

Monte Carlo approximation

Bayesian Methodology in Biostatistics (BST 249)

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Outline

Introduction

Monte Carlo approximation

Example: The Pygmalion effect

Importance sampling (IS) approximation

Example: GPS data with outliers

IS with unknown normalization constants

Basic techniques for generating samples

Inverse c.d.f. method

Rejection sampling

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Introduction

- Sampling-based methods are widely used due to the ease and generality with which they can be applied.
- Basic task: Approximation of expectations such as

$$Eh(X) = \int h(x)p(x)dx$$

in the case of a continuous random variable X with p.d.f. p , or

$$Eh(X) = \sum_x h(x)p(x)$$

in the case of a discrete random variable X with p.m.f. p .

- General principle: Expectations can be approximated by

$$Eh(X) \approx \frac{1}{N} \sum_{i=1}^N h(X_i),$$

where X_1, \dots, X_N are samples from p .

Introduction

- In Bayesian statistics, most inferential tasks require computation of some expectation.
- Examples
 - ▶ posterior probabilities
 - ▶ posterior densities
 - ▶ posterior expected loss
 - ▶ posterior predictive distribution
 - ▶ marginal likelihood
 - ▶ goodness-of-fit statistics
- Samples are also a good way of visualizing where a probability distribution is putting most of its mass.
 - ▶ This is especially useful for distributions on complex/high-dim spaces, e.g., the folding of a protein or RNA strand.

Introduction

- Advantages of sampling-based methods:
 - ▶ easy to implement
 - ▶ general-purpose / widely applicable
 - ▶ reliable
 - ▶ work in complex and high-dimensional spaces
- Disadvantages of sampling-based methods:
 - ▶ slow (require more time to achieve the same level of accuracy)
 - ▶ getting “true” samples may be difficult
 - ▶ can be difficult to assess accuracy

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Monte Carlo approximation

- Suppose we want to know the expectation of a random variable $X \sim P$.
- *Simple Monte Carlo*: Draw samples $X_1, \dots, X_N \stackrel{\text{iid}}{\sim} P$ and use

$$\frac{1}{N} \sum_{i=1}^N X_i$$

as an approximation to $\mathbb{E}X$.

- More generally,

$$\mathbb{E}(h(Y) \mid Z = z) \approx \frac{1}{N} \sum_{i=1}^N h(Y_i)$$

where Y_1, \dots, Y_N are i.i.d. samples from the distribution of $Y \mid Z = z$.

- ▶ This can be viewed as a special case of $\mathbb{E}X$ where X is defined to have the same distribution as $h(Y) \mid Z = z$.

Monte Carlo: Basic properties

- If $E|X| < \infty$, then $\frac{1}{N} \sum X_i$ is a consistent estimator of EX :

$$\frac{1}{N} \sum_{i=1}^N X_i \longrightarrow EX$$

as $N \rightarrow \infty$, with probability 1, by the law of large numbers.

- $\frac{1}{N} \sum X_i$ is an unbiased estimator of EX , that is,

$$E\left(\frac{1}{N} \sum X_i\right) = EX.$$

- Who can tell me the variance of $\frac{1}{N} \sum X_i$?

Monte Carlo: Basic properties

- The variance is $\mathbb{V}(\frac{1}{N} \sum X_i) = \frac{1}{N} \mathbb{V}(X)$.
- Due to unbiasedness, the root-mean-squared-error (RMSE) of $\frac{1}{N} \sum X_i$ equals the standard deviation of $\frac{1}{N} \sum X_i$,

$$\begin{aligned} \text{RMSE} &= \left[\mathbb{E} \left(\left| \frac{1}{N} \sum X_i - \mathbb{E}X \right|^2 \right) \right]^{1/2} \\ &= \left[\mathbb{V} \left(\frac{1}{N} \sum X_i \right) \right]^{1/2} \\ &= \frac{1}{\sqrt{N}} \mathbb{V}(X)^{1/2} = \frac{\sigma(X)}{\sqrt{N}}. \end{aligned} \tag{1}$$

- The RMSE tells us how far the approximation will be from the true value, on average. This tells us that the rate of convergence is of order $1/\sqrt{N}$.

