Sampling and Monte Carlo Integration

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Recap

Learning and inference often involves intractable sums or integrals, e.g.

- Marginalisation

$$p(\mathbf{x}) = \int_{\mathbf{y}} p(\mathbf{x}, \mathbf{y}) \mathrm{d}\mathbf{y}$$

- Expectations

$$\mathbb{E}\left[g(\mathbf{x}) \mid \mathbf{y}_o\right] = \int g(\mathbf{x}) p(\mathbf{x}|\mathbf{y}_o) \mathrm{d}\mathbf{x}$$

  for some function g.

- For unobserved variables, likelihood and gradient of the log lik

$$L(\boldsymbol{\theta}) = p(\mathcal{D}; \boldsymbol{\theta}) = \int_{\mathbf{u}} p(\mathbf{u}, \mathcal{D}; \boldsymbol{\theta}) \mathrm{d}\mathbf{u},$$

$$\nabla_{\boldsymbol{\theta}} \ell(\boldsymbol{\theta}) = \mathbb{E}_{p(\mathbf{u}|\mathcal{D};\boldsymbol{\theta})}\left[\nabla_{\boldsymbol{\theta}} \log p(\mathbf{u}, \mathcal{D}; \boldsymbol{\theta})\right]$$

Recap

- For unnormalised models with intractable partition functions

$$L(\boldsymbol{\theta}) = \frac{\tilde{p}(\mathcal{D}; \boldsymbol{\theta})}{\int_{\mathbf{x}} \tilde{p}(\mathbf{x}; \boldsymbol{\theta}) \mathrm{d}\mathbf{x}}$$

$$\nabla_{\boldsymbol{\theta}} \ell(\boldsymbol{\theta}) \propto \mathbf{m}(\mathcal{D}; \boldsymbol{\theta}) - \mathbb{E}_{p(\mathbf{x};\boldsymbol{\theta})} [\mathbf{m}(\mathbf{x}; \boldsymbol{\theta})]$$

- Combined case of unnormalised models with intractable partition functions and unobserved variables.
- We have seen variational inference as an approach to deal with intractable marginalisations and likelihoods due to unobserved variables.
- Here: methods to approximate integrals and expectations using sampling.

Program

1. Monte Carlo integration
2. Sampling

Program

1. Monte Carlo integration
   - Approximating expectations by averages
   - Importance sampling
   - Effective sample size
2. Sampling

Averages with iid samples

- (From exercises): For Gaussians, the sample average is an estimate (MLE) of the mean (expectation) $\mathbb{E}[x]$

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i \approx \mathbb{E}[x]$$

- Gaussianity not needed: assume x_i are iid observations of $x \sim p(x)$.

$$\mathbb{E}[x] = \int x p(x) \mathrm{d}x \approx \bar{x}_n \qquad \bar{x}_n = \frac{1}{n}\sum_{i=1}^{n} x_i$$

- Subscript n reminds us that we used n samples to compute the average.
- Approximating integrals by means of sample averages is called Monte Carlo integration.

Averages with iid samples

- Sample average is unbiased

$$\mathbb{E}\left[\bar{x}_n\right] = \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}[x_i] \overset{*}{=} \frac{n}{n}\mathbb{E}[x] = \mathbb{E}[x]$$

  ($*$: "identically distributed" assumption is used, not independence)
- Variability

$$\mathbb{V}\left[\bar{x}_n\right] = \frac{1}{n^2}\mathbb{V}\left[\sum_{i=1}^{n} x_i\right] \overset{*}{=} \frac{1}{n^2}\sum_{i=1}^{n}\mathbb{V}[x_i] = \frac{1}{n}\mathbb{V}[x]$$

  ($*$: independence assumption used)
- Expected squared error decreases as $1/n$

$$\mathbb{E}\left[\left(\bar{x}_n - \mathbb{E}[x]\right)^2\right] = \mathbb{V}\left[\bar{x}_n\right] = \frac{1}{n}\mathbb{V}[x]$$

Averages with iid samples

- Weak law of large numbers:

$$\mathbb{P}\left(|\bar{x}_n - \mathbb{E}[x]| \geq \epsilon\right) \leq \frac{\mathbb{V}[x]}{n\epsilon^2}$$

- As $n \to \infty$, the probability for the sample average to deviate from the expected value goes to zero if the variance is finite.
- We say that sample average converges in probability to the expected value.
- Speed of convergence depends on the variance $\mathbb{V}[x]$.
- Different “laws of large numbers” exist that make different assumptions.

Chebyshev's inequality

- Weak law of large numbers is a direct consequence of Chebyshev's inequality
- Chebyshev's inequality: Let s be some random variable with mean $\mathbb{E}[s]$ and variance $\mathbb{V}[s]$.

$$\mathbb{P}\left(|s - \mathbb{E}[s]| \geq \epsilon\right) \leq \frac{\mathbb{V}[s]}{\epsilon^2}$$

- This means that for *all* random variables with finite mean and variance:
  - probability to deviate more than three standard deviation from the mean is less than $1/9 \approx 0.11$ (set $\epsilon = 3\sqrt{\mathbb{V}(s)}$)
  - Probability to deviate more than 6 standard deviations: $1/36 \approx 0.03$.

These are conservative values; for many distributions, the probabilities will be smaller.

