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Academy for PhD Training in Statistics

Computer Intensive Statistics

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Part 1

Introduction, Motivation & Basics

What *is* Computer Intensive Statistics

Computer, *n.* A device or machine for performing or facilitating calculation.
Compare Middle French computeur person who makes calculations (1578).

Intensive, *adj.* Of very high degree or force, vehement.
French intensif, -ive (14–15th cent. in Hatzfeld & Darmesteter).

Statistics, *n.* The systematic collection and arrangement of numerical facts or data of any kind; (also) the branch of science or mathematics concerned with the analysis and interpretation of numerical data and appropriate ways of gathering such data.
In early use after French statistique and German Statistik.

What Makes Statistics Computer Intensive?

Some *good* reasons for using computer-intensive methods:

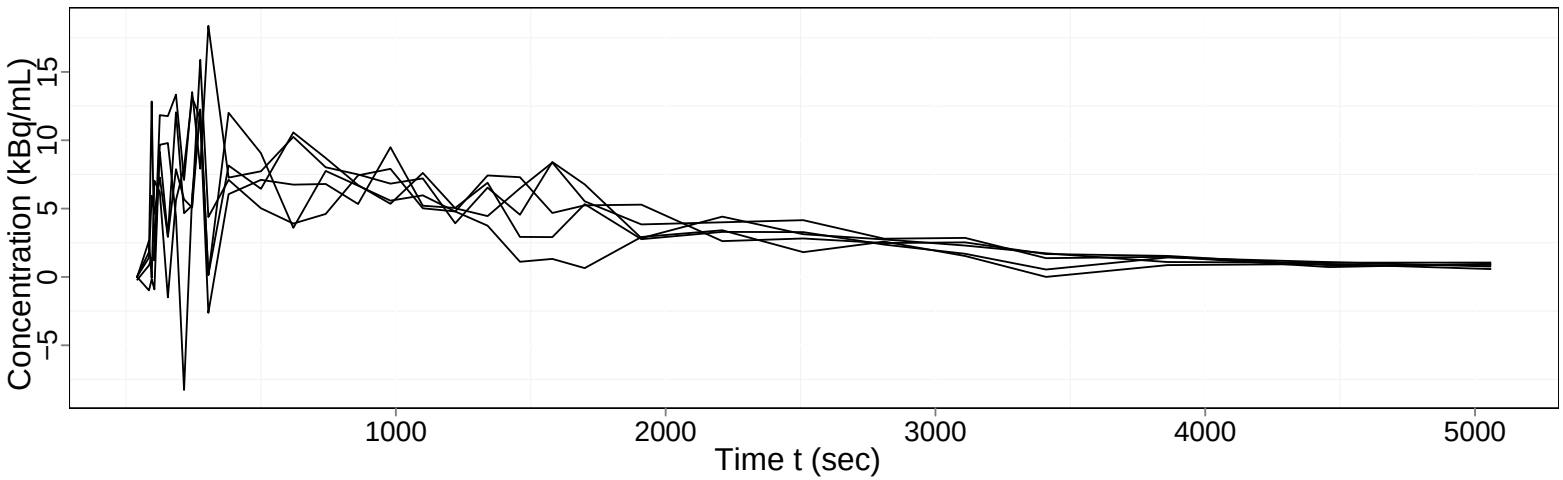
Complexity	Complex models cannot often be dealt with analytically.
Intractability	Models which are not available analytically.
Laziness	Computer time is cheap; human time isn't.
Scale	Large data sets bring fresh challenges.

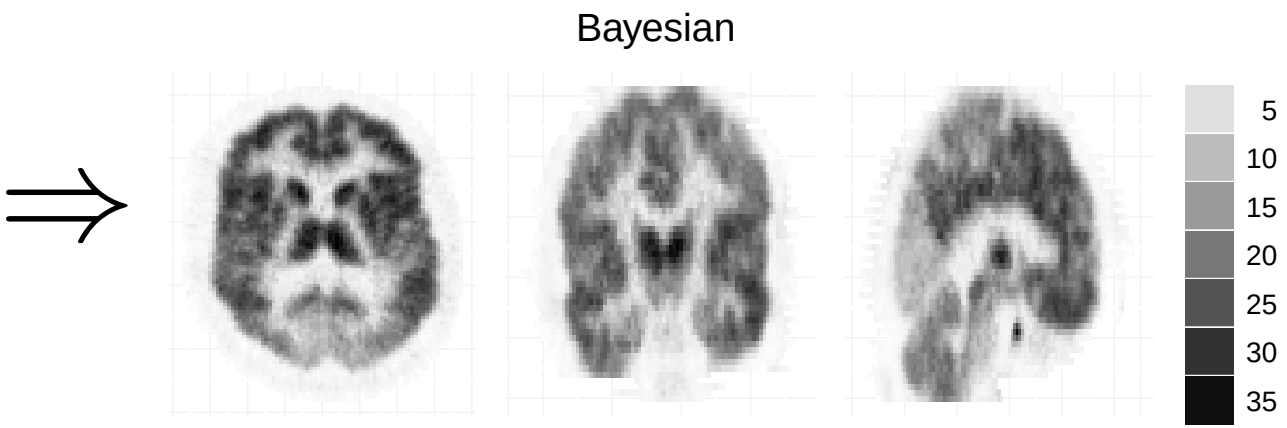
We won't address the *bad* reasons here. . .

Part 1— Section 1

Motivation

Motivating Problem: Positron Emission Tomography I





Motivating Problem: Positron Emission Tomography II

Dynamic model:

$$\frac{\mathrm{d}C_T}{\mathrm{d}t}(s) = AC_T(s) + bC_P(s)$$
$$C_T(0) = \mathbf{0}$$
$$\bar{C_T}(s) = \mathbf{1}^T C_T(t),$$

with solution:

$$\bar{C_T}(t) = \int_0^t C_P(t-s)H_{TP}(s)\mathrm{d}s \tag{1}$$
$$H_{TP}(t) = \sum_{i=1}^{m} \phi_i e^{-\theta_i t},$$

where the ϕ_i and θ_i are functions of A.

Motivating Problem: Positron Emission Tomography III

Interested in the *Volume of Distribution*:

$$V_D := \int_0^\infty H_{TP}(t)\mathrm{d}t = \sum_{i=1}^{m} \frac{\phi_i}{\theta_i}.$$

But have noisy measurements of $\bar{C_T}(t_j)$ for $j = 1, \ldots, n$:

$$y_j = \bar{C_T}(t_j; \phi_{1:m}, \theta_{1:m}) + \sqrt{\frac{\bar{C_T}(t_j; \phi_{1:m}, \theta_{1:m})}{t_j - t_{j-1}}}\varepsilon_j$$

$$\bar{C_T}(t_j; \phi_{1:m}, \theta_{1:m}) = \sum_{i=1}^{m} \phi_i \int_0^{t_j} C_P(s) e^{-\theta_i(t_j - s)} ds.$$

What can we say?

Motivating Problem: Hypothesis Testing

Testing Example: Chi-Squared Test

- $T = \sum_{i=1}^{k} \frac{(O_k - E_k)^2}{E_k}$
- Asymptotic argument:
- $T \overset{d}{\approx} \chi^2_{k-1}$ under regularity conditions.

What if we *don't* have many observations of every category?

What if we want to know whether the *medians* of two populations are *significantly different*?

What if we don't know the form of their distributions?

Motivating Problem: Confidence Intervals

Constructing confidence intervals requires knowledge of sampling distributions.

Confidence Interval: Medians

- $X_1, X_2, \ldots, X_n \overset{\text{iid}}{\sim} f_X$.
- $X_{[1]} \leq X_{[2]} \leq \ldots X_{[n]}$ are the associated order statistics.
- $T = X_{[(n+1)/2]}$ is the sample median
- How can we construct a confidence interval for the median of f_X?
- What if we don't even know the form of f_X?

Motivating Problem: Bayesian Inference

Bayesian statistics

- Data $\mathbf{y}_1, \ldots, \mathbf{y}_n$ and model $f(\mathbf{y}_i|\boldsymbol{\theta})$ where $\boldsymbol{\theta}$ is some parameter of interest.