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Example: The Pygmalion effect

- To compute the posterior probability that the spurters had a larger mean increase in IQ score, we used the Monte Carlo approximation

$$\mathbb{P}(\mu_S > \mu_C \mid \text{data}) \approx \frac{1}{N} \sum_{i=1}^N \mathbb{I}(\mu_S^{(i)} > \mu_C^{(i)}).$$

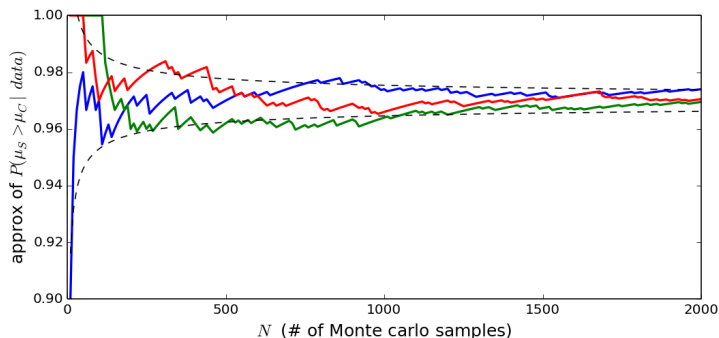
- Using the same approach, we could easily approximate any number of other posterior quantities as well, for example,

$$\mathbb{E}(|\mu_S - \mu_C| \mid \text{data}) \approx \frac{1}{N} \sum_{i=1}^N |\mu_S^{(i)} - \mu_C^{(i)}|$$

$$\mathbb{E}(\mu_S / \mu_C \mid \text{data}) \approx \frac{1}{N} \sum_{i=1}^N \mu_S^{(i)} / \mu_C^{(i)}.$$

- The posterior density can also be approximated using samples from the posterior.

Example: The Pygmalion effect



- The plot shows Monte Carlo approximations for an increasing number of samples, N .
- Red, blue, and green indicate three repetitions using different sequences of Monte Carlo samples.
- Dotted lines indicate the true value \pm the theoretical RMSE of the Monte Carlo estimator.

Approximating the posterior predictive density

- A Monte Carlo approximation to the posterior predictive p.d.f. or p.m.f. can be made using samples from the posterior:

$$\begin{aligned} p(x_{n+1}|x_{1:n}) &= \int p(x_{n+1}|\theta)p(\theta|x_{1:n})d\theta \\ &= \mathbb{E}(p(x_{n+1}|\boldsymbol{\theta}) | x_{1:n}) \\ &\approx \frac{1}{N} \sum_{i=1}^N p(x_{n+1}|\boldsymbol{\theta}_i) \end{aligned}$$

where $\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_N \stackrel{\text{iid}}{\sim} p(\theta|x_{1:n})$.

- This is useful when it is difficult or impossible to evaluate the integral analytically.

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Importance sampling approximation

- Importance sampling (IS) is a more powerful type of Monte Carlo approximation.
- The name “importance sampling” is somewhat misleading, since it is not really a method for drawing samples, but rather, a method for approximating expectations—a better name might be importance-weighted Monte Carlo approximation.
- Advantages of importance sampling over simple Monte Carlo:
 - ▶ Can significantly improve accuracy, by reducing the variance.
 - ▶ Can use samples from a different distribution, say q , to compute expectations with respect to p .
 - ▶ Can compute the normalization constant of p .
- Disadvantages
 - ▶ Need to be able to evaluate the p.d.f.s/p.m.f.s $p(x)$ and $q(x)$, at least up to proportionality constants.
 - ▶ It might be hard to choose a good q .

Importance sampling: Basic idea

- Suppose X is a continuous random variable with p.d.f. $p(x)$.
 - ▶ The same thing works in the discrete case — just replace integrals by sums.
- Let q be another p.d.f. on the same space, such that
 1. we can easily sample from q , and
 2. $q(x) > 0$ wherever $p(x) > 0$.
- (Whiteboard:) An *importance sampling approximation* is

$$\begin{aligned} \mathbb{E}h(X) &= \int h(x)p(x)dx \\ &= \int h(x)\frac{p(x)}{q(x)}q(x)dx \\ &\approx \frac{1}{N} \sum_{i=1}^N h(Y_i)\frac{p(Y_i)}{q(Y_i)} \end{aligned}$$

where $Y_1, \dots, Y_N \stackrel{\text{iid}}{\sim} q$.