Proofs (not examinable)

- Chebyshev's inequality follows from Markov's inequality.
- Markov's inequality: For a random variable $y \geq 0$

$$\mathbb{P}(y \geq t) \leq \frac{\mathbb{E}[y]}{t} \quad (t > 0)$$

- Chebyshev's inequality is obtained by setting $y = |s - \mathbb{E}[s]|$

$$\mathbb{P}\left(|s - \mathbb{E}[s]| \geq t\right) = \mathbb{P}\left((s - \mathbb{E}[s])^2 \geq t^2\right)$$
$$\leq \frac{\mathbb{E}\left[(s - \mathbb{E}[s])^2\right]}{t^2}.$$

Chebyshev's inequality follows with $t = \epsilon$, and because $\mathbb{E}[(s - \mathbb{E}[s]^2)]$ is the variance $\mathbb{V}[s]$ of s.

Proofs (not examinable)

Proof for Markov's inequality: Let t be an arbitrary positive number and y a one-dimensional non-negative random variable with pdf p.
We can decompose the expectation of y using t as split-point,

$$\mathbb{E}[y] = \int_0^\infty u p(u) \mathrm{d}u = \int_0^t u p(u) \mathrm{d}u + \int_t^\infty u p(u) \mathrm{d}u.$$

Since $u \geq t$ in the second term, we obtain the inequality

$$\mathbb{E}[y] \geq \int_0^t u p(u) \mathrm{d}u + \int_t^\infty t p(u) \mathrm{d}u.$$

The second term is t times the probability that $y \geq t$, so that

$$\begin{aligned} \mathbb{E}[y] &\geq \int_0^t u p(u) \mathrm{d}u + t\mathbb{P}(y \geq t) \\ &\geq t\mathbb{P}(y \geq t), \end{aligned}$$

where the second line holds because the first term in the first line is non-negative. This gives Markov's inequality

$$\mathbb{P}(y \geq t) \leq \frac{\mathbb{E}(y)}{t} \quad (t > 0)$$

Averages with correlated samples

- When computing the variance of the sample average

$$\mathbb{V}\left[\bar{x}_n\right] = \frac{\mathbb{V}[x]}{n}$$

  we assumed the samples are identically and independently distributed.
- The variance shrinks with increasing n and the average becomes more and more concentrated around $\mathbb{E}[x]$.
- Corresponding results exist for the case of statistically dependent samples x_i. Known as “ergodic theorems”.
- Out of scope for PMR but important for the theory of Markov chain Monte Carlo methods.

More general expectations

- So far, we have considered

$$\mathbb{E}[x] = \int x p(x) \mathrm{d}x \approx \frac{1}{n} \sum_{i=1}^{n} x_i$$

  where $x_i \sim p(x)$
- This generalises

$$\mathbb{E}[g(\mathbf{x})] = \int g(\mathbf{x}) p(\mathbf{x}) \mathrm{d}\mathbf{x} \approx \frac{1}{n} \sum_{i=1}^{n} g(\mathbf{x}_i)$$

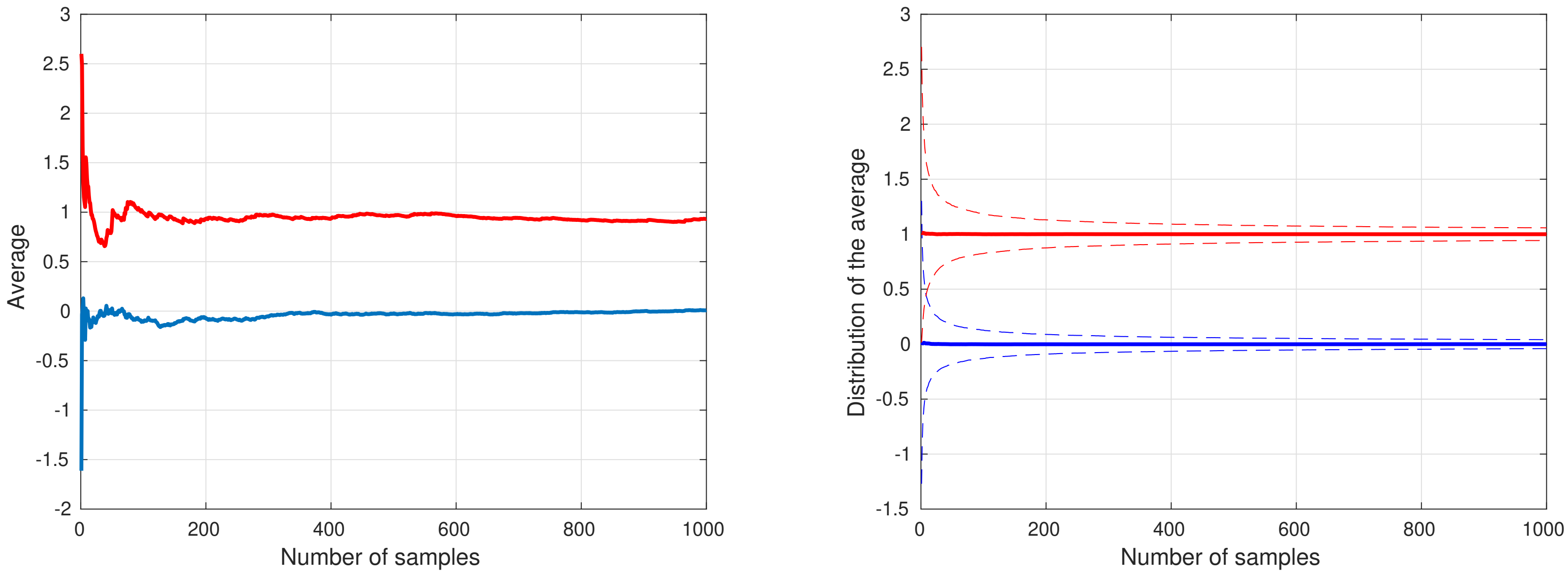
  where $\mathbf{x}_i \sim p(\mathbf{x})$
- Variance of the approximation if the $\mathbf{x}_i$ are iid is $\frac{1}{n}\mathbb{V}[g(\mathbf{x})]$