  $\rightsquigarrow$ Likelihood $l(\mathbf{y}_1, \ldots, \mathbf{y}_n|\boldsymbol{\theta}) = \prod_{i=1}^{n} f(\mathbf{y}_i|\boldsymbol{\theta})$

- In the Bayesian framework $\boldsymbol{\theta}$ is a random variable with prior distribution $f^{\text{prior}}(\boldsymbol{\theta})$. After observing $\mathbf{y}_1, \ldots, \mathbf{y}_n$ the posterior density of f is

$$\begin{aligned} f^{\text{post}}(\boldsymbol{\theta}) &= f(\boldsymbol{\theta}|\mathbf{y}_1, \ldots, \mathbf{y}_n) \\ &= \frac{f^{\text{prior}}(\boldsymbol{\theta}) l(\mathbf{y}_1, \ldots, \mathbf{y}_n|\boldsymbol{\theta})}{\int_\Theta f^{\text{prior}}(\boldsymbol{\vartheta}) l(\mathbf{y}_1, \ldots, \mathbf{y}_n|\boldsymbol{\vartheta})\, d\boldsymbol{\vartheta}} \end{aligned}$$

- Often intractable $\rightsquigarrow$ use of an approximation.

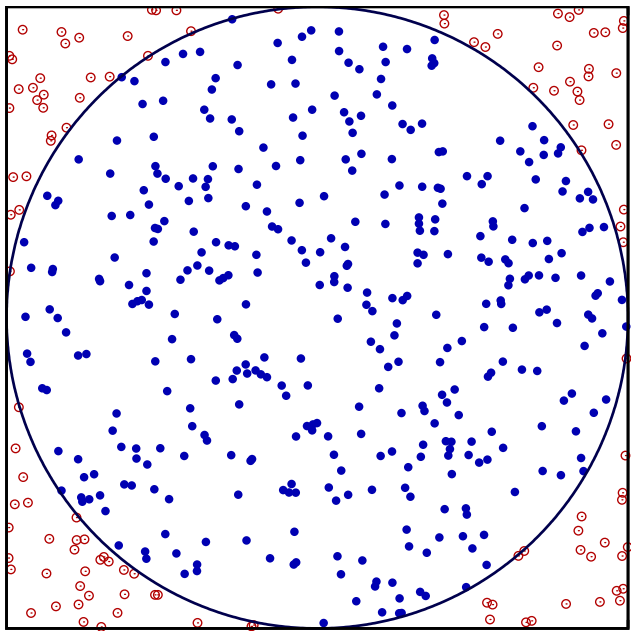
Simulation-based Methods

- Doing statistics backwards:

> *Representing the solution of a problem as a parameter of a hypothetical population, and using a random sequence of numbers to construct a sample of the population, from which statistical estimates of the parameter p values, confidence intervals, or other quantities of interest can be obtained.*

Preliminary Example: Raindrop experiment for π

- Consider "uniform rain" on the square $[-1,1] \times [-1,1]$, i.e. the two coordinates $X, Y \overset{\text{iid}}{\sim} \mathsf{U}[-1,1]$.



- Probability that a rain drop falls in the circle is

$$\mathbb{P}(\text{drop within circle}) = \frac{\text{area of the unit circle}}{\text{area of the square}}$$

$$= \frac{\iint_{\{x^2+y^2 \le 1\}} 1 \, dxdy}{\iint_{\{-1 \le x,y \le 1\}} 1 \, dxdy} = \frac{\pi}{2 \cdot 2} = \frac{\pi}{4}.$$

Preliminary Example: Raindrop experiment for π

- Given π, we can compute $\mathbb{P}(\text{drop within circle}) = \frac{\pi}{4}$.
- Given n independent raindrops, the number of rain drops falling in the circle, Z_n is a binomial random variable:

$$Z_n \sim \text{Bin}\left(n, p = \frac{\pi}{4}\right).$$

- $\rightsquigarrow$ we can estimate p with

$$\widehat{p} = \frac{Z_n}{n}.$$

- and π by

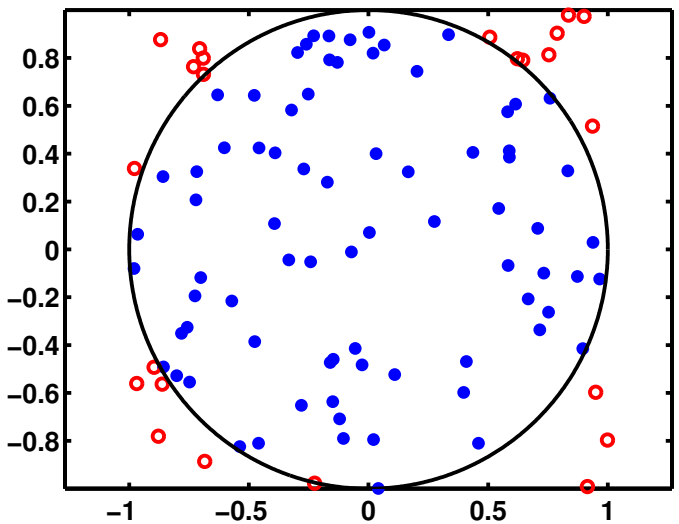
$$\widehat{\pi} = 4\widehat{p} = 4 \cdot \frac{Z_n}{n}.$$

Preliminary Example: Raindrop experiment for π

- Result obtained for $n = 100$ raindrops:
  77 points inside the circle.
- Resulting estimate of π is

$$\widehat{\pi} = \frac{4 \cdot Z_n}{n} = \frac{4 \cdot 77}{100} = 3.08,$$

(rather poor estimate)

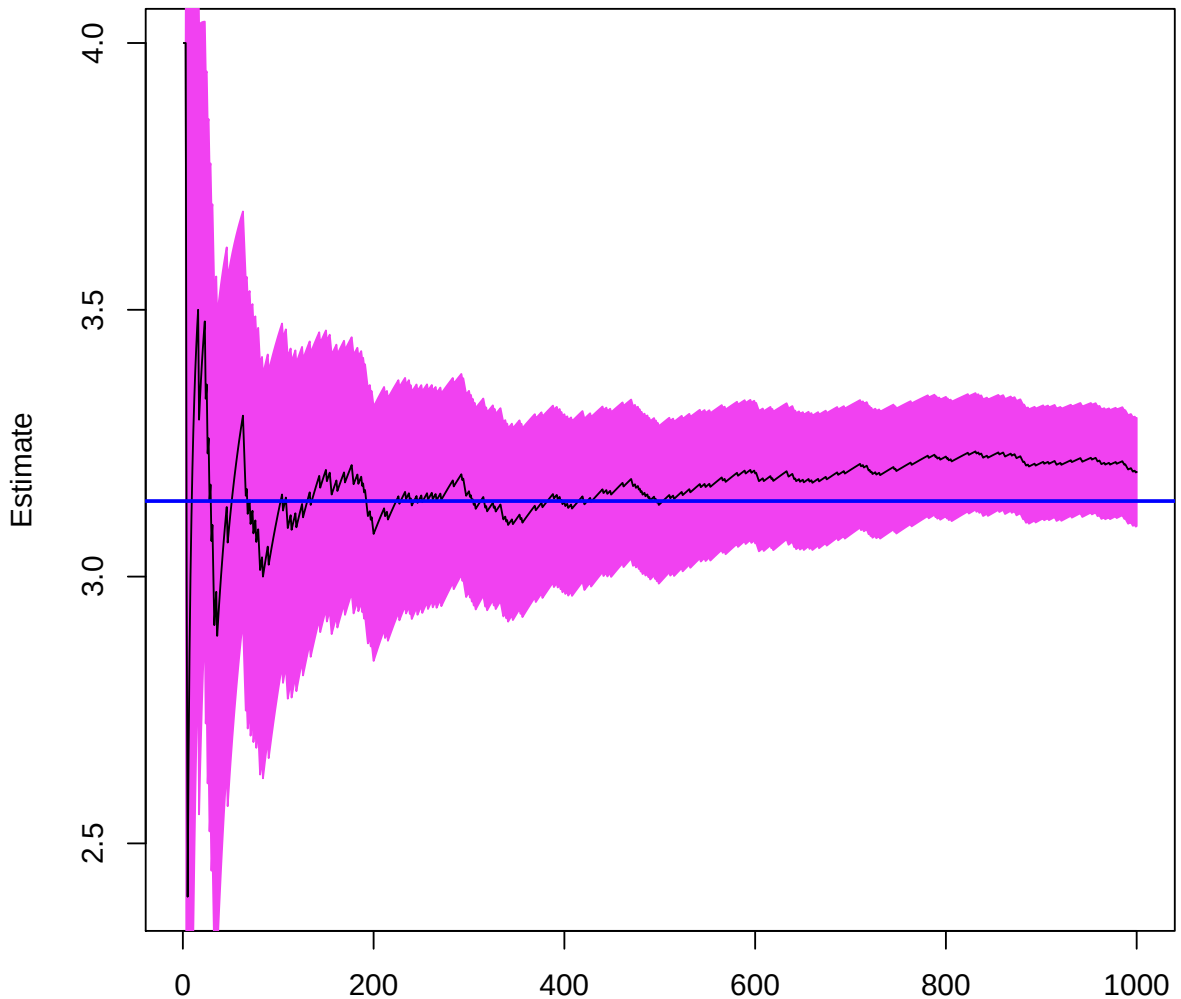


- However: the *law or large numbers* **guarantees** that

$$\widehat{\pi}_n = \frac{4 \cdot Z_n}{n} \to \pi$$

almost surely for $n \to \infty$.