Importance sampling: Basic idea

- Importance sampling: $Eh(X) \approx \frac{1}{N} \sum_{i=1}^N h(Y_i) \frac{p(Y_i)}{q(Y_i)}$.
- The approximation step here is just a simple Monte Carlo approximation, applied to a different function and distribution.
- q is sometimes called the *proposal distribution*.
- The ratios $w(Y_i) := p(Y_i)/q(Y_i)$ are referred to as the *importance weights*.
- Intuitive interpretation: The importance weights correct for the fact that we are sampling from q rather than p .
 - ▶ y 's that occur less frequently under q than p have large importance weight $w(y)$, and vice versa.

Importance sampling: Properties

- Evaluating the IS weights
 - ▶ For the version of IS above, we need to be able to compute $p(x)$ and $q(x)$ in order to get the importance weights.
 - ▶ There is a more general version for which $p(x)$ and $q(x)$ only need to be computable up to constants of proportionality.
- Since the IS approximation is just a simple Monte Carlo approx of $E h(Y)p(Y)/q(Y)$, it has the following properties:
 - ▶ consistent, as long as $E|h(Y)p(Y)/q(Y)| < \infty$, where $Y \sim q$
 - ▶ unbiased
 - ▶ the variance of the estimator is $\frac{1}{N} \mathbb{V}(h(Y)p(Y)/q(Y))$
 - ▶ the RMSE is $\sigma(h(Y)p(Y)/q(Y))/\sqrt{N}$.

Importance sampling: Choosing the proposal distribution

- The rate of convergence is still of order $1/\sqrt{N}$, however, the constant $\sigma(h(Y)p(Y)/q(Y))$ may be smaller or larger.
- How to choose q to minimize RMSE?
- RMSE is minimized when $q(x) \propto h(x)p(x)$, since then $\sigma(h(Y)p(Y)/q(Y)) = 0$.
 - ▶ In other words, the error would be zero after only one sample!
 - ▶ In this case, we could trivially compute $Eh(X)$ since $Eh(X) = \int h(x)p(x)/q(x) q(x) dx$ for almost all x .
- Although this ideal choice of q is unrealistic, it indicates that:
 1. IS can be very accurate if we choose q well, and
 2. we want $q(x)$ to look roughly like $h(x)p(x)$.

Importance sampling: Choosing the proposal distribution

- In practice, we often want to estimate $Eh(X)$ for a variety of different functions h .
- Thus, we often choose $q(x)$ to approximate $p(x)$ rather than $h(x)p(x)$.
 - ▶ That way, we can obtain decent estimators for many h 's.
 - ▶ Plus, we can reuse the same samples Y_i and the same importance weights $w(Y_i) = p(Y_i)/q(Y_i)$.
- When choosing $q(x)$, it is better to err on the side of making it a little more spread out than $p(x)$ (or $h(x)p(x)$).
 - ▶ This is done so that $q(x)$ is not too small in areas where $p(x)$ is large.
 - ▶ Otherwise, we would occasionally encounter very large IS weights $w(Y_i) = p(Y_i)/q(Y_i)$, which would increase the RMSE.

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GPS example: Approximating the marginal likelihood

- Outside of conjugate priors, computing the marginal likelihood can be very hard and is often not recommended.
- If it must be computed, IS and related techniques are one reasonable approach.
- Suppose we are using a Cauchy model, to handle outliers:

$$X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Cauchy}(\theta, s).$$

- The Cauchy distribution with location θ and scale s has p.d.f.

$$\text{Cauchy}(x \mid \theta, s) = \frac{1}{\pi s \left(1 + \left(\frac{x-\theta}{s}\right)^2\right)}.$$

