LECTURE 12: BAYESIAN INFERENCE AND MONTE CARLO METHODS

STAT 545: INTRO. TO COMPUTATIONAL STATISTICS

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BAYESIAN INFERENCE

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Point estimate discards information about uncertainty in θ

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- What is a good prior over θ?
- What is a convenient prior over θ?

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The posterior distribution $p(\theta|X) \propto p(X|\theta)p(\theta)$ summarizes all new information about θ provided by the data

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An exception: ‘Conjugate priors’ for exponential family distributions.

CONJUGATE EXPONENTIAL FAMILY PRIORS

Let observations come from an exponential-family:

$$\begin{aligned} p(x|\theta) &= \frac{1}{Z(\theta)} h(x) \exp(\theta^\top \phi(x)) \\ &= h(x) \exp(\theta^\top \phi(x) - \zeta(\theta)) \quad \text{with } \zeta(\theta) = \log(Z(\theta)) \end{aligned}$$

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$$p(\theta|X) \propto \left(\prod_{i=1}^{N} h(x_i) \exp(\theta^\top \phi(x_i) - \zeta(\theta)) \right) \eta(\theta) \exp(\theta^\top a - \zeta(\theta) b)$$

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CONJUGATE PRIORS (CONTD.)

Prior over θ: exp. fam. distribution with parameters (a, b).

Posterior: same family with parameters $(a + \sum_{i=1}^{N} \phi(x_i), b + N)$.

Rare instance where analytical expressions for posterior exists.

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Note the conjugate prior is an entire family of distributions.

- Actual distribution is chosen by setting the parameters (a, b) (a has the same dimension as ϕ, b is a scalar)
- These might be set by e.g. talking to a domain expert.

CONJUGATE PRIORS: BETA-BERNOULLI EXAMPLE

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&= \exp\left(\mathbb{1}(x=1)\log(\pi) + (1-\mathbb{1}(x=1))\log(1-\pi)\right) \\
&= (1-\pi)\exp\left(\mathbb{1}(x=1)\log\frac{\pi}{1-\pi}\right) \\
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$\theta = \log\frac{\pi}{1-\pi}, \phi(x) = \mathbb{1}(x=1), h(x) = 1, Z(\theta) = (1+\exp(\theta))$.

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Defining $\zeta(\theta) = \log Z(\theta)$ as in the previous slide,

$$p(x|\theta) = \exp\left(\phi(x)\theta - \zeta(\theta)\right)$$

CONJUGATE PRIORS: BETA-BERNOULLI EXAMPLE

When $\theta = \log \frac{\pi}{1-\pi}$ is unknown, a Bayesian places a prior on it.

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Thus, the posterior is in the same family as the prior, but with updated parameters $\left(a_1 + \sum_{i=1}^{N} \mathbb{1}(x_i = 1), a_2 - N\right)$.

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Looking at the prior more carefully, we see:

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&= \pi^{b_1-1}(1-\pi)^{(b_2-1)}
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This is just the Beta(b_1, b_2) distribution, and you can check that the posterior is Beta$\left(b_1 + \sum_{i=1}^{N} \mathbb{1}(x_i = 1), b_2 + \sum_{i=1}^{N} \mathbb{1}(x_i = 0)\right)$.

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b_1 and b_2 are sometimes called pseudo-observations, and capture our prior beliefs: before seeing any x's our prior is as if we saw b_1 successes and b_2 failures. After seeing data, we factor actual observations into the pseudo-observations.

MONTE CARLO METHODS

MONTE CARLO INTEGRATION

What about the situation when the posterior $p(\theta|X)$ is no longer simple/available in closed form?

What information about $p(\theta|X)$ do we really need?

Typically, expectations of different functions g:

$$\mathbb{E}_{\theta|X}[g] = \int \mathrm{d}\theta \, g(\theta) p(\theta|X)$$

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What is g for to calculate 1) mean, 2) variance, 3) $p(\theta > 10|X)$?

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Monte Carlo approximation:

- Obtain points by sampling from $p(x)$: $x_i \sim p$
- Approximate integration with summation

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

MONTE CARLO INTEGRATION

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

If $x_i \sim p$,

$$\mathbb{E}_p[\hat{\mu}] = \frac{1}{N} \sum_{i=1}^{N} \mathbb{E}_p[g] = \mu$$

Unbiased estimate

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$$\mathbb{E}_p[\hat{\mu}] = \frac{1}{N}\sum_{i=1}^{N} \mathbb{E}_p[g] = \mu$$ Unbiased estimate

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

$$\frac{1}{N}\sum_{i=1}^{N} f \rightarrow \mathbb{E}_p(g) = \mu \quad \text{as } N \rightarrow \infty$$ Consistent estimate (LLN)

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  Independent of dimensionality!
- If unbiasedness is important to you.
- Very simple.
- Very modular: easily incorporated into more complex models (Gibbs sampling)

MONTE CARLO SAMPLING (CONTD.)

An aside: Monte Carlo should be your method of last resort!