Preliminary Example: Raindrop experiment for π



Preliminary Example: Raindrop experiment for π

- How fast does $\widehat{\pi}$ converge to π?
  Central limit theorem gives the answer.
- $(1-2\alpha)$ confidence interval for p ($\widehat{p}_n = Z_n/n$):

$$\left[\widehat{p}_n - z_{1-\alpha}\sqrt{\frac{\widehat{p}_n(1-\widehat{p}_n)}{n}}, \widehat{p}_n + z_{1-\alpha}\sqrt{\frac{\widehat{p}_n(1-\widehat{p}_n)}{n}}\right]$$

- $(1-2\alpha)$ confidence interval for π ($\widehat{\pi}_n = 4\widehat{p}_n$):

$$\left[\widehat{\pi}_n - z_{1-\alpha}\sqrt{\frac{\widehat{\pi}_n(4-\widehat{\pi}_n)}{n}}, \widehat{\pi}_n + z_{1-\alpha}\sqrt{\frac{\widehat{\pi}_n(4-\widehat{\pi}_n)}{n}}\right]$$

- Width of the interval is $O(n^{-1/2})$, thus speed of convergence $O_{\mathbb{P}}(n^{-1/2})$.

Preliminary Example: Raindrop experiment for π

Recall the two core elements of this example:

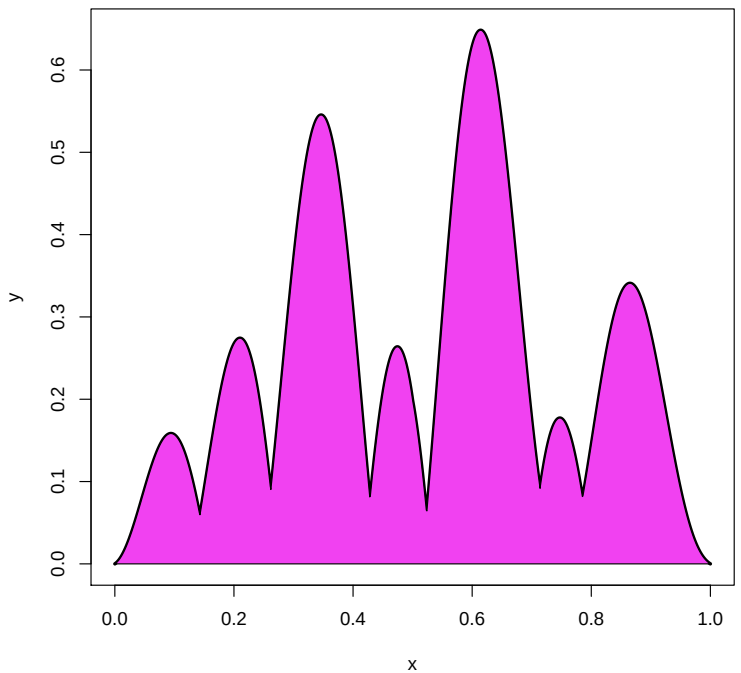
1. Writing the quantity of interest (here π) as an expectation:

$$\pi = 4\mathbb{P}(\text{drop within circle}) = \mathbb{E}\left(4 \cdot \mathbb{I}_{\{\text{drop within circle}\}}\right)$$

2. Replaced this algebraic representation with a sample approximation.
   - SLLN guarantees that the sample approximation converges to the algebraic representation.
   - CLT gives information about the speed of convergence.

The Generalisation to Monte Carlo Integration

$$
\begin{aligned}
& \int_0^1 f(x)\, dx \\
= & \int_0^1 \int_0^{f(x)} 1\, dt\, dx \\
= & \iint\limits_{\{(x,t):t \leq f(x)\}} 1 dt\, dx \\
= & \frac{\iint\limits_{\{(x,t):t \leq f(x)\}} 1\, dt\, dx}{\iint\limits_{\{0 \leq x,t \leq 1\}} 1 dt\, dx}
\end{aligned}
$$



$$f : [0,1] \to [0,1]$$

Comparison of the speed of convergence

- Monte Carlo integration is $O_{\mathbb{P}}(n^{-1/2})$.
- Numerical integration of a *one-dimensional* function by Riemann sums is $O(n^{-1})$.
- Monte Carlo does not compare favourably for one-dimensional problems.
- However:
  - Monte Carlo estimates are often *unbiased*.
  - Order of convergence of Monte Carlo integration is *independent* of dimension.
  - Order of convergence of numerical integration techniqes deteriorates with increasing dimension.

$\rightsquigarrow$ Monte Carlo methods can be a good choice for high-dimensional integrals.

Views of Simulation-Based Inference

Direct approximation of a quantity of interest.

- Careful construction of random experiment for particular task at hand.
- Justify with a dedicated argument in each case.

Approximation of *integrals* of interest.

- Represent quantity of interest as expectation wrt some f.
- Use sample average to approximate expectation.
- Appeal to SLLN and CLT.

Approximation of *distributions* of interest.

- Represent quantity of interest as a function of distribution f.
- Use empirical measure of sample to approximate f.
- Appeal to Glivenko-Cantelli theorem.

Theoretical Motivation of Sample Approximation

Theorem (Strong Law of Large Numbers)

Let $X_1, X_2, \ldots \overset{iid}{\sim} f$, *and let* $\varphi : E \to \mathbb{R}$ *with* $\mathbb{E}\left[|\varphi(X_1)|\right] < \infty$ *then:*

$$\frac{1}{n}\sum_{i=1}^{n} \varphi(X_i) \overset{a.s.}{\to} \mathbb{E}_f\left[\varphi(X_1)\right].$$

Theorem (Central Limit Theorem)

Let $X_1, \ldots \overset{iid}{\sim} f_X$ *and let* $\varphi : E \to \mathbb{R}^k$ *with* $\Sigma = \mathbb{V}ar\left[\varphi(X)\right] < \infty$, *then as* $n \to \infty$*:*

$$\sqrt{n}\left[\frac{1}{n}\sum_{i=1}^{n} \varphi(X_i) - \mathbb{E}\left[\varphi(X_1)\right]\right] \overset{\mathcal{D}}{\to} N(\mathbf{0}, \mathbf{\Sigma}).$$

Theoretical Motivation of Sample Approximation

Theorem (Glivenko-Cantelli)

Let $X_1, \ldots \overset{iid}{\sim} f_X$ *have cdf* F_X.
Let

$$F_n(x) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}_{(-\infty, X_i]}(x)$$

then as $n \to \infty$

$$\sup_x |F_n(x) - F(x)| \overset{a.s.}{\to} 0.$$

Part 1— Section 2

Randomized Testing

Randomized Testing

- One simple example of computer intensive statistics.
- We'll revisit *how* we can implement these things later.
- Art of testing: find a set R_α such that

$$\mathbb{P}\left(T \in R_\alpha; H_0\right) = \alpha$$

and

$$\mathbb{P}\left(T \in R_\alpha; H_1\right) > \alpha$$

.

- What if we don't know f_T?

Is a Die Fair?

- Given n rolls of a die, we want to establish whether it's fair.
- Canonical first-year example of a χ-squared test...
- Compute

$$T = \sum_{k=1}^{K} (O_k - E_k)^2 / E_k$$

- $T \overset{\text{approx}}{\sim} \chi^2_{k-1}$ by asymptotic arguments.
- What if the asymptotics don't hold?

A Randomized Goodness of Fit Test

- Imagine we have 9 measured rolls (and can't easily obtain more):

Value	1	2	3	4	5	6
Count	0	1	0	2	2	4

- If the die is fair we *expect* 1.5 observations of each value.
- The test statistic is:

$$T = \frac{1.5^2 + 0.5^2 + 1.5^2 + 0.5^2 + 0.5^2 + 2.5^2}{1.5} = 7\frac{2}{3}$$

- The asymptotics *certainly* don't hold:

$$(O_k - E_k)^2 \in \{0.5^2, 1.5^2, 2.5^2, 3.5^2, 4.5^2, 5.5^2, 6.5^2, 7.5^2\}.$$

- But we can *simulate* from H_0.

