# Sampling and Monte Carlo Integration

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# Recap

Learning and inference often involves intractable 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
$$L(\boldsymbol{\theta}) = p(\mathcal{D}; \boldsymbol{\theta}) = \int_{\mathbf{u}} p(\mathbf{u}, \mathcal{D}; \boldsymbol{\theta} \mathrm{d}\mathbf{u}),$$
$$\nabla_{\boldsymbol{\theta}} \ell(\boldsymbol{\theta}) = \mathbb{E}_{p(\mathbf{u}|\mathcal{D};\boldsymbol{\theta})} \left[\nabla_{\boldsymbol{\theta}} \log p(\mathbf{u}, \mathcal{D}; \boldsymbol{\theta})\right]$$

Notation: $\mathbb{E}_{p(\mathbf{x})}$ is sometimes used to indicate that the expectation is taken with respect to $p(\mathbf{x})$.

# Recap

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

- For unnormalised models with intractable partition functions

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

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

- Combined case of unnormalised models with intractable partition functions and unobserved variables.
- Evaluation of intractable integrals can sometimes be avoided by using other learning criteria (e.g. score matching).
- Here: methods to approximate integrals like those above using sampling.

# Program

1. Monte Carlo integration
2. Sampling

# Program

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

2. Sampling

# Averages with iid samples

- Tutorial 7: 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

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

(∗: "identically distributed" assumption is used, not independence)

- Variability

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

(∗: independence assumption used)

- Squared error decreases as $1/n$

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

# Averages with iid samples

- Weak law of large numbers:

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

- As $n \to \infty$, the probability for the sample average to deviate from the expected value goes to zero.
- 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 $\mathbb{V}[s]$.

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

- This means that for *all* random variables:
  - 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 $y \geq 0$

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

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

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

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

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

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

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

# 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".
- Important for the theory of Markov chain Monte Carlo methods but requires advanced mathematical theory.

# 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 $\frac{1}{n}\mathbb{V}[g(\mathbf{x})]$

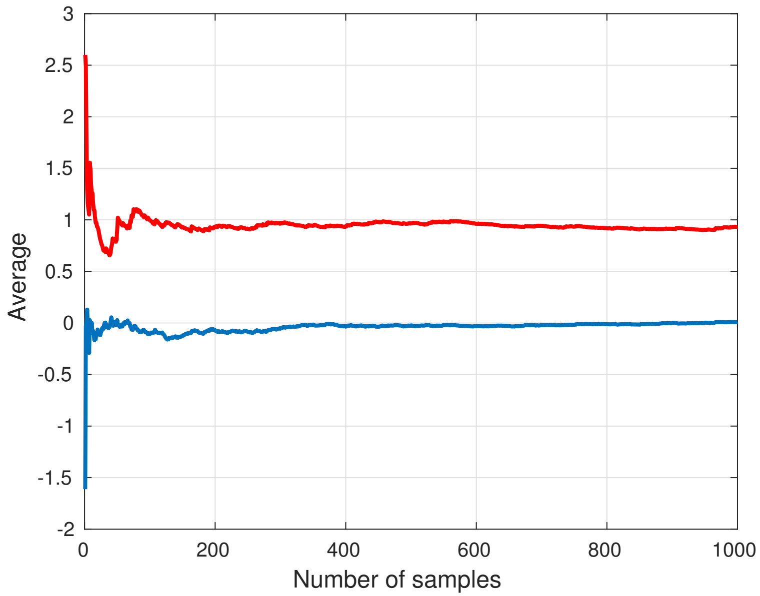
# Example (Based on a slide from Amos Storkey)

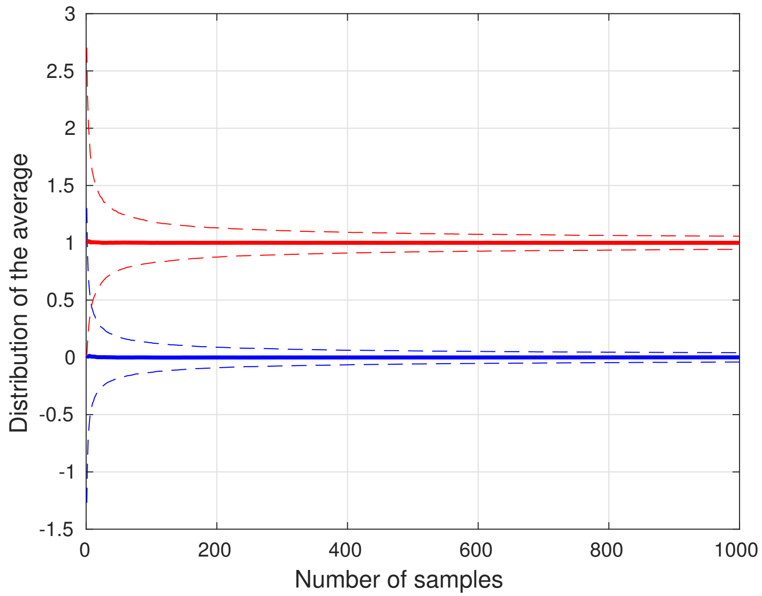
$$\mathbb{E}[g(x)] = \int g(x)\mathcal{N}(x;0,1)\mathrm{d}x \approx \frac{1}{n}\sum_{i=1}^{n} g(x_i) \qquad (x_i \sim \mathcal{N}(x;0,1))$$