- Unfortunately, there is not a nice conjugate prior for θ .
- Let's put a Cauchy prior on θ :

$$\theta \sim \text{Cauchy}(\theta_0, s_0).$$

GPS example: Data

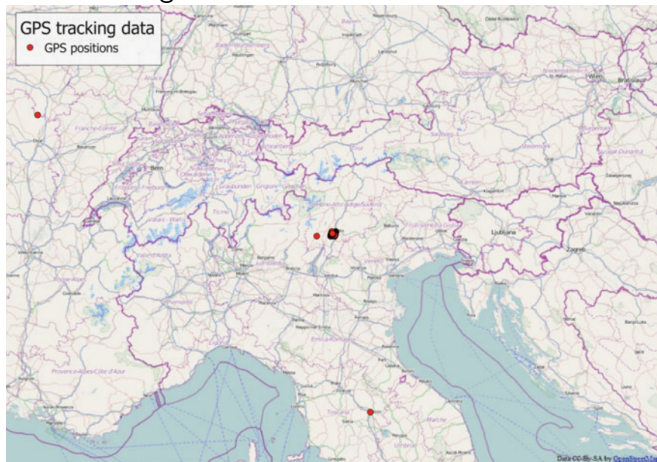
- GPS measurements are usually fairly accurate, but it is not uncommon to get extreme outliers.
- In wildlife management and conservation, animals are tagged with GPS devices in order to track their movements.
- Urbano (2014) provide GPS data on wildlife tracking in northern Italy. Here is a sample of 8 points for illustration:

Latitude	Longitude
36.077916 N	79.009266 W
36.078032 N	79.009180 W
36.078129 N	79.009094 W
36.078048 N	79.008891 W
36.077942 N	79.008962 W
36.089612 N	79.035760 W
36.077789 N	79.008917 W
36.077563 N	79.009281 W

- To keep things simple, let's consider only the latitudes.

GPS example: Data

Animal-tracking GPS measurements with extreme outliers



(Urbano et al., 2014)

GPS example: Approximating the marginal likelihood

- Suppose we need to know the marginal likelihood $p(x_{1:n})$.
- Since we can't compute it analytically (as far as I know), an approximation is needed.
- One approach would be a simple Monte Carlo approximation:

$$p(x_{1:n}) = \int p(x_{1:n}|\theta)p(\theta)d\theta \approx \frac{1}{N} \sum_{i=1}^N p(x_{1:n}|\theta_i)$$

where $\theta_1, \dots, \theta_N \stackrel{\text{iid}}{\sim} p(\theta)$.

- However, this is a poor approximation (the RMSE is large).

GPS example: Approximating the marginal likelihood

- We can do much better with importance sampling if we make a good choice of q :

$$p(x_{1:n}) = \int p(x_{1:n}|\theta) \frac{p(\theta)}{q(\theta)} q(\theta) d\theta \approx \frac{1}{N} \sum_{i=1}^N p(x_{1:n}|\theta_i) \frac{p(\theta_i)}{q(\theta_i)}$$

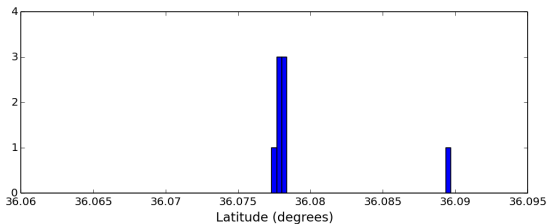
where $\theta_1, \dots, \theta_N \stackrel{\text{iid}}{\sim} q(\theta)$.

- We want $q(\theta)$ to look as much like $p(x_{1:n}|\theta)p(\theta)$ as possible, and if necessary, to err on the side of being a little more spread out.
- By cheating (a little bit) and looking at a plot of the posterior, let's choose

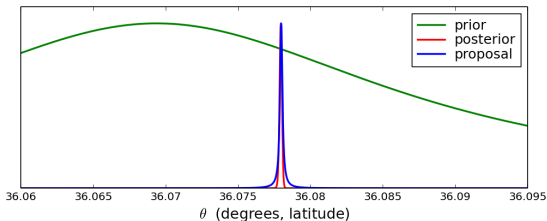
$$q(\theta) = \text{Cauchy}(\theta \mid \text{median}(x_{1:n}), 10^{-4}).$$

GPS example: Approximating the marginal likelihood

Histogram of latitude measurements



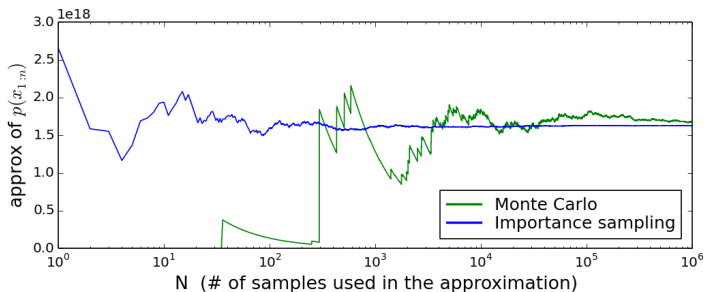
Prior, posterior, and proposal densities



(To make them all visible on one plot, each curve is scaled so that the maximum is 1.)