Example (Based on a slide from Amos Storkey)

$$\mathbb{E}[g(x)] = \int g(x)\mathcal{N}(x;0,1)\mathrm{d}x \approx \frac{1}{n}\sum_{i=1}^{n} g(x_i) \qquad (x_i \sim \mathcal{N}(x;0,1))$$

for $g(x) = x$ and $g(x) = x^2$

Left: sample average as a function of n
Right: Variability (0.5 quantile: solid, 0.1 and 0.9 quantiles: dashed)



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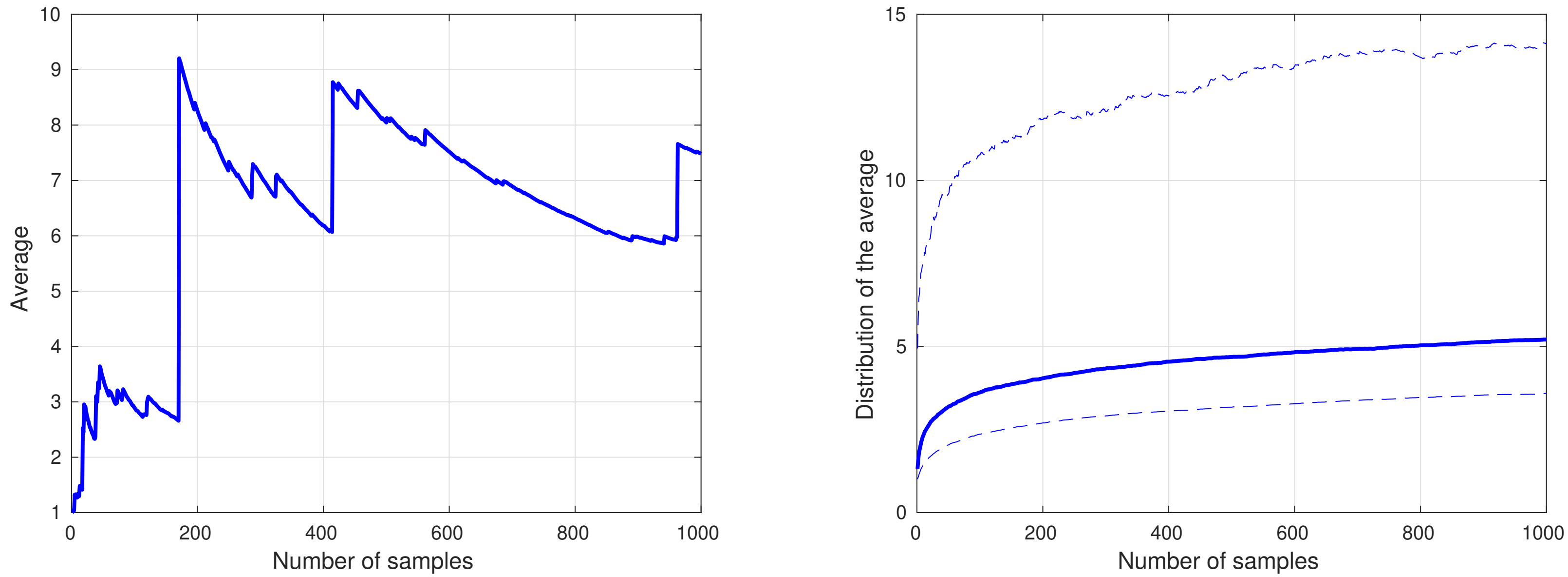
for $g(x) = \exp(0.6x^2)$

Left: sample average as a function of n

Right: Variability (0.5 quantile: solid, 0.1 and 0.9 quantiles: dashed)



Example

- Indicators that something is wrong:
  - Strong fluctuations in the sample average as n increases.
  - Large non-declining variability.
- Note: integral is not finite:

$$\begin{aligned}\int \exp(0.6x^2)\mathcal{N}(x;0,1)\mathrm{d}x &= \frac{1}{\sqrt{2\pi}}\int \exp(0.6x^2)\exp(-0.5x^2)\mathrm{d}x \\ &= \frac{1}{\sqrt{2\pi}}\int \exp(0.1x^2)\mathrm{d}x \\ &= \infty\end{aligned}$$

  but for any n, the sample average is finite and may be mistaken for a good approximation.
- Check variability when approximating the expected value by a sample average!

Importance sampling to approximate integrals

- If the integral does not correspond to an expectation, we can smuggle in a pdf q to rewrite it as an expected value with respect to q

$$
\begin{aligned}
I = \int g(\mathbf{x}) \mathrm{d}\mathbf{x} &= \int g(\mathbf{x}) \frac{q(\mathbf{x})}{q(\mathbf{x})} \mathrm{d}\mathbf{x} \qquad \text{(assume } q(\mathbf{x}) > 0 \text{ when } g(\mathbf{x}) > 0\text{)} \\
&= \int \frac{g(\mathbf{x})}{q(\mathbf{x})} q(\mathbf{x}) \mathrm{d}\mathbf{x} \\
&= \mathbb{E}_{q(\mathbf{x})} \left[\frac{g(\mathbf{x})}{q(\mathbf{x})} \right] \\
&\approx \frac{1}{n} \sum_{i=1}^{n} \frac{g(\mathbf{x}_i)}{q(\mathbf{x}_i)}
\end{aligned}
$$

  with $x_i \sim q(\mathbf{x})$ (iid)
- This is the basic idea of importance sampling.
- q is called the importance (or proposal) distribution