An R Implementation

Randomized Goodness of Fit Testing: Setup

```
p  <- 1/6 * c(1,1,1,1,1,1)
n  <- 9
r  <- 10000
ob <- rmultinom(r,n,p)
ex <- n*p
T  <- colSums((ob - ex)^2/ex)
```

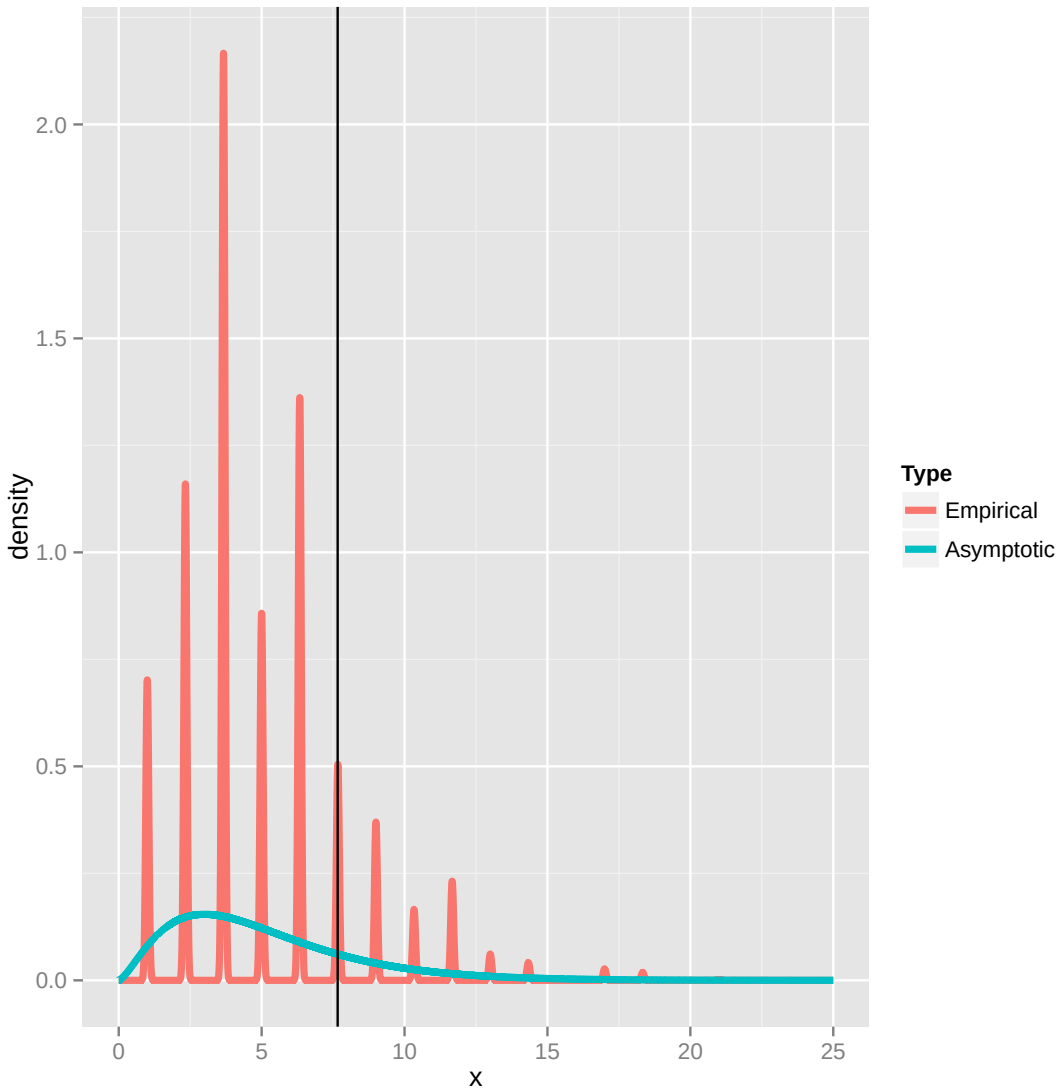
How many elements in T are larger than the observed value?

Randomized Goodness of Fit Testing: Comparison

```
t <- 7.66
m <- sum(T >= (t - 0.001)) #T discrete
print(m/r)
```

A Startling (Anti)climax

Empirical p-value: 0.1848
Asymptotic p-value: 0.1860



Randomized Test in General

- Given a hypothesis, H_0 and an alternative, H_1, and data $\mathbf{x}$ which realises $\mathbf{X}$ under H_0:
  - Obtain a realisation $\mathbf{u}$ of $\mathbf{U}$ ($\mathbf{U}|\mathbf{X} \sim f_{\mathbf{U}|\mathbf{X}}$ from some known distribution).
  - Compute R_α such that $\mathbb{P}\left((\mathbf{X}, \mathbf{U}) \in R_\alpha; H_0\right) = \alpha$.
  - Reject H_0 if $(\mathbf{x}, \mathbf{u}) \in R_\alpha$.

Goodness of Fit Test in General Form

- Let $f_{\mathbf{U}|\mathbf{X}}(\mathbf{u}|\mathbf{x}) = \prod_{i=1}^{r} f_T(u_i; H_0)$.
  By sampling $\mathbf{Z}_i \overset{\text{iid}}{\sim} f_{\mathbf{X}}(\cdot; H_0)$ and setting $U_i = g(\mathbf{Z}_i)$.
- Let $R_\alpha = \{(\mathbf{x}, \mathbf{u}) : g(\mathbf{x}) > u_{[r(1-\alpha)]}\}$.
  Where g is such that $T = g(\mathbf{X})$; $u_{[i]}$ is the i^{th} order statistic.

Are Those Medians Different (Part I)?

- Consider testing for different medians:

$$H_0: \quad X_1, \ldots, X_{n_X} \overset{\text{iid}}{\sim} f_X(\cdot; m) \quad Y_1, \ldots, Y_{n_Y} \overset{\text{iid}}{\sim} f_Y(\cdot; m)$$
$$H_1: \quad X_1, \ldots, X_{n_X} \overset{\text{iid}}{\sim} f_X(\cdot; m) \quad Y_1, \ldots, Y_{n_Y} \overset{\text{iid}}{\sim} f_Y(\cdot; m')$$

- Here, lets consider the two-sided version: $m' \neq m$.
- And we'll assume that we know the form of the two distributions:

$$f_X(x; m) = f_Y(x; m) = \frac{1}{2}\exp(-|x - m|)$$

- Letting $\widetilde{X} = X_{[(n_X+1)/2]}$ and $\widetilde{Y} = Y_{[(n_Y+1)/2]}$:

$$\begin{aligned}\widetilde{X} - \widetilde{Y} =& (\widetilde{X} - m) - (\widetilde{Y} - m) \\ =& (X - m)_{[(n_X+1)/2]} - (Y - m)_{[(n_Y+1)/2]}\end{aligned}$$

- So the distribution of $\widetilde{X} - \widetilde{Y}$ is *independent* of $m|H_0$.

- A Randomized test:
  - Let $T = \widetilde{X} - \widetilde{Y}$.
  - Draw $i = 1 : r$ copies of $\mathbf{X}$ and $\mathbf{Y}$ with $m = 0$:

$$X'^{,j}_{1,\ldots,n_X} \overset{\text{iid}}{\sim} f_X(\cdot; 0),$$
$$Y'^{,j}_{1,\ldots,n_Y} \overset{\text{iid}}{\sim} f_Y(\cdot; 0).$$

  - Compute the difference between their medians:

$$i = 1, \ldots, r: \qquad T'_i = X'^{,i}_{[(n_X+1)/2]} - Y'^{,i}_{[(n_Y+1)/2]}.$$

  - Let $p = (1 + |\{i : T'_i \geq T\}|)/(r + 1)$.
  - Reject H_0 if $p < \alpha$.

But surely this is cheating: what if we *don't* know so much?

Permutation Tests

- Consider the hypotheses:

$$
\begin{aligned}
H_0: \quad & X_1, \ldots, X_{n_X} \overset{\text{iid}}{\sim} f_X(\cdot) && Y_1, \ldots, Y_{n_Y} \overset{\text{iid}}{\sim} f_X(\cdot) \\
& F_X^{-1}(0.5) = F_Y^{-1}(0.5) && \\
H_1: \quad & X_1, \ldots, X_{n_X} \overset{\text{iid}}{\sim} f_X(\cdot) && Y_1, \ldots, Y_{n_Y} \overset{\text{iid}}{\sim} f_Y(\cdot) \\
& F_X^{-1}(0.5) \neq F_Y^{-1}(0.5) &&
\end{aligned}
$$

  where f_X and f_Y are unknown.
- Here, F_X^{-1} and F_Y^{-1} are assumed to exist.
- Sample medians are a natural test statistics, but:
  - We don't know their distribution under H_0.
  - And can't sample from that distribution.
- What can we do?