GPS example: Approximating the marginal likelihood

Convergence of Monte Carlo and IS approximations as N increases



- The IS approximations appear to converge much more quickly, by several orders of magnitude.

GPS example: Approximating the marginal likelihood

- Why does IS do so much better than Monte Carlo here?
- The prior is so spread out, compared to the likelihood, that samples from the prior very rarely land in the small region where the likelihood is large.
- So most of the terms in the Monte Carlo approximation are essentially zero, and a small number of terms are enormous.
- **Caution: Approximating the marginal likelihood can be a tricky business, and I would avoid it unless strictly necessary.**

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IS with unknown normalization constants

- Often, we cannot compute p and q , but we can compute functions \tilde{p} and \tilde{q} proportional to p and q .
- Fortunately, there is a neat trick that still allows us to make an IS approximation in this situation.
- Suppose

$$p(x) = \tilde{p}(x)/Z_p$$
$$q(x) = \tilde{q}(x)/Z_q$$

where $\tilde{p}(x)$ and $\tilde{q}(x)$ are easy to compute (but Z_p and Z_q may be intractable).

- Further, assume that $\tilde{q}(x) > 0$ wherever $\tilde{p}(x) > 0$.

IS with unknown normalization constants

- Define

$$\tilde{w}(x) = \begin{cases} \tilde{p}(x)/\tilde{q}(x) & \text{if } \tilde{q}(x) > 0 \\ 0 & \text{if } \tilde{q}(x) = 0. \end{cases}$$

- The general form of the IS approximation is then

$$\begin{aligned} \mathbb{E}h(X) &= \int h(x)p(x)dx \approx \frac{\frac{1}{N} \sum_{i=1}^N h(Y_i)\tilde{w}(Y_i)}{\frac{1}{N} \sum_{i=1}^N \tilde{w}(Y_i)} \\ &= \sum_{i=1}^N h(Y_i) \left(\frac{\tilde{w}(Y_i)}{\sum_{j=1}^N \tilde{w}(Y_j)} \right) \end{aligned}$$

where $Y_1, \dots, Y_N \stackrel{\text{iid}}{\sim} q$.

- This can be interpreted as a weighted average of the $h(Y_i)$'s, with weights $\tilde{w}(Y_i)/\sum_j \tilde{w}(Y_j)$.

Example: Approximating posterior expectations

- Consider the animal-tracking GPS example, and now suppose we would like to estimate the posterior mean. Define

$$\pi(\theta) := p(\theta|x_{1:n})$$

$$\tilde{\pi}(\theta) := p(x_{1:n}|\theta)p(\theta)$$

$$Z_\pi := p(x_{1:n}) = \int p(x_{1:n}|\theta)p(\theta)d\theta = \int \tilde{\pi}(\theta)d\theta.$$

- Then $\pi(\theta) = \tilde{\pi}(\theta)/Z_\pi$, and using the general IS formula,

$$\begin{aligned} E(\theta|x_{1:n}) &= \int \theta p(\theta|x_{1:n})d\theta = \int \theta \pi(\theta)d\theta \\ &\approx \frac{\frac{1}{N} \sum_{i=1}^N \theta_i \tilde{w}(\theta_i)}{\frac{1}{N} \sum_{i=1}^N \tilde{w}(\theta_i)}. \end{aligned}$$

where $\theta_1, \dots, \theta_N \stackrel{\text{iid}}{\sim} q$ and $\tilde{w}(\theta) = \tilde{\pi}(\theta)/q(\theta)$.

- For the GPS data, this yields $E(\theta|x_{1:n}) \approx 36.0780$.