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)

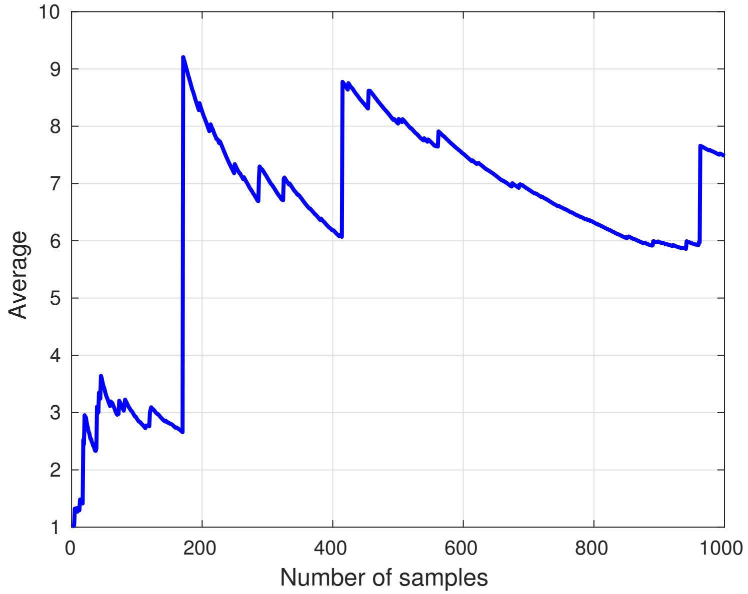


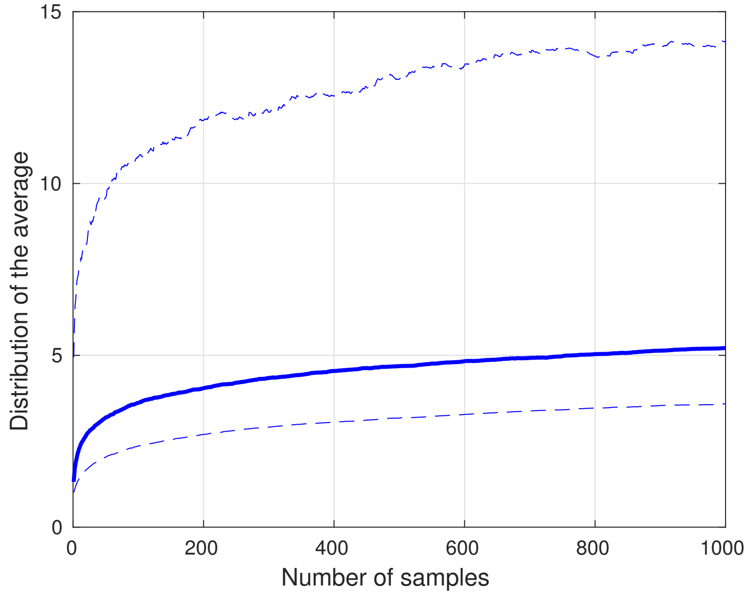



$$\mathbb{E}[g(x)] = \int g(x)\mathcal{N}(x;0,1)\mathrm{d}x \approx \frac{1}{n}\sum_{i=1}^{n} g(x_i) \qquad (x_i \sim \mathcal{N}(x;0,1))$$

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

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:

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

  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!

# Approximating general 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 $q$

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

  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 compute the partition function

