LECTURE 11: BAYESIAN INFERENCE AND MONTE CARLO METHODS

STAT 545: Intro. to Computational Statistics

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Point estimate discards information about uncertainty in θ

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An exception: ‘Conjugate priors’.

Conjugate exponential family priors

Let observations come from an exponential-family:

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

Place a prior over θ:

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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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$$\propto \eta(\theta) \exp\left(\theta^\top \left(a + \sum_{i=1}^{N} \phi(x_i) \right) - \zeta(\theta)(b + N) \right)$$

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.

In most cases a simple prior quickly leads to a complicated posterior, requiring Monte Carlo methods.

Conjugate priors: Beta-Bernoulli example

Let $x \sim \text{Bern}(\pi)$, so that

$$
\begin{aligned}
p(x|\pi) &= \pi^{\mathbb{1}(x=1)}(1-\pi)^{\mathbb{1}(x=2)} \\
&= \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) \\
&= \frac{1}{1+\exp(\theta)}\exp\left(\phi(x)\theta\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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$\theta = \log\frac{\pi}{1-\pi}, \phi(x) = \mathbb{1}(x=1), h(x) = 1, Z(\theta) = (1+\exp(\theta))$.
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

If the parameter θ (or equivalently π) is unknown, Bayesian inference places a prior on it.

As before, define an exp. fam. prior with parameters $\vec{a}$:

$$p(\theta|\vec{a}) \propto \exp(a_1\theta + a_2\zeta(\theta))$$

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Then given data $X = (x_1, \ldots, x_N)$,

$$\begin{aligned} p(\theta|\vec{a}, X) &\propto p(\theta, X|\vec{a}) \\ &\propto \exp\left(\left(a_1 + \sum_{i=1}^{N} \mathbb{1}(x_i = 1)\right)\theta + (a_2 - N)\zeta(\theta)\right) \end{aligned}$$

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

Looking at the prior more carefully, we see:

$$\begin{aligned}
p(\theta|\vec{a}) &\propto \exp(a_1\theta + a_2\zeta(\theta)) \\
&\propto \exp\left(a_1 \log \frac{\pi}{1-\pi} + a_2 \log(1-\pi)\right) \\
&\propto \pi^{a_1}(1-\pi)^{(a_2-a_1)} \\
&= \pi^{b_1-1}(1-\pi)^{(b_2-1)}
\end{aligned}$$

This is just the Beta(b_1, b_2) distribution, and you can check that the posterior is Beta$\left(b_1 + \sum_{i=1}^{N} \mathbb{1}(x_i = 1), b_2 + \sum_{i=1}^{N} \mathbb{1}(x_i = 2)\right)$.

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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 ones and b_2 twos. After seeing data, we factor actual observations into the pseudo-observations.

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E.g.: probability 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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Where is the next observation marginalizing out hidden state?

$$P(Y_{t+1}|Y_{1:t}) \propto \int \mathrm{d}X_t \int \mathrm{d}X_{t+1} P(Y_{t+1}|X_{t+1}) P(X_{t+1}|X_t) P(X_t|Y_{1:t})$$

Monte Carlo integration

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Calculate 'posterior expectations':

$$\mathbb{E}_{\theta|X}[f] = \int \mathrm{d}\theta {\color{red}f(\theta)} P(\theta|X) \propto \int \mathrm{d}\theta f(\theta) P(X|\theta) P(\theta)$$

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Monte Carlo approximation:

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

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

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

If $x_i \sim p$,

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

Unbiased estimate

Monte Carlo integration

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

If $x_i \sim p$,

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

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

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

Monte Carlo Sampling

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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)

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- Careful with batch/parallel processing.

R has a bunch of random number generators.

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

What if we want samples from some other distribution?

Inverse transform sampling

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

Let:

$$X \sim p(\cdot)$$

$$U = F(X)$$

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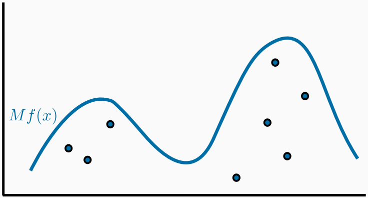
E.g. $-\log(U)$ is $\texttt{Exponential}(1)$.
Usually hard to compute F^{-1}.

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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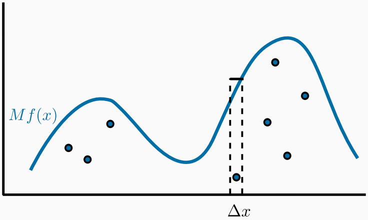

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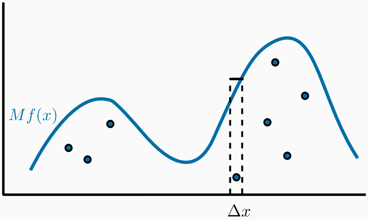

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How to do this (without sampling from p)?