Derivation of the general IS formula

(Whiteboard activity)

Derivation of the general IS formula (1/2)

- Letting $S = \{x : \tilde{p}(x) > 0\}$, we have

$$\begin{aligned} \mathbb{E}h(X) &= \int h(x)p(x)dx \\ &\stackrel{(a)}{=} \int_S h(x) \frac{\tilde{p}(x)}{Z_p} \frac{Z_q}{\tilde{q}(x)} q(x) dx \\ &\stackrel{(b)}{=} \frac{Z_q}{Z_p} \int h(x) \tilde{w}(x) q(x) dx \\ &\stackrel{(c)}{\approx} \frac{Z_q}{Z_p} \frac{1}{N} \sum_{i=1}^N h(Y_i) \tilde{w}(Y_i). \end{aligned}$$

- In step (a), we use the fact that $\tilde{q}(x) > 0$ whenever $\tilde{p}(x) > 0$.
- In step (b), we use the fact that $\tilde{w}(x) = 0$ for any $x \notin S$.
- Step (c) is a simple Monte Carlo approximation.

Derivation of the general IS formula (2/2)

- Similarly, for the ratio of normalizing constants Z_p/Z_q ,

$$\begin{aligned}\frac{Z_p}{Z_q} &= \frac{1}{Z_q} \int_S \tilde{p}(x) dx \\ &= \frac{1}{Z_q} \int_S \frac{\tilde{p}(x)}{\tilde{q}(x)} \tilde{q}(x) dx \\ &= \int_S \frac{\tilde{p}(x)}{\tilde{q}(x)} q(x) dx \\ &= \int \tilde{w}(x) q(x) dx \\ &\approx \frac{1}{N} \sum_{i=1}^N \tilde{w}(Y_i).\end{aligned}$$

- Plugging this into the equation on the previous slide yields the result.

Group activity: Check your understanding

Go to breakout rooms and work together to answer these questions:

<https://forms.gle/NKwmWrwNMF6ezoBm6>

(Three people per room, randomly assigned. 15 minutes.)

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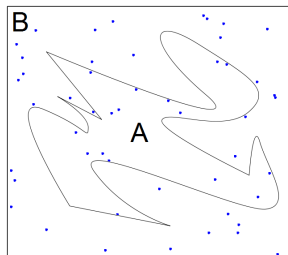
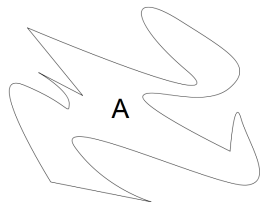
Inverse c.d.f. method / Smirnov transform

- The *inverse c.d.f. method* is a common way of generating random samples from univariate probability distributions when the inverse of the c.d.f. can be easily computed.
- The basic idea is that if G is the inverse (in a generalized sense) of the c.d.f. F , and $U \sim \text{Uniform}(0, 1)$, then $G(U)$ is a random variable with c.d.f. F .
- $\text{Exp}(\theta)$ example:
 - ▶ The $\text{Exp}(\theta)$ c.d.f. is $F(x) = (1 - e^{-\theta x})\mathbf{I}(x > 0)$.
 - ▶ F is invertible on $(0, \infty)$, with inverse $G(u) = -(1/\theta) \log(1 - u)$ for $u \in (0, 1)$.
 - ▶ Therefore, if $U \sim \text{Uniform}(0, 1)$ then $G(U) \sim \text{Exp}(\theta)$.
- Precise statement: Let F be a c.d.f. on \mathbb{R} , and define $G(u) = \inf\{x \in \mathbb{R} : F(x) \geq u\}$ for $u \in (0, 1)$. If $U \sim \text{Uniform}(0, 1)$, then $G(U) \sim F$.

Rejection sampling

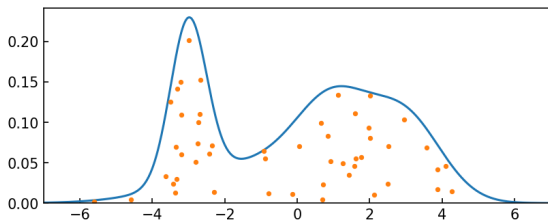
- Rejection sampling is a method for drawing samples when the p.d.f. can be evaluated up to a constant of proportionality.
- Rejection sampling can be applied in multivariate settings, but one has to design a good proposal distribution q .
 - ▶ Finding a good q can be difficult, especially in high-dim cases.
- The method relies on two principles:
 1. **The rejection principle:** Rejecting results in conditional samples. That is, if we reject any samples falling outside of a given set, the remaining samples are distributed according to the conditional distribution on that set.
 2. **The projection principle:** If we sample uniformly from the region under the p.d.f. of a distribution (or a function proportional to it), and discard the “height”, then we obtain a sample from that distribution.