Don't hesitate using numerical integration

- Numerical integration can be much faster and more accurate

Contrast

```
> integrate(function(x) x * exp(-x), lower = 0, upper = Inf)
```

with

```
> mean(rexp(1000))
```

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- Careful with batch/parallel processing.

GENERATING RANDOM VARIABLES

`R` has a bunch of random number generators.

`rnorm`, `rgamma`, `rbinom`, `rexp`, `rpoiss` etc.

What if we want samples from some other distribution?

GENERATING RANDOM VARIABLES

Inverse transform sampling

Let X have pdf $p(x)$, and cdf $F(x) = P(X \leq x) = \int_{-\infty}^{x} p(u) \mathrm{d}u$

Let:

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Equivalently, sample $U \sim \texttt{Unif}(0, 1)$, and let $X = F^{-1}(U)$
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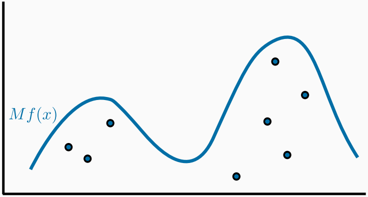
E.g. $-\log(U)$ is $\texttt{Exponential}(1)$.
Usually hard to compute F^{-1}.

REJECTION SAMPLING

Let $p(x) = \frac{f(x)}{Z}$.

Probability of a sample in $[x_0, x_0 + \Delta x] = p(x_0)\Delta x$.



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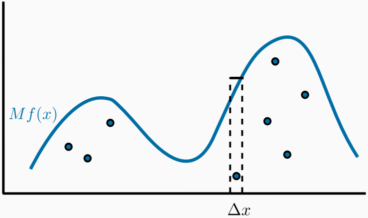

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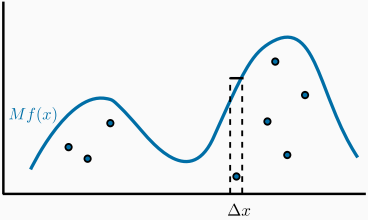

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Probability of a sample in $[x_0, x_0 + \Delta x] = \frac{Mf(x_0)\Delta X}{\int_X Mf(x_0)\mathrm{d}x} = p(x_0)\Delta x$.
How to do this (without sampling from p)?

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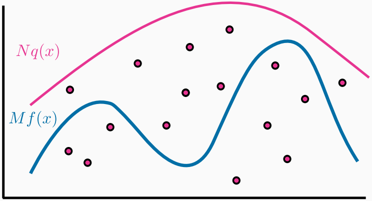

If $Mf(x) \leq Nq(x)$ $\forall x$ for constant N and distribution $q(\cdot)$
Sample points uniformly under $Nq(x)$.
(sample $x_0 \sim q(\cdot)$, and assign it a uniform height in $[0, Nq(x_0)]$

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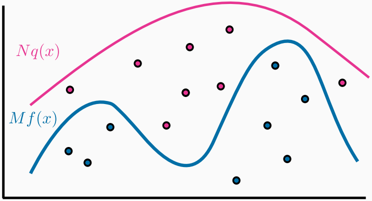
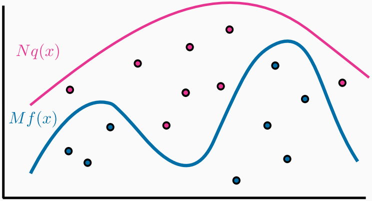


If $Mf(x) \leq Nq(x)$ $\forall x$ for constant N and distribution $q(\cdot)$
Sample points uniformly under $Nq(x)$.
Keep only points under $Mf(x)$.

REJECTION SAMPLING

Let $p(x) = \frac{f(x)}{Z}$.
Probability of a sample in $[x_0, x_0 + \Delta x] = p(x_0)\Delta x$.



Equivalent algorithm: (convince yourself)

- Propose $x^* \sim q(\cdot)$
- Accept with probability $Mf(x^*)/Nq(x^*)$

REJECTION SAMPLING

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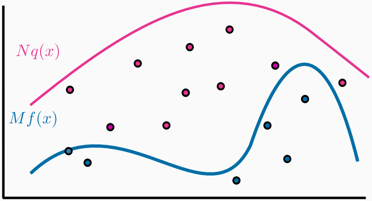

We need a bound on $f(x)$.
A loose bound leads to lots of rejections.
Probability of acceptance = $\frac{MZ}{N}$.

INTRACTABLE NORMALIZATION CONSTANTS

A probability density takes the form $p(x) = \frac{f(x)}{Z}$

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However, rejection sampling doesn't need Z or $p(x)$

REJECTION SAMPLING (CONTD.)

Example 1:

$$p(x) \propto \exp(-x^2/2)|\sin(x)|$$

Example 2 (truncated normal):

$$p(x) \propto \exp(-x^2/2)1_{\{x>c\}}$$

What is M for each case? What can we say about efficiency?