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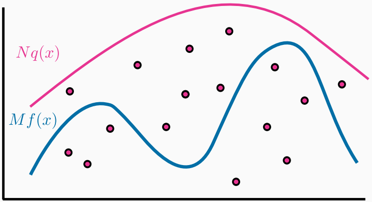

If $Mf(x) \leq Nq(x)\ \forall x$ for constant N and distribution $q(\cdot)$
Sample points uniformly under $Nq(x)$.
(sample $x_0 \sim q(\cdot)$, and assign it a uniform height in $[0, Nq(x_0)]$

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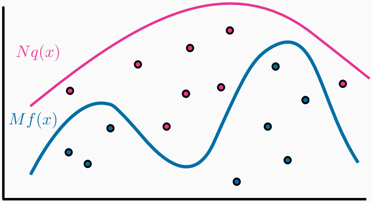

If $Mf(x) \leq Nq(x)$ $\forall x$ for constant N and distribution $q(\cdot)$
Sample points uniformly under $Nq(x)$.
Keep only points under $Mf(x)$.

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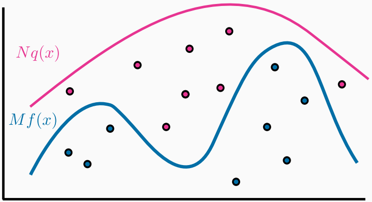

Equivalent algorithm:

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

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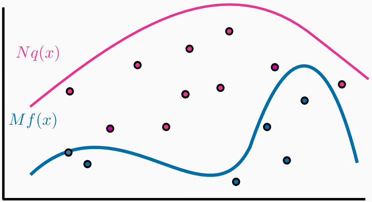

We need a bound on $f(x)$.

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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- Ensures probability integrates to 1

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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

Rather that accept/reject, assign weights to samples.

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

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Draw proposal x from $q(\cdot)$ and assign weight $w(x) = p(x)/q(x)$.
Use approximation

$$\int_{\mathcal{X}} g(x)p(x)\mathrm{d}x \approx \frac{1}{N}\sum_{i=1}^{N} w(x_i)g(x)$$

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Draw proposal x from $q(\cdot)$ and assign weight $w(x) = p(x)/q(x)$.
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$$\int_{\mathcal{X}} g(x)p(x)\mathrm{d}x \approx \frac{1}{N}\sum_{i=1}^{N} w(x_i)g(x)$$

Since $w(x) = p(x)/q(x) = \frac{f(x)}{Zq(x)}$, we need normalizn constant Z

We don't need a bounding envelope.

Importance Sampling (contd)

When does this make sense?
Sometimes it's easier to simulate from $q(x)$ than $p(x)$.

Importance Sampling (contd)

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

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

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

Importance sampling:

Sample proposals $x^* \sim q(\cdot)$ and assign weights $w(x) = p(x)/q(x)$.

$$\int f(x)p(x)\mathrm{d}x \approx \frac{1}{N}\sum_{s=1}^{N} f(x_s)w(x_s)$$

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

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Let $X = (x_1, \ldots, x_{100})$ be a hundred dice.
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Rejection sampling (from $p(x)$) leads to high rejection.

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

Importance sampling:

Define $S_X = \sum x_i$

$$p(S \geq 550) = \sum_{y \in \text{ all configs of 100 dice}} \delta(\sum y \geq 550) p(y)$$

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

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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$$\begin{aligned}\text{Var}[\mu_{imp}] &= \mathbb{E}[\mu_{imp}^2] - \mu^2 \\ &= \mathbb{E}\left[\left(\frac{1}{N}\sum_{i=1}^{N} w_i g(x_i)\right)^2\right] - \mu^2\end{aligned}$$

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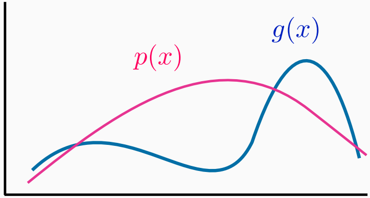
&\geq \left(\int_{\mathcal{X}} q(x)\frac{p(x)g(x)}{q(x)}\mathrm{d}x\right)^2 - \mu^2 \\
&= 0 \qquad\qquad (!)
\end{aligned}
$$

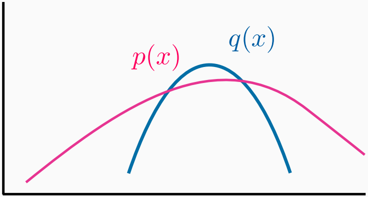
Importance sampling (contd)



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.



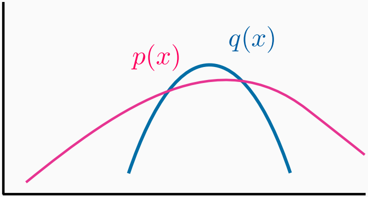
We want a small variance in the weights $w(x_i)$.

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

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

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 $\rightarrow$ Large variability in w's $\rightarrow$ 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 $N \to \infty$.