The Permutation Approach

- If $\exists m \text{s.t. } \mathbb{P}(X_i \leq m) = \mathbb{P}(Y_i \leq m) = 0.5$,
- then $F_X^{-1}(0.5) = F_Y^{-1}(0.5) = m$
- and $F_X(m) = F_Y(m) = 0.5$
- so $\alpha F_X(m) + (1-\alpha)F_Y(m) = 0.5$.
- In fact, under H_0, the distribution of $\tilde{X}$ and $\tilde{Y}$ should be invariant under label permutations.

- Let $\mathbf{Z} = (X_1, \ldots, X_{n_X}, Y_1, \ldots, Y_{n_Y})$ be an $n = n_X + n_Y$ vector.
- Now let

$$T(\mathbf{Z}) = \text{median}(Z_1, \ldots, Z_{n_X}) - \text{median}(Z_{n_X+1}, \ldots, Z_n)$$

- And let $\pi \in \mathcal{P} \subset \{1, \ldots, n\}^n$ denote a permutation, writing:

$$\pi Z := (Z_{\pi_1}, Z_{\pi_2}, \ldots, Z_{\pi_n})$$

- Now, under H_0:

$$\forall \pi \in \mathcal{P}: \qquad T(\pi Z) \overset{\mathcal{D}}{=} T(Z)$$

- So if $T(\mathbf{Z}) > T(\pi\mathbf{Z})$ for $100(1-\alpha)\%$ of π we can reject H_0.
- We *just* need to compute $T(\pi\mathbf{Z})$ for every $\pi \in \mathcal{P}$...

A Randomized Permutation Test

- We can sample elements uniformly from $\mathcal{P}$:
  - Sample $\pi_1 \sim \mathsf{U}(1, \ldots, n)$.
  - Sample $\pi_2 \sim \mathsf{U}(\{1, \ldots, n\} \setminus \{\pi_1\})$.
  - $\vdots$
  - Sample $\pi_n \sim \mathsf{U}(\{1, \ldots, n\} \setminus \{\pi_1, \ldots, \pi_{n-1}\})$.
- We can do this many times to approximate the law of $T(\pi \mathbf{z})$ when $\pi \sim \mathsf{U}(\mathcal{P})$:
  - Sample $\pi_1, \ldots, \pi_k \overset{\text{iid}}{\sim} \mathsf{U}(\mathcal{P})$.
  - Compute $T_1 = T(\pi_1 \mathbf{z}), \ldots, T_k = T(\pi_k \mathbf{z})$.
  - Use the empirical distribution of $(T_1, \ldots, T_k)$ to approximate the law of $T(\pi \mathbf{z})$.
- This provides a general strategy for nonparametric testing.

Part 1— Section 3

Bootstrap Methods

Bootstrap Methods

- Randomized tests: use empirical distribution of T.
- Permutation tests: use *resampling*-based empirical distribution of T.
- Bootstrap methods: use *resampling*-based empirical distribution of $\hat{\theta}$ to characterise the sampling distribution of $\hat{\theta}$.

The Bootstrap Ansatz

If $X_1, \ldots, X_n \overset{\text{iid}}{\sim} F_X$ and n is large then "$\hat{F}_X^n \approx F$"
$\Longrightarrow$ sampling from $\hat{F}_X^N$ is "close" to sampling from F
$\Longrightarrow$ samples from $\hat{F}_X^N$ might be suitable for approximating F!

The Basis of the Bootstrap

- Given a simple random sample $X_1, \ldots, X_n$
- Repeat the following for $b = 1 : B$:
  - Sample n times from $\hat{F}_X^n(x)$ i.e. sample n times uniformly with replacement from $X_1, \ldots, X_n$ to obtain $\hat{X}_1^b, \ldots, \hat{X}_n^b$.
- Given a function $g : E^n \to \mathbb{R}$ approximate the distribution of g under F using the sample $g(\hat{X}_1^1, \ldots, \hat{X}_n^1), \ldots, g(\hat{X}_1^B, \ldots, \hat{X}_n^B)$.
- Glivenko-Cantelli (and extensions) tells us that $\hat{F}_X^n(x) \overset{a.s.}{\to} F_X(x)$.

NB Regularity conditions must hold in order for this to work.

Approximating the Sampling Distribution of the Median

- Given $X_1, \ldots, X_n$ a simple random sample:
- Compute $T = \text{median}(X_1, \ldots, X_n)$.
- For $b = 1 : B$
  - Sample n times with replacement from $X_1, \ldots, X_n$ to obtain $\hat{X}_1^b, \ldots, \hat{X}_n^b$.
  - Compute $\hat{T}^b = \text{median}(\hat{X}_1^b, \ldots, \hat{X}_n^b)$.
- Treat the empirical distribution of $\hat{T}^1, \ldots, \hat{T}^B$ as a proxy for the sampling distribution of T.

Bootstrap Bias Correction

- Given $x_1, \ldots, x_n$ and,
- estimator $T : E^n \to \mathbb{R}$ of θ
- computer $t = T(x_1, \ldots, x_n)$.
- For $b = 1 : B$
  - Sample n times with replacement from $X_1, \ldots, X_n$ to obtain $\hat{X}_1^b, \ldots, \hat{X}_n^b$.
  - Compute $\hat{T}^b = T(\hat{X}_1^b, \ldots, \hat{X}_n^b)$.
- Treat the empirical distribution of $\hat{T}^1 - t, \ldots, \hat{T}^B$ as a proxy for the sampling distribution of $T(X_1, \ldots, X_n) - \theta$.
- Obtain *bias-corrected* estimate:

$$t - \frac{1}{B}\sum_{b=1}^{B}(\hat{T}^b - t) = 2t - \frac{1}{B}\sum_{b=1}^{B}\hat{T}^b.$$

Naïve Bootstrap Confidence Intervals 1: The Asymptotic Approach

- For some T we might expect T to have an asymptotically normal distribution.
- So, estimate it's variance:

$$\hat{\sigma}_T^2 = \frac{1}{B-1}\sum_{b=1}^{B}\left(\hat{T}^b - \frac{1}{B}\sum_{b=1}^{B}\hat{T}^b\right)^2$$

- And use the normal confidence interval:

$$\left[T - z_{\alpha/2}\hat{\sigma}_T, T + z_{\alpha/2}\hat{\sigma}_T\right]$$

  with approximate coverage α.
- Depends on asymptotic normality.
- Further approximation for finite samples.

Naïve Bootstrap Confidence Intervals 2: Bootstrap Percentile Confidence Intervals

- We could use the bootstrap distribution of T directly:

$$[\hat{T}^{[B(\alpha/2)]}, \hat{T}^{[B(1-\alpha/2)]}]$$

- These are known as *bootstrap percentile confidence intervals*.
- Depend on the *bootstrap* approximation; no additional approximations.

Bootstrap "pivotal" Confidence Intervals

- Using bootstrap approximations of (approximate) pivots can be more elegant.
- Assume that T is an estimator of some real population parameter, θ.
- Define $R = T - \theta$.
- Let F_R denote the cdf of R, then:

$$\begin{aligned}\mathbb{P}(L \leq \theta \leq U) =& \mathbb{P}(L - T \leq \theta - T \leq U - T) \\ =& \mathbb{P}(T - U \leq R \leq T - L) \\ =& F_R(T - L) - F_R(T - U).\end{aligned}$$

Suggests using:

$$[T - F_R^{-1}(1 - \alpha/2), T - F_R^{-1}(\alpha/2)]$$

- We can't use this interval directly because we don't know F_R and we certainly don't know F_R^{-1}.

Bootstrap "pivotal" Confidence Intervals

- We can invoke the bootstrap idea again:
- Compute $T = g(X_1, \ldots, X_n)$.
- For $b = 1 : B$
  - Sample n times with replacement from $X_1, \ldots, X_n$ to obtain $\hat{X}_1^b, \ldots, \hat{X}_n^b$.
  - Compute $\hat{T}^b = g(\hat{X}_1^b, \ldots, \hat{X}_n^b)$.
- Claim that "$\hat{T}^1, \ldots, \hat{T}^B$ are to T as T is to θ".
- Set $\hat{R}^b = \hat{T}^b - T$.
- Use the empirical distribution, $\hat{F}_R$, of $\hat{R}^1, \ldots, \hat{R}^B$ instead of F_R:

$$[T - \hat{F}_R^{-1}(1 - \alpha/2), T - \hat{F}_R^{-1}(\alpha/2)]$$

Summary of Part 1

- Motivation: Bayesian inference, Fisherian inference, ...
- Towards simulation-based inference (see later).
- Randomized Tests
- Permutation Tests
- Boostrap Characterisation of Estimators.
- Bootstrap Confidence Intervals.

