

LECTURE 14: 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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E.g. consider the likelihood $p(X|\theta) = N(X|\theta, 1)$

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

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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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

Let $x_i \in \{0, 1\}$ indicate if a new drug works for subject i .

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

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

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 $\left(a_1 + \sum_{i=1}^N \mathbb{1}(x_i = 1), a_2 - N \right)$.

CONJUGATE PRIORS: BETA-BERNOULLI EXAMPLE

Looking at the prior more carefully, we see:

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

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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

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 :

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

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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 Integration

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Monte Carlo approximation:

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

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

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

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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Unbiased estimate

$$\text{Var}_p[\hat{\mu}] = \frac{1}{N} \text{Var}_p[g],$$

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.

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 $F(x) = P(X \leq x) = \int_{-\infty}^x p(u)du$

Let:

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

$$U = F(X)$$

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Equivalently, sample $U \sim \text{unif}(0, 1)$, and let $X = F^{-1}(U)$

Then $X \sim p(\cdot)$ (see wikipedia for proof)

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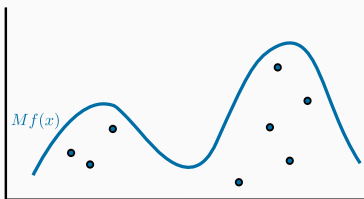
E.g. $-\log(U)$ is $\text{Exponential}(1)$.

Usually hard to compute F^{-1} .

REJECTION SAMPLING

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

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

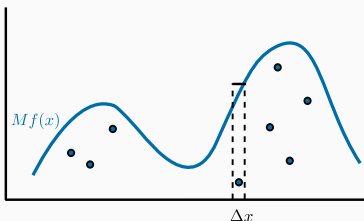


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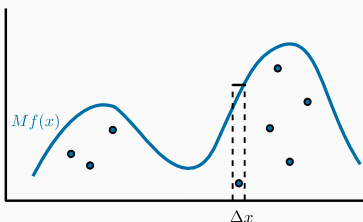
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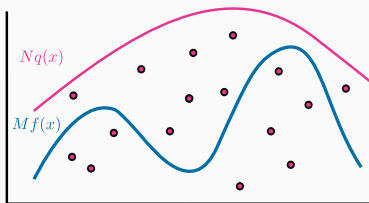
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How to do this (without sampling from p)?

REJECTION SAMPLING

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If $Mf(x) \leq Nq(x) \forall x$ for constant N and distribution $q(\cdot)$

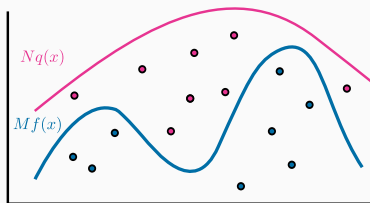
Sample points uniformly under $Nq(x)$.

(sample $x_0 \sim q(\cdot)$, and assign it a uniform height in $[0, Nq(x_0)]$)

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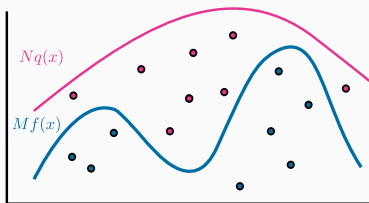
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Keep only points under $Mf(x)$.

REJECTION SAMPLING

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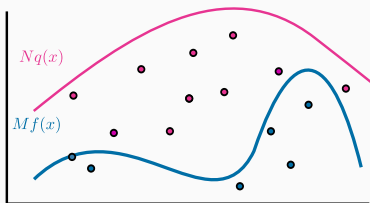
Equivalent algorithm: (convince yourself)

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

REJECTION SAMPLING

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



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

A loose bound leads to lots of rejections.

Probability of acceptance = $\frac{MZ}{N}$.

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

- $Z = \int_{\mathcal{X}} f(x)dx$ is the normalization constant
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Often Z is difficult to calculate (intractable integral over $f(x)$)

Consequently, evaluating $p(x)$ is hard

INTRACTABLE NORMALIZATION CONSTANTS

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

- $Z = \int_{\mathcal{X}} f(x)dx$ is the normalization constant
- Ensures probability integrates to 1

Often Z is difficult to calculate (intractable integral over $f(x)$)

Consequently, evaluating $p(x)$ is hard

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

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 $w(x) = \frac{p(x)}{q(x)}$.

$$\int g(x)p(x)dx \approx \frac{1}{N} \sum_{s=1}^N w(x_s)g(x_s)$$

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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 normalizing constant Z (but see later).

IMPORTANCE SAMPLING (CONTD)

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Let $x \sim (0, 1)$

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

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

A better choice might be to bias the dice.

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

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

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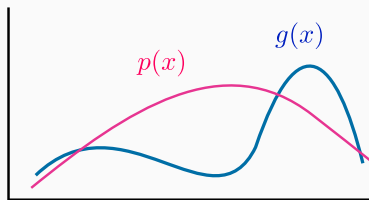
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IMPORTANCE SAMPLING (CONTD)

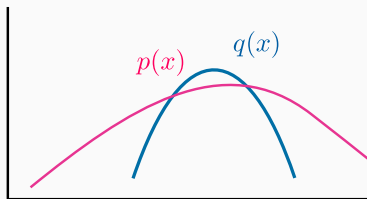


We achieve this lower bound when $q(x) \propto p(x)g(x)$.
A slightly useless result, because

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

requires solving the integral we care about.

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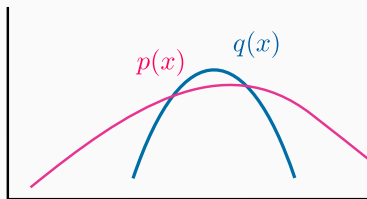
We want a small variance in the weights $w(x_i)$.

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

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

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 \rightarrow Large variability in w 's \rightarrow bad estimate.

Large ESS promises you nothing!

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

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

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