10: Introduction to Bayesian Computation

10/28/19

Introduction

This chapter gives an overview for how to approximate intractable quantities such as posterior expectations and predictions.

Definitions

Numerical integration methods approximate integrals.

These methods can be loosely categorized as either **stochastic** or **deterministic** (e.g. quadrature methods).

Deterministic Methods

Deterministic methods don't draw samples, and instead approximate the integral by summing up approximate volumes:

$$E[h(\theta) \mid y] = \int h(\theta)p(\theta \mid y)\mathrm{d}\theta \approx \frac{1}{S}\sum_{s=1}^{S} w_s h(\theta^s)p(\theta^s \mid y)$$

Approximating the posterior on a grid

We used this method earlier for the rat tumor example!

Given that we can evaluate the unnormalized target $p(\theta, y) = p(y \mid \theta)p(\theta)$, we choose a nonrandom grid of points (think `seq`) $\theta_1, \ldots, \theta_S$, and then we approximate the the continuous posterior with a discrete random variable with pmf equal to

$$\tilde{p}(\theta_j \mid y) = \frac{p(y \mid \theta_j)p(\theta_j)}{\sum_{s=1}^{S} p(y \mid \theta_s)p(\theta_s)}$$

for any $\theta_j \in \{\theta_1, \ldots, \theta_S\}$. Then

$$E[h(\theta) \mid y] \approx \sum_{j=1}^{S} h(\theta_j)\tilde{p}(\theta_j \mid y).$$

Stochastic Methods

Stochastic methods involve sample averages of simulated draws from some distribution. There are **many** ways to do this, but here are a couple examples that we've seen:

$$E[h(\theta) \mid y] = \int h(\theta)p(\theta \mid y)\mathrm{d}\theta \approx \frac{1}{S}\sum_{s=1}^{S} h(\theta^s)$$

with $\theta^s \sim p(\theta \mid y)$, or

$$E[h(\tilde{y}) \mid y] = \int h(\tilde{y})p(\tilde{y} \mid y)\mathrm{d}\tilde{y} \approx \frac{1}{S}\sum_{s=1}^{S} h(\tilde{y}^s)$$

with $\tilde{y} \sim p(\tilde{y} \mid y)$

Stochastic Methods

Drawing $\tilde{y}$ samples can be done in a two-stage way:

1. draw $\theta^s \sim p(\theta \mid y)$
2. draw $\tilde{y}^s \sim p(\tilde{y} \mid \theta^s)$

Stochastic Methods

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1. draw $\theta^s \sim p(\theta \mid y)$
2. draw $\tilde{y}^s \sim p(\tilde{y} \mid \theta^s)$

If you can derive $E\left(h(\tilde{y}) \mid \theta\right)$, you should probably use a Rao-Blackwellized procedure:

$$E[h(\tilde{y}) \mid y] = E[E\left(h(\tilde{y}) \mid \theta\right) \mid y] \approx \frac{1}{S}\sum_{s=1}^{S} E\left(h(\tilde{y}) \mid \theta^s\right)$$

with $\theta^s \sim p(\theta \mid y)$

The general setup

From now on we will write the posterior in terms of an unnormalized density $q(\theta \mid y)$. In other words:

$$p(\theta \mid y) = \frac{q(\theta \mid y)}{\int q(\theta \mid y) \mathrm{d}\theta}$$

Most (maybe all) of the sampling techniques will assume that we can't evaluate $p(\theta \mid y)$, but that we can evaluate $q(\theta \mid y)$

Rejection Sampling aka Accept-Reject sampling

Setup

1. $p(\theta \mid y)$ the target, posterior
2. $q(\theta \mid y) = p(y \mid \theta)p(\theta)$ the unnormalized target
3. $g(\theta)$ the "instrumental" or "proposal" distribution
4. need $q(\theta \mid y)/g(\theta) \leq M$ uniformly
5. need $g \gg q$ i.e. the proposal "dominates" your target (won't divide by 0)

We are free to choose our own $g(\theta)$. For the time being, we assume that $\int g(\theta)\mathrm{d}\theta = 1$.