Part 2

Simulation and the Monte Carlo Method

Simulation

- We've seen *motivation* of simulation for inference.
- We've seen *examples* of simulation-based methods.
- We *need* methods for addressing broad classes of problems.
- We *need* methods for obtaining the necessary samples.

Part 2— Section 4

The Monte Carlo Method

Monte Carlo Method

- A generic scheme for approximating expectations.
- To approximate $I = \mathbb{E}_f [\varphi(X)]$,
- Draw $X_1, \ldots, X_n \overset{\text{iid}}{\sim} f$,
- Use $\hat{I}_{\text{mc}} = \frac{1}{n} \sum_{i=1}^{n} \varphi(X_i)$.
- Convergence follows from SLLN, CLT, ...

Recall: The Three Views of the Monte Carlo Method

Direct Approximation Design an experiment such that:

$$\varphi(X) \sim f_{\varphi(X)}$$

constructed such that it has the expectation of interest.

Integral Approximation We're interested in

$$\mathbb{E}_f\left[\varphi(X)\right]$$

and know how to approximate such.

Distributional Approximation We're interested in

$$\mathbb{E}_f\left[\varphi(X)\right]$$

so obtain an approximation of f which we can compute expectationts with respect to.

Contrasting Views of Monte Carlo

- Usual explanation of the Monte Carlo Method, with $X_1, \ldots \overset{\text{iid}}{\sim} f$ approximate the integral:

$$\frac{1}{n}\sum_{i=1}^{n}\varphi(X_i) \overset{a.s.}{\to} \mathbb{E}_f\left[\varphi(X)\right]$$

- Another perspective, approximate the distribution:
  - let $\hat{f}^n = \frac{1}{n}\sum_{i=1}^{n}\delta_{X_i}$
  - if $\hat{f}^n \Rightarrow f$
  - then we automatically have that

$$\mathbb{E}_{\hat{f}^n}\left[\varphi(X)\right] \to \mathbb{E}_f\left[\varphi(X)\right]$$

  for every continuous bounded φ.

Part 2— Section 5

PRNGs

Problem: (how) can computers produce random numbers?

von Neumann's perspective

> *Any one who considers artithmetical methods of reproducing random digits is, of course, in a state of sin. . . . there is no such thing as a random number — there are only methods of producing random numbers, and a strict arithmetic procedure is of course not such a method.*

As in so many other areas, von Neumann was completely correct.

Three Resolutions of this Philosophical Paradox

1. Use Exogeneous Randomness (TRNGs)
   See `www.random.org` or `http://en.wikipedia.org/wiki/Hardware_random_number_generator`.
2. Pseudorandom Number Generators (PRNGs; cf. *Statistical Computing* module)
   Sacrifice randomness whilst mimicking its *relevant statistical properties*.
3. Quasirandom Number Sequences (QRNSs)
   Sacrifice randomness in exchange for *minimising discrepancy*.

All have advantages and disadvantages; we'll focus on PRNGs.

Part 2— Section 6

Sampling From Distributions

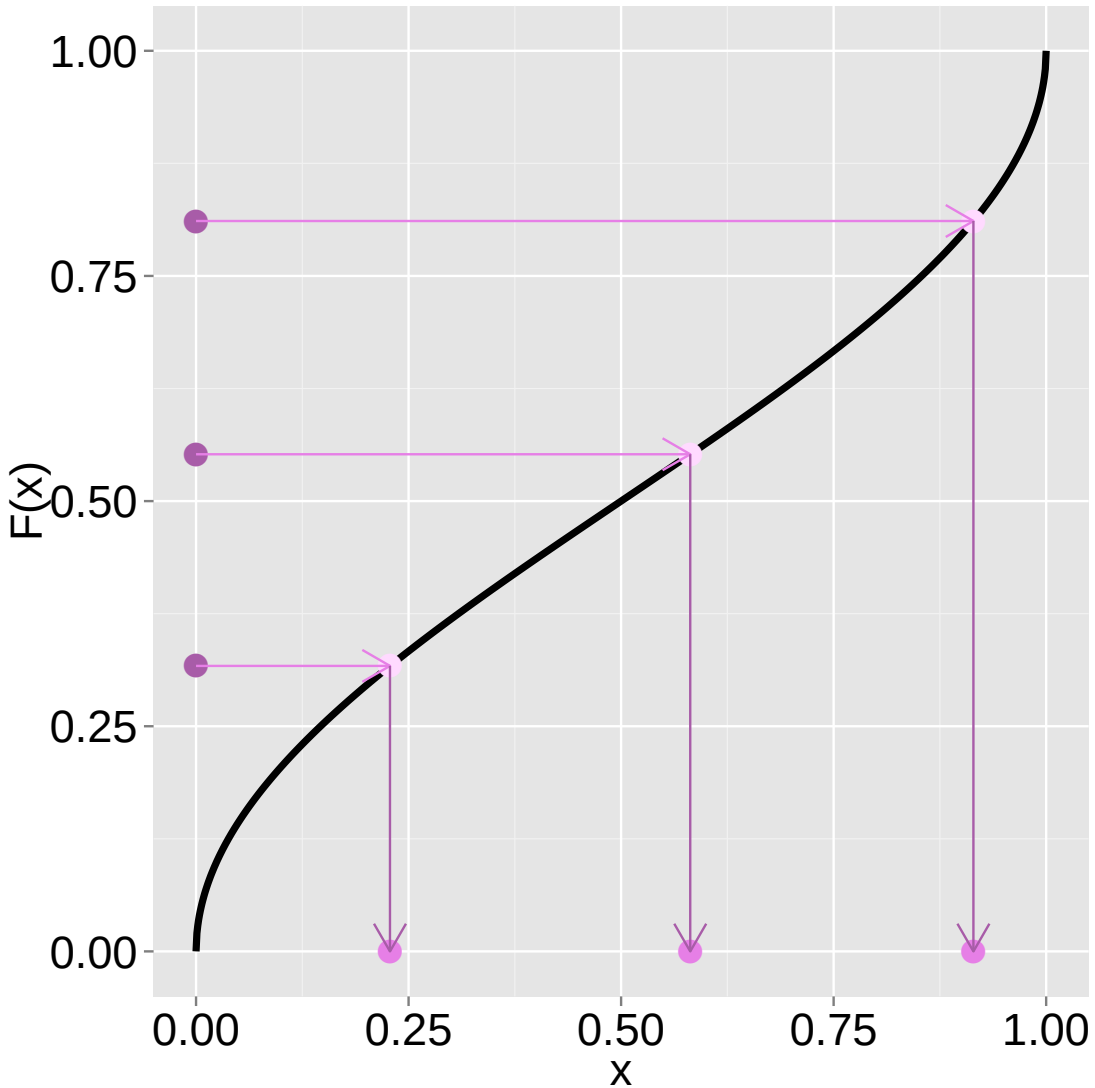
Transformation Methods

- Assume we have a *good* PRNG.
- How can we obtain (pseudo)samples from other distributions?
- General framework:
  - Treat output of PRNG as a stream of iid $\mathrm{U}[0, 1]$ RVs.
  - Use laws of probability to transform these to obtain RVs with other distributions.
  - Treat transformed PRNG output as RVs of the target distribution.
- But, how?

Inversion Sampling

The Inversion method

Let $U \sim \mathrm{U}[0,1]$ and let F be an invertible CDF. Then $F^{-1}(U)$ has the CDF F.



Inversion Sampling

The Inversion method

Let $U \sim \mathsf{U}[0,1]$ and F be an invertible CDF.
Then $F^{-1}(U)$ has the CDF F.