Choice of the importance distribution

- Call the approximation $\widehat{I}$,

$$\widehat{I} = \frac{1}{n}\sum_{i=1}^{n} \frac{g(\mathbf{x}_i)}{q(\mathbf{x}_i)}$$

- $\widehat{I}$ is unbiased by construction

$$\mathbb{E}[\widehat{I}] = \mathbb{E}\left[\frac{g(\mathbf{x})}{q(\mathbf{x})}\right] = \int \frac{g(\mathbf{x})}{q(\mathbf{x})} q(\mathbf{x}) \mathrm{d}\mathbf{x} = \int g(\mathbf{x}) \mathrm{d}\mathbf{x} = I$$

- Variance

$$\mathbb{V}\left[\widehat{I}\right] = \frac{1}{n}\mathbb{V}\left[\frac{g(\mathbf{x})}{q(\mathbf{x})}\right] = \frac{1}{n}\mathbb{E}\left[\left(\frac{g(\mathbf{x})}{q(\mathbf{x})}\right)^2\right] - \frac{1}{n}\underbrace{\left(\mathbb{E}\left[\frac{g(\mathbf{x})}{q(\mathbf{x})}\right]\right)^2}_{I^2}$$

Depends on the second moment.

Choice of the importance distribution

- The second moment is

$$\mathbb{E}\left[\left(\frac{g(\mathbf{x})}{q(\mathbf{x})}\right)^2\right] = \int \left(\frac{g(\mathbf{x})}{q(\mathbf{x})}\right)^2 q(\mathbf{x})\mathrm{d}\mathbf{x} = \int \frac{g(\mathbf{x})^2}{q(\mathbf{x})}\mathrm{d}\mathbf{x}$$
$$= \int |g(\mathbf{x})| \frac{|g(\mathbf{x})|}{q(\mathbf{x})}\mathrm{d}\mathbf{x}$$

- Bad: $q(\mathbf{x})$ is small when $|g(\mathbf{x})|$ is large. Gives large variance.
- Good: $q(\mathbf{x})$ is large when $|g(\mathbf{x})|$ is large.
- Optimal q equals

$$q^*(\mathbf{x}) = \frac{|g(\mathbf{x})|}{\int |g(\mathbf{x})|\mathrm{d}\mathbf{x}}$$

- Optimal q cannot be computed, but justifies the heuristic that $q(\mathbf{x})$ should be large when $|g(\mathbf{x})|$ is large, or that the ratio $|g(\mathbf{x})|/q(\mathbf{x})$ should be approximately constant.

Proof (not examinable)

Since the variance of a random variable $|x|$ is non-negative and can be written as

$$\mathbb{V}[|x|] = \mathbb{E}[x^2] - (\mathbb{E}[|x|])^2,$$

we have

$$\mathbb{E}[x^2] \geq \mathbb{E}[|x|]^2$$

The smallest second moment achieves equality. We now verify that for $q^*(\mathbf{x})$, we have

$$\mathbb{E}\left[\left(\frac{g(\mathbf{x})}{q^*(\mathbf{x})}\right)^2\right] = \mathbb{E}\left[\left|\frac{g(\mathbf{x})}{q^*(\mathbf{x})}\right|\right]^2$$

Proof (not examinable)

Indeed, for the optimal q, we have

$$\mathbb{E}\left[\left(\frac{g(\mathbf{x})}{q^*(\mathbf{x})}\right)^2\right] = \int |g(\mathbf{x})| \frac{|g(\mathbf{x})|}{q^*(\mathbf{x})} \mathrm{d}\mathbf{x}$$
$$= \int |g(\mathbf{x})| \mathrm{d}\mathbf{x} \int |g(\mathbf{x})|^2 \frac{1}{|g(\mathbf{x})|} \mathrm{d}\mathbf{x}$$
$$= \left(\int |g(\mathbf{x})| \mathrm{d}\mathbf{x}\right)^2$$

and

$$\mathbb{E}\left[\left|\frac{g(\mathbf{x})}{q^*(\mathbf{x})}\right|\right]^2 = \left(\int \left|\frac{g(\mathbf{x})}{q^*(\mathbf{x})}\right| q^*(\mathbf{x}) \mathrm{d}\mathbf{x}\right)^2$$
$$= \left(\int |g(\mathbf{x})| \mathrm{d}\mathbf{x}\right)^2,$$

which concludes the proof.

Importance sampling to approximate the partition function

We can use importance sampling to approximate the partition function for unnormalised models $\tilde{p}(\mathbf{x}; \boldsymbol{\theta})$.

$$
\begin{aligned}
Z(\boldsymbol{\theta}) &= \int \tilde{p}(\mathbf{x}; \boldsymbol{\theta}) \mathrm{d}\mathbf{x} \\
&= \int \tilde{p}(\mathbf{x}; \boldsymbol{\theta}) \frac{q(\mathbf{x})}{q(\mathbf{x})} \mathrm{d}\mathbf{x} && \text{(assume } q(\mathbf{x}) > 0 \text{ when } \tilde{p}(\mathbf{x}) > 0\text{)} \\
&= \int \frac{\tilde{p}(\mathbf{x}; \boldsymbol{\theta})}{q(\mathbf{x})} q(\mathbf{x}) \mathrm{d}\mathbf{x} \\
&\approx \frac{1}{n} \sum_{i=1}^{n} \frac{\tilde{p}(\mathbf{x}_i; \boldsymbol{\theta})}{q(\mathbf{x}_i)} && (\mathbf{x}_i \sim q(\mathbf{x}) \text{ iid})
\end{aligned}
$$