Rejection Sampling aka Accept-Reject sampling

To (potentially) produce one draw:

1. propose the draw $\theta^s \sim g(\theta)$
2. accept θ^s with probability $\frac{q(\theta^s|y)}{g(\theta^s)M}$

Rejection Sampling aka Accept-Reject sampling

To (potentially) produce one draw:

1. propose the draw $\theta^s \sim g(\theta)$
2. accept θ^s with probability $\frac{q(\theta^s|y)}{g(\theta^s)M}$

Note this is the same as

1. propose the draw $\theta^s \sim g(\theta)$
2. draw $U \sim \text{Uniform}(0, 1]$
3. accept θ^s if $U < q(\theta^s \mid y)/\{g(\theta^s)M\}$

Proof

$$
\begin{aligned}
P\left(\theta \le t \,\middle|\, U \le \frac{q(\theta \mid y)}{Mg(\theta)}\right) &= \frac{P\left(\theta \le t, U \le \frac{q(\theta|y)}{Mg(\theta)}\right)}{P\left(U \le \frac{q(\theta|y)}{Mg(\theta)}\right)} \\
&= \frac{\int_{-\infty}^{t} \int_{0}^{\frac{q(\theta|y)}{Mg(\theta)}} g(\theta) 1 \mathrm{d}u \mathrm{d}\theta}{\int_{-\infty}^{\infty} \int_{0}^{\frac{q(\theta|y)}{Mg(\theta)}} g(\theta) 1 \mathrm{d}u \mathrm{d}\theta} \\
&= \frac{\int_{-\infty}^{t} g(\theta) \frac{q(\theta|y)}{Mg(\theta)} \mathrm{d}\theta}{\int_{-\infty}^{\infty} g(\theta) \frac{q(\theta|y)}{Mg(\theta)} \mathrm{d}\theta} \\
&= \frac{\int_{-\infty}^{t} q(\theta \mid y) \mathrm{d}\theta}{\int_{-\infty}^{\infty} q(\theta \mid y) \mathrm{d}\theta} \\
&= P(\theta \le t \mid y).
\end{aligned}
$$

Example 1

Assume $y \sim \text{Normal}(\theta, 1)$, and $p(\theta) = \frac{1}{\pi(1+\theta^2)}$. Our goal is to draw from

$$
\begin{aligned}
p(\theta \mid y) &\propto q(\theta \mid y) \\
&= p(y \mid \theta) p(\theta) \\
&= \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}(y-\theta)^2\right] \frac{1}{\pi(1+\theta^2)} \\
&\propto \exp\left[-\frac{(\theta-y)^2}{2} - \log(1+\theta^2)\right],
\end{aligned}
$$

Example 1

Let's assume that we want to use our prior distribution as a proposal: $g(\theta) = p(\theta)$. Then we have to find M:

$$\begin{aligned}
\frac{q(\theta \mid y)}{g(\theta)} &= \frac{p(y \mid \theta)p(\theta)}{p(\theta)} \\
&= p(y \mid \theta) \\
&= \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}(y-\theta)^2\right] \\
&\leq \frac{1}{\sqrt{2\pi}} \stackrel{\text{def}}{=} M
\end{aligned}$$

Our acceptance probability for draw θ^s is then

$$q(\theta^s \mid y)/\{g(\theta^s)M\} = p(y \mid \theta^s)/M = \exp\left[-\frac{1}{2}(y-\theta^s)^2\right]$$