The rejection principle



- How to draw samples from the uniform distribution on A ?
- Rejection-based approach: Draw samples uniformly from B and keep only those that are in A .
- To minimize rejections, we want the bounding region B to be as small as possible, while still containing A .
- More generally, if we sample X , and reject unless $X \in A$, we get samples from the conditional distribution $X \mid X \in A$.

The projection principle



- Suppose we want to sample from a distribution on \mathbb{R}^d with p.d.f. $\pi(x) = \tilde{\pi}(x)/Z_\pi$.
- Consider the region of \mathbb{R}^{d+1} under $\tilde{\pi}$:

$$A = \left\{ (x, y) : x \in \mathbb{R}^d, 0 < y < \tilde{\pi}(x) \right\}.$$

- It turns out that if $(X, Y) \sim \text{Uniform}(A)$, then $X \sim \pi$.

The projection principle

- To see why, first note that the volume of A is

$$\text{Vol}(A) = \int \tilde{\pi}(x) dx = \int Z_{\pi} \pi(x) dx = Z_{\pi}.$$

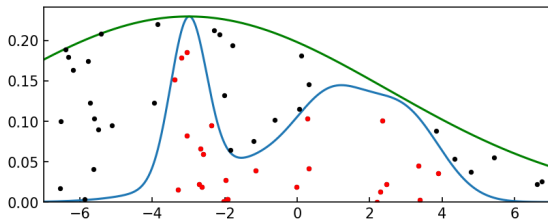
- Since the p.d.f. of the uniform distribution on A is constant, we have

$$p(x, y) = \text{Uniform}(x, y | A) = \frac{\mathbf{I}(0 < y < \tilde{\pi}(x))}{Z_{\pi}}.$$

- Therefore,

$$\begin{aligned} p(x) &= \int_{-\infty}^{\infty} p(x, y) dy = \int_{-\infty}^{\infty} \frac{\mathbf{I}(0 < y < \tilde{\pi}(x))}{Z_{\pi}} dy \\ &= \frac{1}{Z_{\pi}} \int_0^{\tilde{\pi}(x)} dy = \frac{\tilde{\pi}(x)}{Z_{\pi}} = \pi(x). \end{aligned}$$

Rejection sampling procedure



- Combining these two principles leads to rejection sampling.
- Basic idea: Generate samples uniformly under a curve that dominates $\tilde{p}(x)$, and only keep samples that land under $\tilde{p}(x)$.
- This generates samples from $p(x) \propto \tilde{p}(x)$.

Rejection sampling procedure

- Objective: Generate samples from a distribution on \mathbb{R}^d with p.d.f. $p(x) \propto \tilde{p}(x)$.
- Choose a proposal distribution q that is easy to sample from, and is as close as possible to being proportional to \tilde{p} .
- Choose $c > 0$ such that $c q(x) \geq \tilde{p}(x)$ for all x .
- Then, to draw a sample from p :
 1. Sample $X \sim q$.
 2. Sample $Y \sim \text{Uniform}(0, c q(X))$.
 3. If $Y \geq \tilde{p}(X)$, then go back to step 1.
 4. Otherwise, output X as a sample.

References and supplements

- Urbano, F., Basille, M., and Cagnacci, F. Data Quality: Detection and Management of Outliers. Spatial Database for GPS Wildlife Tracking Data. Springer International Publishing, 2014. 115-137.
- Radford Neal (2008), The Harmonic Mean of the Likelihood: Worst Monte Carlo Method Ever.
<https://radfordneal.wordpress.com/2008/08/17/the-harmonic-mean-of-the-likelihood-worst-monte-carlo-method-ever/>

Individual activity: Exit ticket

Answer these questions individually:

<https://forms.gle/mQeZJHMFZdz1oUAh6>