Example

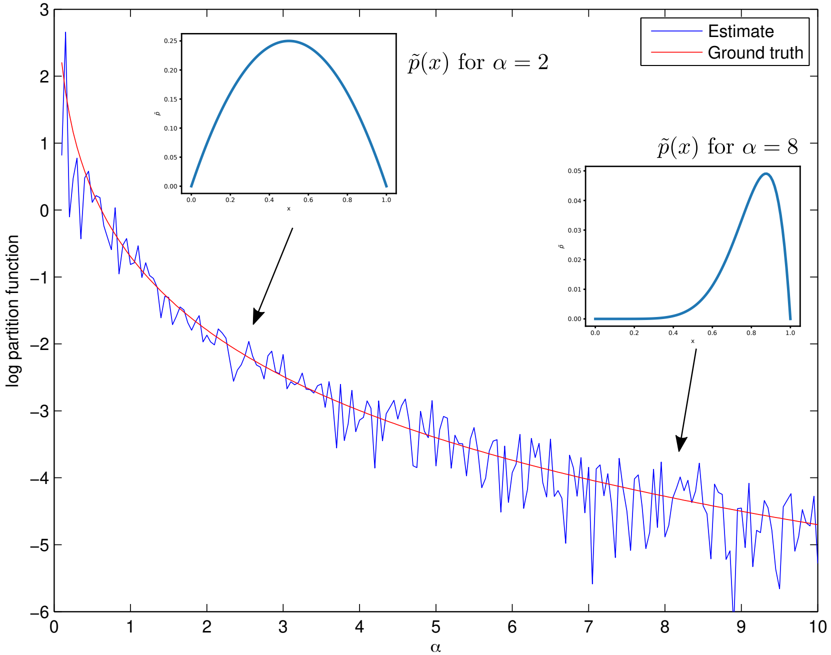
Approximating the log partition function of the unnormalised beta-distribution

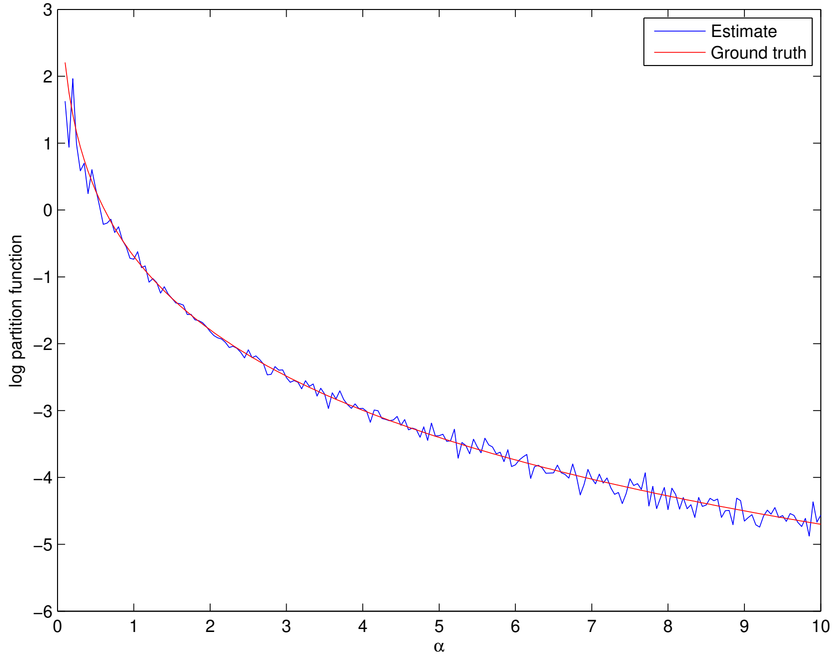
$$\tilde{p}(x; \alpha, \beta) = x^{\alpha-1}(1-x)^{\beta-1}, \qquad x \in [0, 1]$$

for β fixed to $\beta = 2$.

Importance distribution: uniform distribution on $[0, 1]$

Left: $n = 10$, right: $n = 100$.





Importance sampling to approximate expectations

- Assume you would like to approximate $\mathbb{E}_{p(\mathbf{x})}[g(\mathbf{x})]$ by a sample average but sampling from $p(\mathbf{x})$ is difficult.
- We can write

$$\begin{aligned}
\mathbb{E}_{p(\mathbf{x})}[g(\mathbf{x})] &= \int g(\mathbf{x})p(\mathbf{x})\mathrm{d}\mathbf{x} \\
&= \int g(\mathbf{x})\frac{p(\mathbf{x})}{q(\mathbf{x})}q(\mathbf{x})\mathrm{d}\mathbf{x} \qquad \text{(assume } q(\mathbf{x}) > 0 \text{ when } g(\mathbf{x})p(\mathbf{x}) > 0\text{)} \\
&= \mathbb{E}_{q(\mathbf{x})}\left[g(\mathbf{x})\frac{p(\mathbf{x})}{q(\mathbf{x})}\right] \\
&\approx \frac{1}{n}\sum_{i=1}^{n} g(\mathbf{x}_i)\frac{p(\mathbf{x}_i)}{q(\mathbf{x}_i)}
\end{aligned}$$

  where $\mathbf{x}_i \sim q(\mathbf{x})$ (iid)
- The $w_i = p(\mathbf{x}_i)/q(\mathbf{x}_i)$ are called the importance weights.