Rejection Sampling aka Accept-Reject sampling

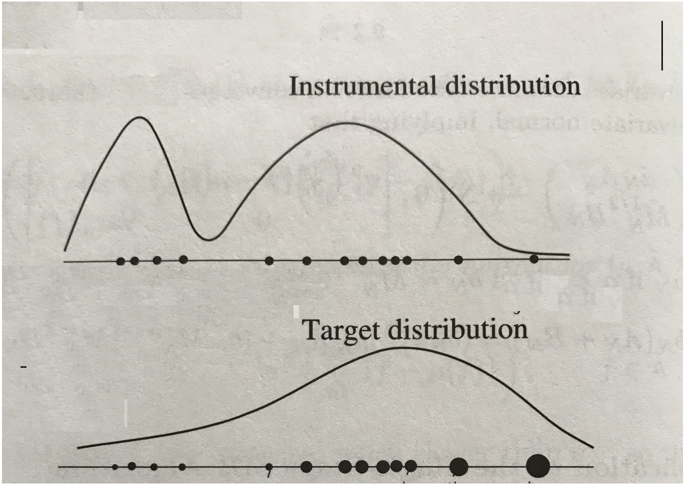
Generally a good strategy is work with logarithms, and then exponentiate as late as possible.

```
y <- 2 # fake data
num_trials <- 1000
theta_proposals <- rt(num_trials, 1)
us <- runif(num_trials, min = 0, max = 1)
log_accept_prob <- function(theta){
  -.5*(y - theta)^2
}
probs <- exp(log_accept_prob(theta_proposals))
accepts <- us < probs
hist(theta_proposals[accepts]) # only the accepted draws
#hist(theta_proposals) # all draws!
```

Importance Sampling

importance sampling also involves ratios like the previous algorithm. However, instead of using those ratios to either accept or discard samples, it uses the ratios to weight samples.

Importance Sampling



Original, unedited image is from
`https://www.springer.com/us/book/9780387402642`

Importance Sampling

Setup

1. $p(\theta \mid y)$ the target, posterior
2. $q(\theta \mid y) = p(y \mid \theta)p(\theta)$ the unnormalized target
3. $g(\theta)$ the "instrumental" or "proposal" distribution
4. $g \gg q$ i.e. the proposal dominates your target

We are free to choose our own $g(\theta)$. For the time being, we assume that $\int g(\theta)\mathrm{d}\theta = 1$.

Importance Sampling

Algorithm: for each iteration s

1. draw $\theta^s \sim g(\theta)$
2. calculate unnormalized weight $\tilde{w}(\theta^s) = \frac{q(\theta^s|y)}{g(\theta^s)}$
3. calculate normalized weights $w(\theta^s) = \tilde{w}(\theta^s) / \sum_r \tilde{w}(\theta^r)$

Final calculation:

$$E_q[h(\theta) \mid y] \approx \sum_s w(\theta^s) h(\theta^s)$$

Importance Sampling

Motivation:

$$
\begin{aligned}
E_q[h(\theta) \mid y] &= \int h(\theta) p(\theta \mid y) \mathrm{d}\theta \\
&= \frac{\int h(\theta) q(\theta \mid y) \mathrm{d}\theta}{\int q(\theta \mid y) \mathrm{d}\theta} \\
&= \frac{\int h(\theta) \frac{q(\theta|y)}{g(\theta)} g(\theta) \mathrm{d}\theta}{\int \frac{q(\theta|y)}{g(\theta)} g(\theta) \mathrm{d}\theta}
\end{aligned}
$$

Importance Sampling

Motivation:

$$E_q[h(\theta) \mid y] = \int h(\theta)p(\theta \mid y)\mathrm{d}\theta$$
$$= \frac{\int h(\theta)q(\theta \mid y)\mathrm{d}\theta}{\int q(\theta \mid y)\mathrm{d}\theta}$$
$$= \frac{\int h(\theta)\frac{q(\theta|y)}{g(\theta)}g(\theta)\mathrm{d}\theta}{\int \frac{q(\theta|y)}{g(\theta)}g(\theta)\mathrm{d}\theta}$$