Inversion Sampling: A simple algorithm for drawing $X \sim F$

1. Draw $U \sim \mathsf{U}[0,1]$.
2. Set $X = F^{-1}(U)$.

Example: Exponential distribution

The exponential distribution with rate $\lambda > 0$ has the CDF ($x \geq 0$)

$$\begin{aligned} F_\lambda(x) &= 1 - \exp(-\lambda x) \\ F_\lambda^{-1}(u) &= -\log(1-u)/\lambda. \end{aligned}$$

So we have a simple algorithm for drawing $X \sim \text{Exp}(\lambda)$:

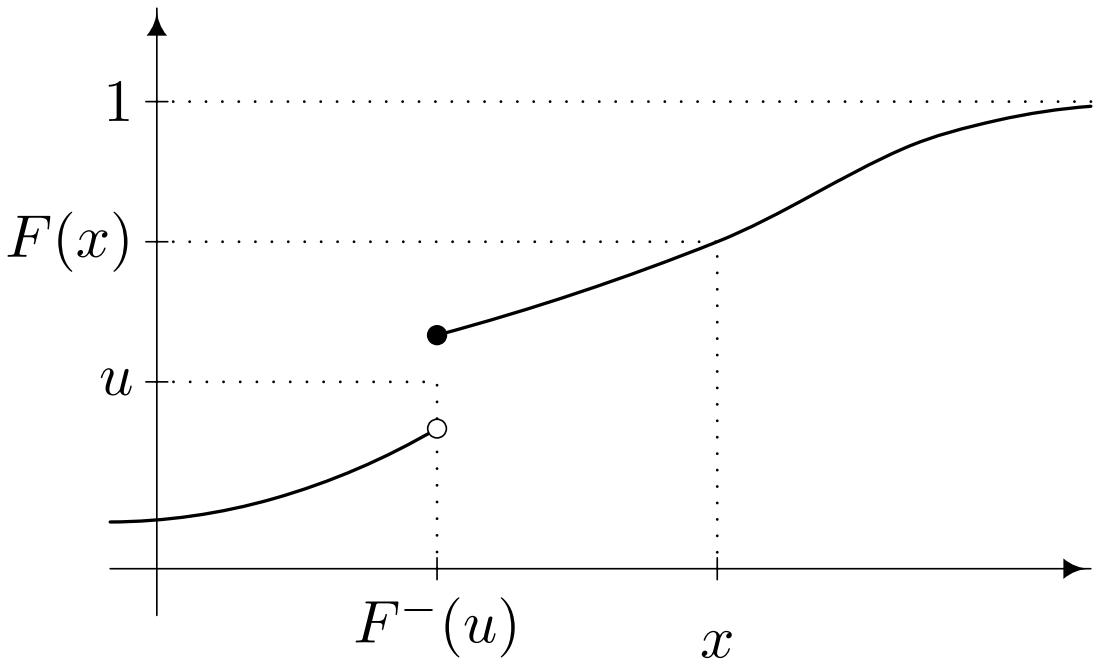
1. Draw $U \sim \text{U}[0,1]$.
2. Set $X = -\dfrac{\log(1-U)}{\lambda}$.

Actually, setting $X = -\dfrac{\log(U)}{\lambda}$ makes more sense.

The Generalised Inverse of the CDF

Generalised inverse of the CDF

$$F^-(u) := \inf\{x : \ F(x) \geq u\}$$



Replacing F^{-1} with F^- yields a generally-applicable inversion sampling algorithm — key is $F^-(u) \leq x \Leftrightarrow u \leq F(x)$.

Box-Muller: Fast Normally-Distributed Random Variables

- Consider (X_1, X_2) their polar representation (R, θ):

$$X_1 = R \cdot \cos(\theta), \qquad X_2 = R \cdot \sin(\theta)$$

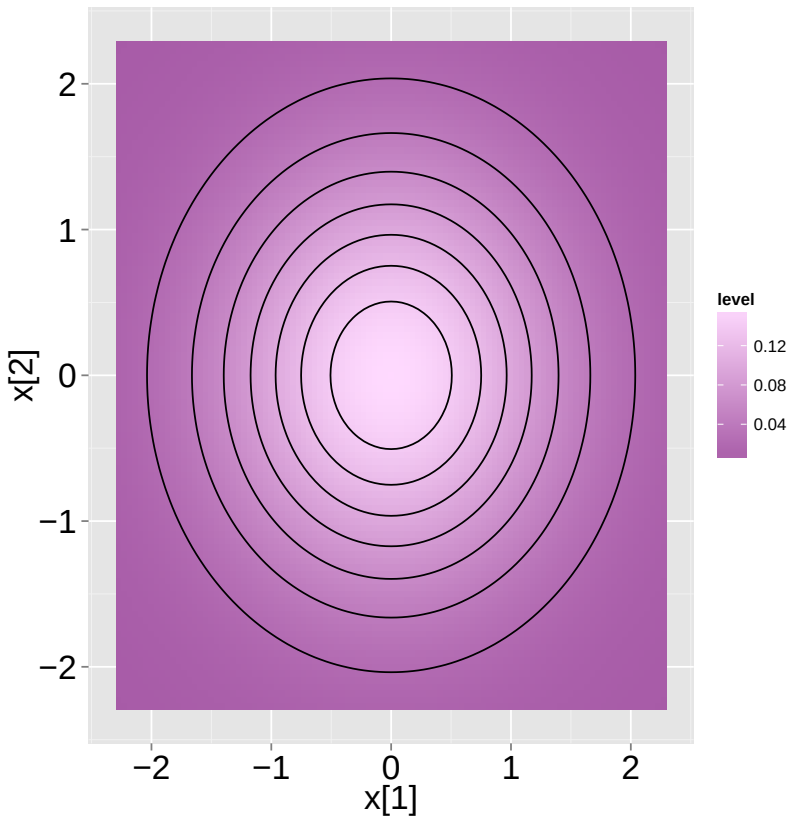
- The following equivalence holds (with θ, R independent):
  $X_1, X_2 \overset{\text{iid}}{\sim} \mathsf{N}(0,1) \iff \theta \sim \mathsf{U}[0, 2\pi]$ and $R^2 \sim \mathsf{Expo}(1/2)$
- Given $U_1, U_2 \overset{\text{iid}}{\sim} \mathsf{U}[0,1]$ set

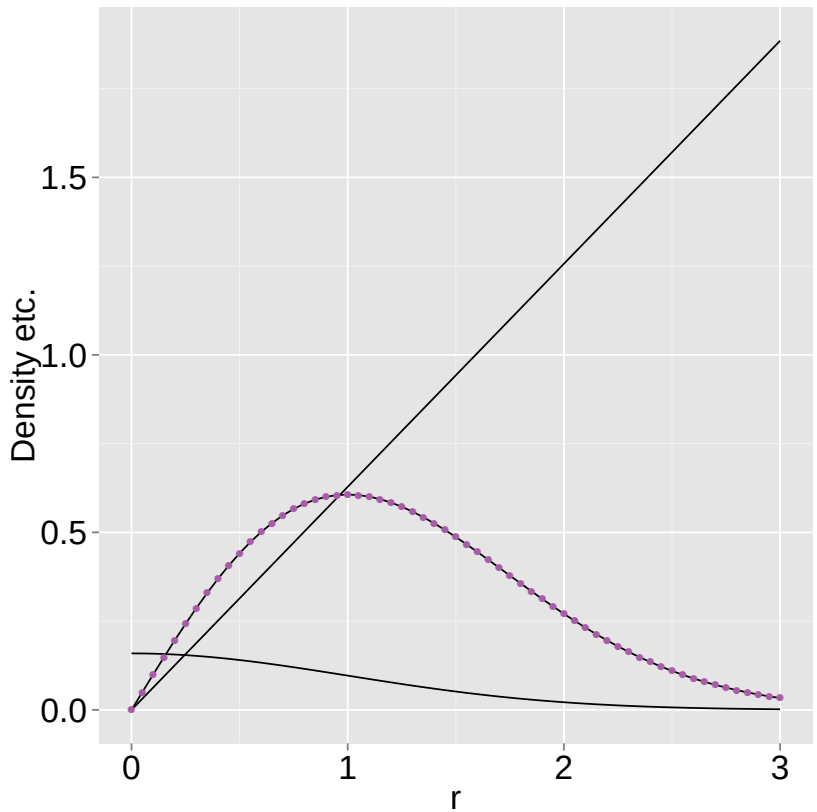
$$R = \sqrt{-2\log(U_1)}, \qquad \theta = 2\pi U_2,$$

- By substitution

$$\begin{aligned} X_1 &= \sqrt{-2\log(U_1)} \cdot \cos(2\pi U_2) \\ X_2 &= \sqrt{-2\log(U_1)} \cdot \sin(2\pi U_2) \end{aligned}$$

The Geometry of Box-Muller Transformation





Box-Muller: Algorithm

Box-Muller method

1. Draw
$$U_1, U_2 \overset{\text{iid}}{\sim} \mathsf{U}[0,1].$$
2. Set
$$\begin{aligned} X_1 &= \sqrt{-2\log(U_1)} \cdot \cos(2\pi U_2), \\ X_2 &= \sqrt{-2\log(U_1)} \cdot \sin(2\pi U_2). \end{aligned}$$
3. Output $X_1, X_2 \overset{\text{iid}}{\sim} \mathsf{N}(0,1)$.

The Limitations of Simple Transformations...

- When F^- is available and cheap to evaluate, inversion sampling is very efficient. But:
  - We often don't have access to F;
  - if we do F^- may be difficult/impossible to obtain.
  - The multivariate case can be even harder.
- Clever custom transformations:
  - are costly to develop
  - require considerable ingenuity
  - are completely infeasible in complicated scenarios
- We need alternatives.

The Fundamental Theorem of simulation

Fundamental Theorem of Simulation

Sampling from a density f is equivalent to sampling uniformly from the area between f and the ordinal axes and discarding the "vertical" component.