Self/auto-normalised importance sampling

- We can combine the above ideas to approximate

$$\mathbb{E}_{p(\mathbf{x})}[g(\mathbf{x})] = \int g(\mathbf{x})p(\mathbf{x})\mathrm{d}\mathbf{x}$$

by importance sampling even if we only know $\tilde{p}(\mathbf{x}) \propto p(\mathbf{x})$ and

$$p(\mathbf{x}) = \frac{\tilde{p}(\mathbf{x})}{\int \tilde{p}(\mathbf{x})\mathrm{d}\mathbf{x}}$$

- Write

$$\begin{aligned}
\int g(\mathbf{x})p(\mathbf{x})\mathrm{d}\mathbf{x} &= \frac{\int g(\mathbf{x})\tilde{p}(\mathbf{x})\mathrm{d}\mathbf{x}}{\int \tilde{p}(\mathbf{x})\mathrm{d}\mathbf{x}} \\
&= \frac{\int g(\mathbf{x})\frac{\tilde{p}(\mathbf{x})}{q(\mathbf{x})}q(\mathbf{x})\mathrm{d}\mathbf{x}}{\int \frac{\tilde{p}(\mathbf{x})}{q(\mathbf{x})}q(\mathbf{x})\mathrm{d}\mathbf{x}} \\
&= \frac{\mathbb{E}_{q(\mathbf{x})}\left[g(\mathbf{x})\frac{\tilde{p}(\mathbf{x})}{q(\mathbf{x})}\right]}{\mathbb{E}_{q(\mathbf{x})}\left[\frac{\tilde{p}(\mathbf{x})}{q(\mathbf{x})}\right]}
\end{aligned}$$

Self/auto-normalised importance sampling

- Since

$$\int g(\mathbf{x})p(\mathbf{x})\mathrm{d}\mathbf{x} = \frac{\mathbb{E}_{q(\mathbf{x})}\left[g(\mathbf{x})\frac{\tilde{p}(\mathbf{x})}{q(\mathbf{x})}\right]}{\mathbb{E}_{q(\mathbf{x})}\left[\frac{\tilde{p}(\mathbf{x})}{q(\mathbf{x})}\right]}$$

$$= \frac{\mathbb{E}_{q(\mathbf{x})}\left[g(\mathbf{x})\frac{\tilde{p}(\mathbf{x})}{\tilde{q}(\mathbf{x})}\right]}{\mathbb{E}_{q(\mathbf{x})}\left[\frac{\tilde{p}(\mathbf{x})}{\tilde{q}(\mathbf{x})}\right]}$$

we only need to know the importance distribution $q(\mathbf{x})$ up to normalisation constant.

- Approximate both expectations by a sample average

$$\int g(\mathbf{x})p(\mathbf{x})\mathrm{d}\mathbf{x} \approx \frac{\frac{1}{n}\sum_{i=1}^{n} g(\mathbf{x}_i)\frac{\tilde{p}(\mathbf{x}_i)}{\tilde{q}(\mathbf{x}_i)}}{\frac{1}{n}\sum_{i=1}^{n}\frac{\tilde{p}(\mathbf{x}_i)}{\tilde{q}(\mathbf{x}_i)}} = \frac{\sum_{i=1}^{n} g(\mathbf{x}_i)w_i}{\sum_{i=1}^{n} w_i}$$

where $w_i = \frac{\tilde{p}(\mathbf{x}_i)}{\tilde{q}(\mathbf{x}_i)}$ and $\mathbf{x}_i \sim q(\mathbf{x})$ (iid)

Self/auto-normalised importance sampling

$$w_i = \frac{\tilde{p}(\mathbf{x}_i)}{\tilde{q}(\mathbf{x}_i)}, \quad \mathbf{x}_i \overset{\text{iid}}{\sim} q(\mathbf{x})$$

- Called self-normalised or auto-normalised importance sampling

$$\int g(\mathbf{x})p(\mathbf{x})\mathrm{d}\mathbf{x} \approx \sum_{i=1}^{n} W_i g(\mathbf{x}_i) \qquad W_i = \frac{w_i}{\sum_{k=1}^{n} w_k}$$

Note: $\sum_{i=1}^{n} W_i = 1$

- Interpretation in terms of a Dirac-delta approximation of $p(\mathbf{x})$,

$$p(\mathbf{x}) \approx \sum_{i=1}^{n} W_i \delta_{\mathbf{x}_i}(\mathbf{x}) \qquad \mathbf{x}_i \overset{\text{iid}}{\sim} q(\mathbf{x})$$

($\equiv$ mixture of Gaussians with mixture probabilities W_i, expected values $\mathbf{x}_i$, and infinitesimally small variances)

Effective sample size

$$w_i = \frac{\tilde{p}(\mathbf{x}_i)}{\tilde{q}(\mathbf{x}_i)}, \quad \mathbf{x}_i \overset{\text{iid}}{\sim} q(\mathbf{x})$$

- If the weights w_i are constants, the weighted average $\sum_{i=1}^{n} W_i g(\mathbf{x}_i)$ becomes a standard average

$$W_i = \frac{w_i}{\sum_{k=1}^{n} w_k} \overset{w_i=c}{==} \frac{c}{\sum_{k=1}^{n} c} = \frac{1}{N}$$

- But the w_i are typically not all equal, so that some x_i contribute more to the average than others, e.g.

$$w_1 = 10^6, w_k = 1, k > 1 \Longrightarrow W_1 \approx 1, W_k \approx 0, k > 1$$

  We would effectively "average" over 1 data point!
- When working with a weighted average, always compute the"effective sample size" (ESS),

$$\text{ESS} = \frac{\left(\sum_{i=1}^{n} w_i\right)^2}{\sum_{i=1}^{n} w_i^2} = \frac{1}{\sum_{i=1}^{n} W_i^2} \in [1, N]$$

  Small ESS means the average is unreliable (high variance).