IMPORTANCE SAMPLING

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Use Monte Carlo approximation to the latter expectation:

- Draw proposal x from $q(\cdot)$ and calculate weight $w(x) = \frac{p(x)}{q(x)}$.

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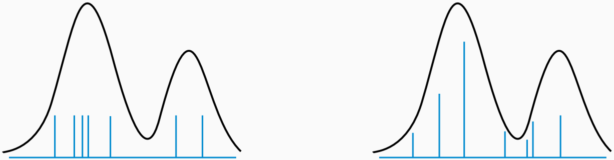
Since $w(x) = p(x)/q(x) = \frac{f(x)}{Zq(x)}$:

- We don't need a bounding envelope.
- We need normalizn constant Z (but see later).

Importance sampling vs simple Monte Carlo



Simple Monte Carlo/MCMC (left) uses sampling approximation

Importance sampling (right) weights the samples

IMPORTANCE SAMPLING (CONTD)

When does this make sense?

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

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

Let $x \sim (0, 1)$

- What is $P(X > 5)$?

IMPORTANCE SAMPLING:

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IMPORTANCE SAMPLING:

Let $X = (x_1, \ldots, x_{100})$ be a hundred dice.
What is $p(\sum x_i \geq 550)$?

Rejection sampling (from $p(x)$) leads to high rejection.

A better choice might be to bias the dice.
E.g. $q(x_i = v) \propto v \quad (\text{for } v \in \{1, \ldots 6\})$

IMPORTANCE SAMPLING:

Define $S_X = \sum x_i$

$$
\begin{aligned}
p(S \geq 550) &= \sum_{y \in \text{ all configs of 100 dice}} \delta(\sum y \geq 550) p(y) \\
&= \sum_{y \in \text{ all configs of 100 dice}} \frac{p(y)}{q(y)} \delta(\sum y \geq 550) q(y)
\end{aligned}
$$

For a proposal $X^* \sim q$,

$$
w(X^*) = \frac{p(X^*}{q(X^*)} = \frac{(1/6)^{100}}{\prod_i q(x_i^*)}
$$

Use approximation $p(S \geq 550) \approx \sum_{j=1}^{N} w(X_j) \delta(\sum x_i^j \geq 550)$

IMPORTANCE SAMPLING (CONTD)

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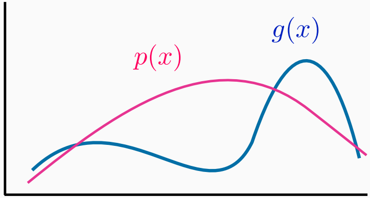
&= 0 \qquad\qquad\qquad\qquad\qquad\qquad (!)
\end{aligned}$$

IMPORTANCE SAMPLING (CONTD)

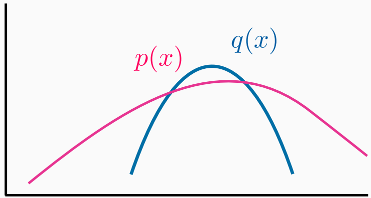


We achieve this lower bound when $q(x) \propto p(x)g(x)$.
A slightly useless result, because

$$q(x) = \frac{p(x)g(x)}{\int_{\mathcal{X}} p(x)g(x)\mathrm{d}x}$$

requires solving the integral we care about.

IMPORTANCE SAMPLING (CONTD)



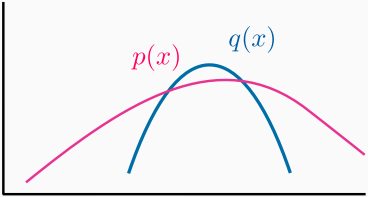
We want a small variance in the weights $w(x_i)$.

Easy to check at $\mathbb{E}_q[w(x)] = 1$.

$$\begin{aligned}\mathrm{Var}_q[w(x)] &= \mathbb{E}_q[w(x)^2] - \mathbb{E}_q[w(x)]^2 \\ &= \int_{\mathcal{X}} \left(\frac{p(x)}{q(x)}\right)^2 q(x)\mathrm{d}x - 1 \qquad = \int_{\mathcal{X}} \frac{p(x)^2}{q(x)}\mathrm{d}x - 1\end{aligned}$$

Can be unbounded. E.g. $p = \mathcal{N}(0, 2)$ and $q = \mathcal{N}(0, 1)$.

IMPORTANCE SAMPLING (CONTD)



A popular diagnosis statistic: effective sample size (ESS).

$$ESS = \frac{\left(\sum_{i=1}^{N} w(x_i)\right)^2}{\sum_{i=1}^{N} w(x_i)^2}$$

Small ESS → Large variability in w's → bad estimate.

Large ESS promises you nothing!

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Reuse samples from the proposal distribution $q(x)$:

$$\hat{Z} = \frac{1}{N}\sum_{i=1}^{N} \frac{f(x_i)}{q(x_i)} = \frac{1}{N}\sum_{i=1}^{N} \tilde{w}(x_i)$$

Can use to approximate importance sampling weights $w(x_i)$:

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Is biased for finite N, but consistent as $N \to \infty$.