrm{d}w$$

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Monte Carlo integration

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Sampling approximation: rather than visit all points in $\mathcal{X}$, calculate a summation over a finite set.

Monte Carlo approximation:

- Obtain points by sampling from $p(x)$

$$x_i \sim p$$

$$\hat{\mu} \approx \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

Is this a good idea?

- Very simple
- Unbiased

Monte Carlo integration

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If $x_i \sim p$,

$$\mathbb{E}_p[\hat{\mu}] = \mathbb{E}_p\left[\frac{1}{N}\sum_{i=1}^{N} f(x)\right] = \frac{1}{N}\sum_{i=1}^{N}\mathbb{E}_p[f] = \mu \qquad \text{Unbiased estimate}$$

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$$\mathrm{Var}_p[\hat{\mu}] = \frac{1}{N}\mathrm{Var}_p[f], \qquad \text{Error = StdDev} \propto N^{-1/2}$$

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Independent of dimensionality!

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set.seed(1)
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- Careful with batch/parallel processing.

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In `R` we generate uniform random variables via `runif`

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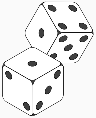
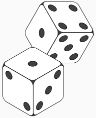
In practice, finding this f is too hard. Need other approaches.

There is a whole subfield of statistics addressing this.



x, y are a pair of dice. What is $p(x, y)$?



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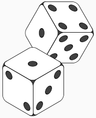
What is $\mathbb{E}[\min(x, y)] = \sum_{i=1}^{6} \sum_{j=1}^{6} \min(x, y) p(x, y)$



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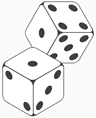

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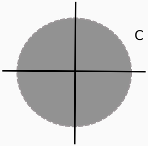
Don't really need Monte Carlo here (but what if we had a 100 dice?), but let's try it anyway. How?

Roll a pair of dice N times. Call the ith outcome (x_i, y_i). Then

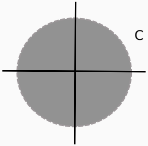
$$\mathbb{E}[\min(x, y)] \approx \frac{1}{N} \sum_{i=1}^{N} \min(x_i, y_i)$$



Let C be the unit disc, i.e. all points (x, y) with $x^2 + y^2 \leq 1$.

$$\text{Its area is } A(C) = \int\int_{x,y\in C} \mathrm{d}x\mathrm{d}y = \int_0^\infty \int_0^\infty \delta_C\left((x,y)\right)\mathrm{d}x\mathrm{d}y$$

Here $\delta_C\left((x,y)\right) = 1$ if $x^2 + y^2 \leq 1$, else it equals 0



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How might we try to approximate this using Monte Carlo?

- What is the f and p?

A (BAD) WAY OF ESTIMATING THE AREA OF A CIRCLE

One way: choose some probability distribution $p(x, y)$
(e.g. both x and y are Gaussian distributed)

Then:

$$
\begin{aligned}
A(C) &= \int_0^\infty \int_0^\infty \delta_C\left((x, y)\right) \mathrm{d}x\mathrm{d}y \\
&= \int_0^\infty \int_0^\infty \frac{\delta_C\left((x, y)\right)}{p(x, y)} p(x, y)\mathrm{d}x\mathrm{d}y \\
&\approx \frac{1}{N} \sum_{i=1}^{N} \frac{\delta_C((x_i, y_i))}{p(x_i, y_i)} \quad \text{(Monte Carlo, with } (x_i, y_i) \sim p\text{)}
\end{aligned}
$$

A (bad) way of estimating the area of a circle

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Then:

$$\begin{aligned} A(C) &= \int_0^\infty \int_0^\infty \delta_C\left((x, y)\right) \mathrm{d}x\mathrm{d}y \\ &= \int_0^\infty \int_0^\infty \frac{\delta_C\left((x, y)\right)}{p(x, y)} p(x, y)\mathrm{d}x\mathrm{d}y \\ &\approx \frac{1}{N} \sum_{i=1}^{N} \frac{\delta_C((x_i, y_i))}{p(x_i, y_i)} \quad \text{(Monte Carlo, with } (x_i, y_i) \sim p\text{)} \end{aligned}$$

In words, sample N points (x_i, y_i) from some distribution p, and plug them into the last equation above

A (BAD) WAY OF ESTIMATING THE AREA OF A CIRCLE

```r
N <- 1000   # Number of Monte Carlo simulations
x <- rnorm(N); y <- rnorm(N)  # Sample N Gaussian pairs (x,y)
px <- dnorm(x); py <- dnorm(y)
pp <- px * py         # Calculate their probabiliy
dd <- sqrt(x^2+y^2)
mc_est <- 1/N * sum(1/pp[dd<1])  # Monte Carlo estimate
```

Let $X = (x_1, \ldots, x_{100})$ be a hundred dice.
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Let $X = (x_1, \ldots, x_{100})$ be a hundred dice.
What is $p(\text{Sum}(X) \geq 450)$?
(where $\text{Sum}(X) = \sum_{d=1}^{100} x_d$)

Rare event simulation:

Let $X = (x_1, \ldots, x_{100})$ be a hundred dice.
What is $p(\mathrm{Sum}(X) \geq 450)$?
(where $\mathrm{Sum}(X) = \sum_{d=1}^{100} x_d$)

$$p(\mathrm{Sum}(X) \geq 450) = \sum \delta(\mathrm{Sum}(X) \geq 450) p(X)$$
$$= \mathbb{E}_p[\delta(\mathrm{Sum}(X) \geq 450)]$$

- $\delta(\cdot)$ is the indicator function
- $\delta(\mathit{condition}) = 1$ if *condition* is true, else 0.

Naive Monte Carlo sampling

- Propose from $p(x)$
- Calculate $\frac{1}{N}\sum_{i=1}^{N}\delta(\mathrm{Sum}(X_i))$

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Most $\delta(\mathrm{Sum}(X_i))$ terms will be 0

High variance

Importance sampling

Importance sampling: assigns importance weights to samples.

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Scheme:

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$$\mu = \int_{\mathcal{X}} f(x)p(x)\mathrm{d}x = \int_{\mathcal{X}} f(x)\frac{p(x)}{q(x)}q(x)\mathrm{d}x \approx \frac{1}{N}\sum_{i=1}^{N} w_i f(x_i) := \mu_{imp}$$

When does this make sense?

Sometimes it's easier to simulate from $q(x)$ than $p(x)$

Importance Sampling (contd)

When does this make sense?

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Sometimes it's better to simulate from $q(x)$ than $p(x)$!

To reduce variance. E.g. rare event simulation.

For 100 dice, what is $p(\text{Sum} > 450)$? A better choice might be to bias the dice.

E.g. $\quad q(x_i = v) \propto v \quad (\text{for } v \in \{1, \dots 6\})$

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E.g. $\quad q(x_i = v) \propto v \quad (\text{for } v \in \{1, \ldots 6\})$

- Propose from $q(x)$
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Gives a better estimate of
$p(\text{Sum}(X) \geq 500) = \sum \delta(\text{Sum}(X) \geq 500)p(X)$