Program

1. Monte Carlo integration
   - Approximating expectations by averages
   - Importance sampling
   - Effective sample size
2. Sampling

Program

1. Monte Carlo integration

2. Sampling
   - Simple univariate sampling
   - Rejection sampling
   - Ancestral sampling
   - Gibbs sampling

Assumption

- We assume that we are able to generate iid samples from the uniform distribution on $[0, 1]$.
- How to do that: see e.g.
  `https://statweb.stanford.edu/~owen/mc/Ch-unifrng.pdf`
  (not examinable)

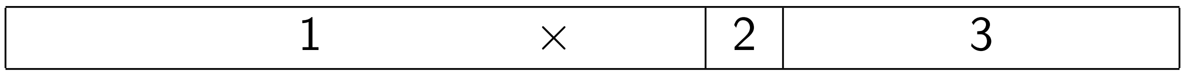
Sampling for univariate discrete random variables

(Based on a slide from David Barber)

- Consider the one dimensional discrete distribution $p(x)$ with $x \in \{1, 2, 3\}$, with

$$p(x) = \begin{cases} 0.6 & x = 1 \\ 0.1 & x = 2 \\ 0.3 & x = 3 \end{cases}$$

- Divide $[0, 1]$ into chunks $[0, 0.6)$, $[0.6, 0.7)$, $[0.7, 1]$



- We then draw a sample u uniformly from $[0, 1]$
- We return the label of the partition in which u fell.
- Example: if $u = 0.53$, we return the sample "1"

Sampling for univariate continuous random variables

- A similar method as the one above exists for continuous random variables.
- Called inverse transform sampling.
- Recall: the cumulative distribution function (cdf) of a random variable x with pdf p_x is

$$F_x(\alpha) = \mathbb{P}(x \le \alpha) = \int_{-\infty}^{\alpha} p_x(u)\mathrm{d}u$$

- To generate n iid samples from x with cdf F_x:
  - calculate the inverse F_x^{-1}
  - sample n iid random variables uniformly distributed on $[0, 1]$: $y_i \sim \mathcal{U}(0, 1)$, $i = 1, \ldots, n$.
  - transform each sample by F_x^{-1}: $x_i = F_x^{-1}(y_i)$, $i = 1, \ldots, n$.

(see exercises for derivation)

Basic principle of rejection sampling

- Assume you can draw iid samples $\mathbf{x}_i \sim q(\mathbf{x})$.
- For each sampled $\mathbf{x}_i$, you draw a Bernoulli random variable $y_i \in \{0, 1\}$ whose success probability depends on $\mathbf{x}_i$

$$\mathbb{P}(y_i = 1|\mathbf{x}_i) = f(\mathbf{x}_i)$$

- You get samples $(y_i, \mathbf{x}_i)$ with joint distribution

$$q(\mathbf{x})f(\mathbf{x})^y(1 - f(\mathbf{x}))^{(1-y)}$$

- Conditional pdf of $\mathbf{x}|y = 1$ is proportional to $q(\mathbf{x})f(\mathbf{x})$
- Keep/"accept" the $\mathbf{x}_i$ with $y_i = 1$, "reject" those with $y_i = 0$.
- Accepted samples follow

$$\mathbf{x}_i \sim \frac{q(\mathbf{x})f(\mathbf{x})}{\int q(\mathbf{x})f(\mathbf{x})\mathrm{d}\mathbf{x}}$$

- Denominator equals the marginal probability of acceptance

$$\mathbb{P}(y = 1) = \mathbb{E}_{q(\mathbf{x})}\mathbb{P}(y = 1|\mathbf{x}) = \int q(\mathbf{x})f(\mathbf{x})\mathrm{d}\mathbf{x}$$

Sampling from the posterior by rejection sampling

- Conditional acceptance probability $f(\mathbf{x}) \in [0, 1]$ can be used to shape the distribution of the samples from $q(\mathbf{x})$
- Consider Bayesian inference: prior $p(\boldsymbol{\theta})$, likelihood $L(\boldsymbol{\theta})$
- Using $L(\boldsymbol{\theta})/(\max L(\boldsymbol{\theta}))$ as acceptance probability f transforms the samples $\boldsymbol{\theta}_i$ from the prior into samples from the posterior.
- Accepted parameters follow

$$\boldsymbol{\theta}_i \sim \frac{p(\boldsymbol{\theta})L(\boldsymbol{\theta})}{\int p(\boldsymbol{\theta})L(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}} = p(\boldsymbol{\theta}|\mathcal{D})$$

- More likely parameter configurations are more likely accepted.

Sampling from the posterior by rejection sampling

- For discrete random variables $L(\boldsymbol{\theta}) = \mathbb{P}(\mathbf{x} = \mathcal{D}; \boldsymbol{\theta}) \in [0, 1]$.
- Accepting a $\boldsymbol{\theta}_i$ with probability $L(\boldsymbol{\theta})$ can be implemented by checking whether data simulated from the model with parameter value $\boldsymbol{\theta}_i$ equals the observed data.
- Samples from the posterior = samples from the prior that produce data equal to the observed one.
  (see slides "Basic of Model-Based Learning")

Side-note (not examinable): enables Bayesian inference when the likelihood is intractable (e.g. due to unobserved variables) but sampling from the model is possible. Forms the basis of a set of methods called approximate Bayesian computation, for an introductory review paper see `https://michaelgutmann.github.io/assets/papers/Lintusaari2017.pdf`.