So first:

$$\frac{1}{S}\sum_{s=1}^{S}\frac{q(\theta^s \mid y)}{g(\theta^s)} \to E_g\left[\frac{q(\theta \mid y)}{g(\theta)}\right] = \int \frac{q(\theta \mid y)}{g(\theta)}g(\theta)\mathrm{d}\theta = \int q(\theta \mid y)\mathrm{d}\theta$$

Importance Sampling

1. $E_q[h(\theta) \mid y] = \frac{\int h(\theta)q(\theta|y)\mathrm{d}\theta}{\int q(\theta|y)\mathrm{d}\theta}$
2. $\frac{1}{S}\sum_{s=1}^{S} \frac{q(\theta^s|y)}{g(\theta^s)} \to \int q(\theta \mid y)\mathrm{d}\theta$ (for the denominator)

And second:

$$\frac{1}{S}\sum_{s=1}^{S} h(\theta^s)\frac{q(\theta^s \mid y)}{g(\theta^s)} \to E_g\left[h(\theta)\frac{q(\theta \mid y)}{g(\theta)}\right] = \int h(\theta)q(\theta \mid y)\mathrm{d}\theta$$

which converges to the numerator

Importance Sampling

1. $E_q[h(\theta) \mid y] = \frac{\int h(\theta)q(\theta|y)\mathrm{d}\theta}{\int q(\theta|y)\mathrm{d}\theta}$
2. $\frac{1}{S}\sum_{s=1}^{S} \frac{q(\theta^s|y)}{g(\theta^s)} \to \int q(\theta \mid y)\mathrm{d}\theta$
3. $\frac{1}{S}\sum_{s=1}^{S} h(\theta^s)\frac{q(\theta^s|y)}{g(\theta^s)} \to \int h(\theta)q(\theta \mid y)\mathrm{d}\theta$

So finally

$$\sum_{i=1}^{S} w(\theta^s)h(\theta^s) = \frac{\sum_{s=1}^{S} h(\theta^s)\frac{q(\theta^s|y)}{g(\theta^s)}}{\sum_{r=1}^{S} \frac{q(\theta^r|y)}{g(\theta^r)}} = \frac{\frac{1}{S}\sum_{s=1}^{S} h(\theta^s)\frac{q(\theta^s|y)}{g(\theta^s)}}{\frac{1}{S}\sum_{r=1}^{S} \frac{q(\theta^r|y)}{g(\theta^r)}} \to E[h(\theta) \mid y]$$

where $w(\theta^s) = \frac{q(\theta^s|y)}{g(\theta^s)} \Big/ \sum_{r=1}^{S} \frac{q(\theta^r|y)}{g(\theta^r)}$ are the self-normalized weights

Example 2

Assume $y \sim \text{Normal}(\theta, 1)$, and $p(\theta) = \frac{1}{\pi(1+\theta^2)}$. Approximate $E_q[\theta \mid y]$ using proposal $g(\theta) = p(\theta)$.

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If we sample from $g(\theta) = p(\theta) = \frac{1}{\pi(1+\theta^2)}$ then the unnormalized weights are

$$
\begin{aligned}
\tilde{w}(\theta^s) &= \frac{q(\theta^s \mid y)}{g(\theta^s)} \\
&= p(y \mid \theta^s) \\
&= \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}(y - \theta^s)^2\right]
\end{aligned}
$$

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&= \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}(y - \theta^s)^2\right]
\end{aligned}
$$

then normalize these...