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

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

# Example

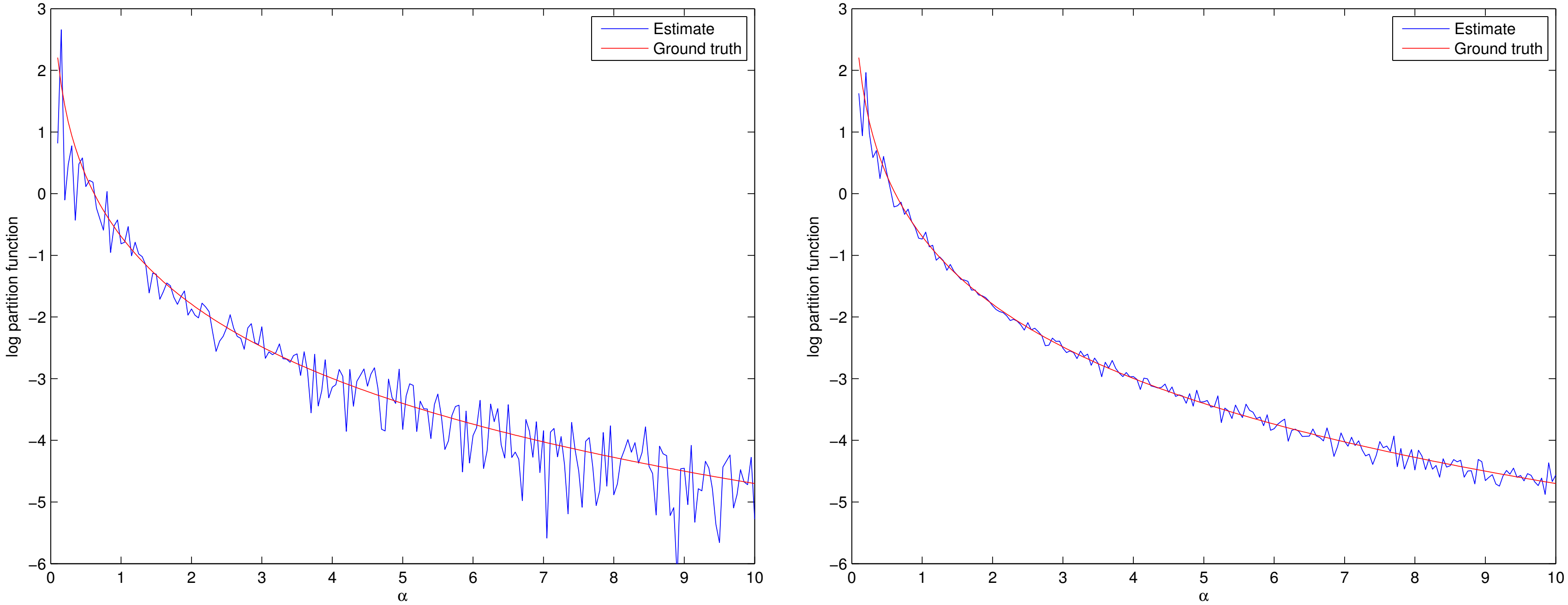
Approximating the log partition function of the unnormalised beta-distribution

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

for $\beta$ fixed to $\beta = 2$.

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

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



# Importance sampling to compute 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

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

  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.

# Normalised importance weights

- 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

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

# Normalised importance weights

- 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 sample average

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

  where $\mathbf{x}_i \sim q(\mathbf{x})$ (iid)

# Normalised importance weights

- With importance weights

$$w_i = \frac{\tilde{p}(\mathbf{x}_i)}{\tilde{q}(\mathbf{x}_i)},$$

where $\mathbf{x}_i \overset{\text{iid}}{\sim} q(\mathbf{x})$, we can write

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

- Same weights in numerator and denominator.
- The quantities

$$\frac{w_i}{\sum_{i=1}^{n} w_i}$$

are called normalised importance weights.

# Program

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

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

$$F_x(\alpha) = \Pr(x \leq \alpha) = \int_{-\infty}^{\alpha} p_x(u) \mathrm{d}u$$

- 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 Tutorial 8 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 $\mathbf{x}_i$

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

- 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 or "accept" the $\mathbf{x}_i$ with $y_i = 1$, "reject" those with $y_i = 0$.
- Accepted samples follow

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

# 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 $L(\boldsymbol{\theta}) = \Pr(\mathbf{x} = \mathcal{D}; \boldsymbol{\theta}) \in [0, 1]$.
- 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.

# Standard formulation of rejection sampling

- Rejection sampling is typically presented (slightly) differently.
- Goal is to generate samples from a target distribution $p(\mathbf{x})$ known up to normalisation constant 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 $f(\mathbf{x}) \propto p(\mathbf{x})/q(\mathbf{x})$
- See Barber 27.1.2.

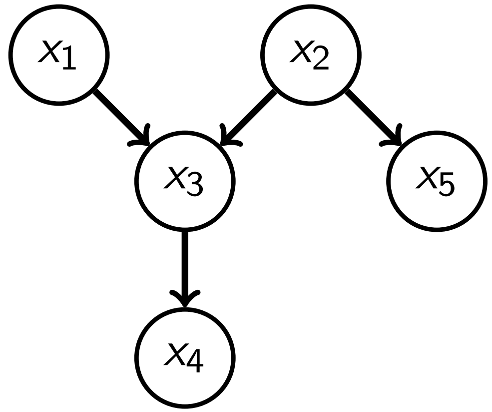
# Multivariate by univariate sampling

- Rejection sampling is limited to low-dimensional cases (see Barber 27.1.2)
- 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.
- We did that in ancestral 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 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 $\mathbf{x}^2$,

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

- 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.

  ($\mathrm{MB}(x_i)$ denotes the Markov blanket of $x_i$, see slides on directed and undirected graphical models.)
- Samples are not independent.
- Gibbs sampling is an example of a Markov chain Monte Carlo method (see Barber 27.3 and 27.4).

# Program recap

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

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