Standard formulation of rejection sampling

- Rejection sampling is typically presented (slightly) differently.
- Goal is to generate samples from $p(\mathbf{x})$ when being able to sample from $q(\mathbf{x})$.
- Since accepted samples follow

$$\mathbf{x}_i \sim \frac{q(\mathbf{x})f(\mathbf{x})}{\int q(\mathbf{x})f(\mathbf{x})\mathrm{d}\mathbf{x}}$$

  choose conditional acceptance probability $f(\mathbf{x}) \propto p(\mathbf{x})/q(\mathbf{x})$
- To determine the proportionality factor, note that $f(\mathbf{x})$ must be ≤ 1 since it is a conditional probability. Hence:

$$f(\mathbf{x}) = \frac{1}{M}\frac{p(\mathbf{x})}{q(\mathbf{x})} \qquad\qquad M = \max_{\mathbf{x}} \frac{p(\mathbf{x})}{q(\mathbf{x})}$$

- Acceptance probability: $\mathbb{P}(y=1) = \int q(\mathbf{x})f(\mathbf{x})\mathrm{d}\mathbf{x} = \frac{1}{M}$.

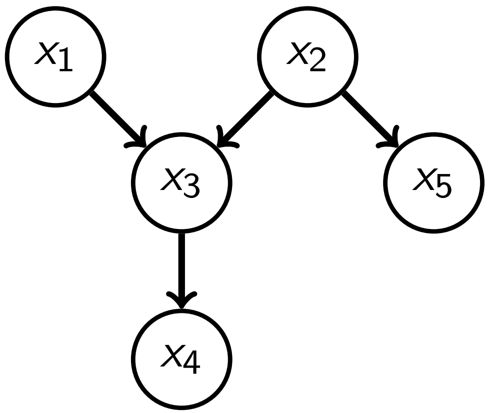
Multivariate by univariate sampling

- Rejection sampling may scale poorly because M increases with dimensionality so that acceptance probability goes down.
- Sampling from high-dimensional multivariate distributions is generally difficult.
- One way to approach the problem of multivariate sampling is to translate it into the task of solving several lower dimensional sampling problems.
- Examples:
  - Ancestral sampling
  - Gibbs sampling

Ancestral sampling

- Factorisation provides a recipe for data generation / sampling from $p(\mathbf{x})$
- Example:
  $p(x_1, \ldots, x_5) = p(x_1)p(x_2)p(x_3|x_1, x_2)p(x_4|x_3)p(x_5|x_2)$
- We can generate samples from the joint distribution $p(x_1, x_2, x_3, x_4, x_5)$ by sampling

  1. $x_1 \sim p(x_1)$
  2. $x_2 \sim p(x_2)$
  3. $x_3 \sim p(x_3|x_1, x_2)$
  4. $x_4 \sim p(x_4|x_3)$
  5. $x_5 \sim p(x_5|x_2)$



- Sets of univariate sampling problems.

Gibbs sampling

(Based on a slide from David Barber)

- Gibbs sampling also reduces the problem of multivariate sampling to the problem of univariate sampling.
- Goal: generate samples $\mathbf{x}^{(k)}$ from $p(\mathbf{x}) = p(x_1, \ldots, x_d)$.
- By product rule

$$\begin{aligned} p(\mathbf{x}) &= p(x_i | x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_d) p(x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_d) \\ &= p(x_i | \mathbf{x}_{\setminus i}) p(\mathbf{x}_{\setminus i}) \end{aligned}$$

- Given a joint initial state $\mathbf{x}^{(1)}$ from which we can read off the 'parental' state $\mathbf{x}^{(1)}_{\setminus i}$

$$\mathbf{x}^{(1)}_{\setminus i} = (x^{(1)}_1, \ldots, x^{(1)}_{i-1}, x^{(1)}_{i+1}, \ldots, x^{(1)}_d),$$

  we can draw a sample $x^{(2)}_i$ from $p(x_i | \mathbf{x}^{(1)}_{\setminus i})$.
- We assume this distribution is easy to sample from since it is univariate.

Gibbs sampling

(Based on a slide from David Barber)

- We call the new joint sample in which only x_i has been updated $\mathbf{x}^{(2)}$,

$$\mathbf{x}^{(2)} = (x_1^{(1)}, \ldots, x_{i-1}^{(1)}, x_i^{(2)}, x_{i+1}^{(1)}, \ldots, x_d^{(1)}).$$

- One then selects another variable x_j to sample and, by continuing this procedure, generates a set $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(n)}$ of samples in which each $\mathbf{x}^{(k+1)}$ differs from $\mathbf{x}^{(k)}$ in only a single component.
- Since $p(x_i|\mathbf{x}_{\setminus i}) = p(x_i|\mathrm{MB}(x_i))$, we can sample from $p(x_i|\mathrm{MB}(x_i))$ which is easier. ($\mathrm{MB}(x_i)$ is the Markov blanket of x_i)
- Samples are not independent.
- Gibbs sampling is an example of a Markov chain Monte Carlo method (see Barber 27.4 and 27.3.1, and the exercises, not examinable).

Program recap

1. Monte Carlo integration
   - Approximating expectations by averages
   - Importance sampling
   - Effective sample size

2. Sampling
   - Simple univariate sampling
   - Rejection sampling
   - Ancestral sampling
   - Gibbs sampling