Example 2

```
y <- 2 # fake data
num_samples <- 1000000
theta_draws <- rt(num_samples , 1)
log_unnorm_weight <- function(theta){
  # can ignore sqrt(2pi) because it will cancel out
  -.5*(y - theta)^2
}
lunws <- log_unnorm_weight(theta_draws)
norm_weights <- exp(lunws)/sum(exp(lunws))
sum(norm_weights * theta_draws)
hist(norm_weights)
```

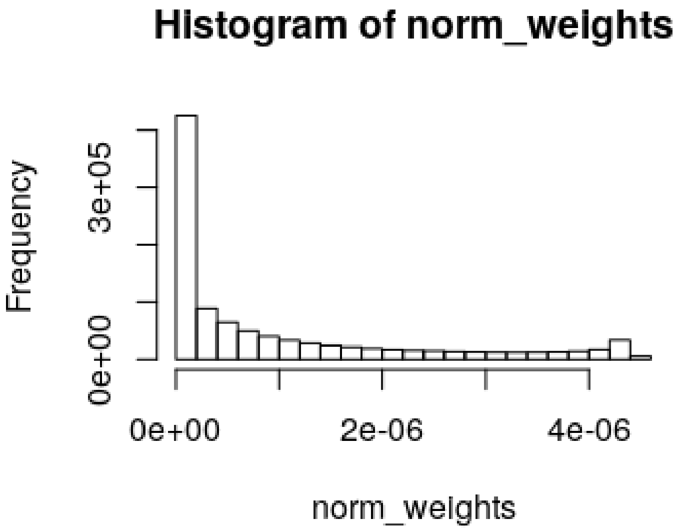
Example 2

The choice of proposal is very important.

$$\text{Var}_g\left(\sum_{s=1}^{S} w(\theta^s)h(\theta^s)\right) \approx \sum_{s=1}^{S} E_g\left[w(\theta^s)(h(\theta^s) - E_q[h(\theta)])\right]^2$$

Beware of proposals that have tails that are thin relative to the target!

Example 2


Histogram of norm_weights
Frequency
0e+00
3e+05
0e+00
2e-06
4e-06
norm_weights

Example 2

Beware of bad proposal distributions!

A sample estimator of this approximate variance is

$$\sum_{s=1}^{S} w(\theta^s)^2 \left(h(\theta^s) - \hat{E}[h(\theta)] \right)^2$$

where $\hat{E}[h(\theta)] = \sum_s w(\theta^s) h(\theta^s)$.

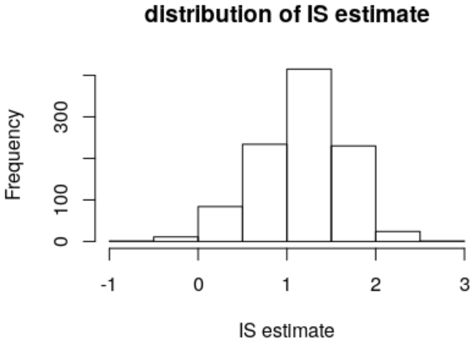
Note the weights aren't the same for each sample, like a "standard" estimation of the sample variance.

Example 2

```
y <- 2 # fake data
log_unnorm_weight <- function(theta){
  # can ignore sqrt(2pi) because it will cancel out
  -.5*(y - theta)^2 }
getISEstimator <- function(num_samples){
  theta_draws <- rt(num_samples, 1)
  lunws <- log_unnorm_weight(theta_draws)
  norm_weights <- exp(lunws)/sum(exp(lunws))
  estimator <- sum(norm_weights * theta_draws)
  list("estimate" = estimator,
       "approx_var" =
       sum( norm_weights^2*(theta_draws - estimator)^2) ) }
```

Example 2

```
hist(
  replicate(1000,
            getISEstimator(num_samps_per_estimate)$estimate),
  xlab = "IS estimate",
  main = "distribution of IS estimate")
```



Example 2

Two ways to calculate standard errors

```
num_samps_per_estimate <- 10
sqrt(getISEstimator(num_samps_per_estimate)$approx_var)
sd(replicate(1000,
    getISEstimator(num_samps_per_estimate)$estimate))
```

Effective Sample Size

Calculating

$$\mathrm{ESS} = \frac{1}{\sum_{s=1}^{S} w(\theta^s)^2}$$

will tell you, effectively, how many iid samples you have.