- Follows from the identity

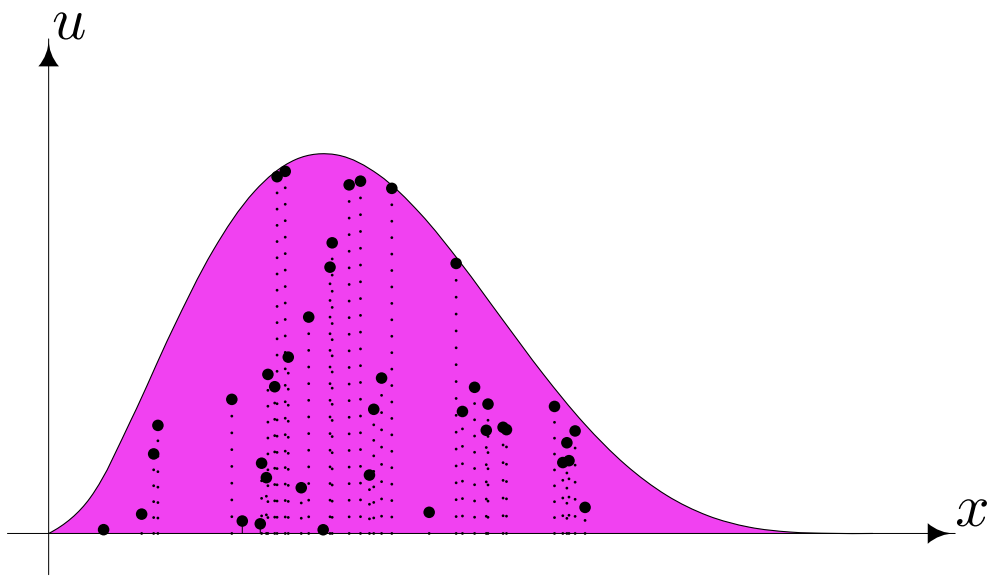
$$f(x) = \int_0^{f(x)} 1 \, du = \int_0^{\infty} \underbrace{1_{0<u<f(x)}}_{=f(x,u)} du.$$

- i.e. $f(x)$ can be interpreted as the marginal density of a uniform distribution on the area under the density $f(x)$:

$$\{(x, u) : \ 0 \leq u \leq f(x)\}.$$

First element of rejection sampling

- We can sample from f by sampling from the area under the density.



- If $(X, U) \sim \mathsf{U}(\{(x, u) : 0 \leq u \leq f(x)\})$ then $X \sim f$.

Second Element of Rejection Sampling

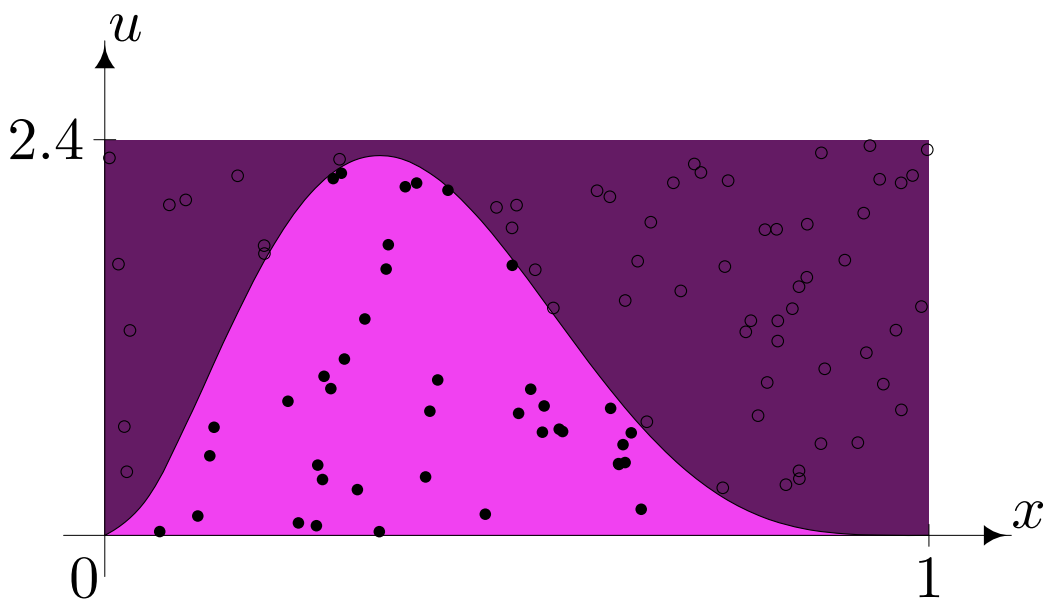
- Generally $\mathcal{G} = \{(x, u) : 0 \leq u \leq f(x)\}$ is complicated: we can't sample uniformly from it — at least not directly.
- Idea: Instead:
  - Sample from some $\mathcal{A} \supset \mathcal{G}$.
  - Keep only those points which lie within $\mathcal{G}$.
  - *Reject* the rest.

Example: Sampling from a Beta$(3, 5)$ distribution (1)

1. Draw (X, U) from the dark rectangle, i.e.:

$$X \sim \mathsf{U}(0, 1) \qquad U \sim \mathsf{U}(0, 2.4) \qquad X \perp U.$$

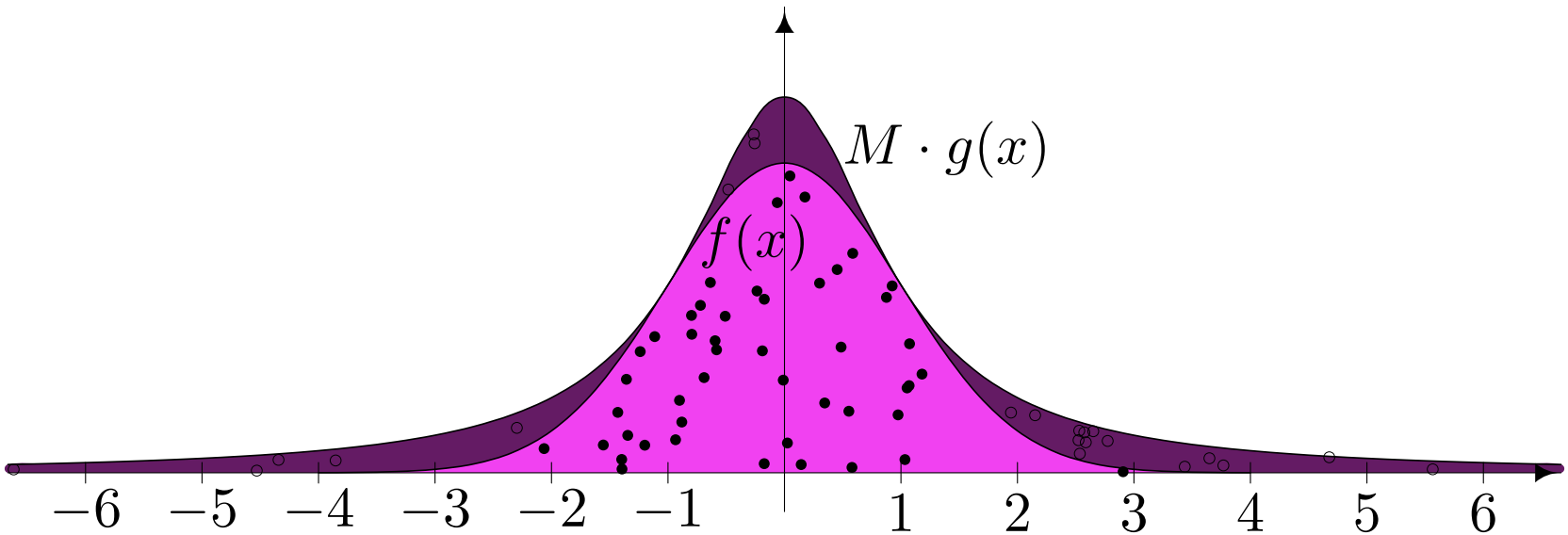
2. Accept X as a sample from f if (X, U) lies under the density.



Step 2 is equivalent to: Accept X if $U < f(X)$,
i.e. accept X with probability $\mathbb{P}(U < f(X)|X = x) = f(X)/2.4$.

Example: Sampling from a Beta$(3, 5)$ distribution (2)

- Algorithm:
  1. Draw $X \sim \mathrm{U}(0, 1)$.
  2. Accept X as a sample from Beta$(3, 5)$ w.p. $f(X)/2.4$.
- Not every density can be bounded by a box.
- Natural generalisation: replace M times U$[0, 1]$ with M times another density g.



A General Algorithm

Algorithm: Rejection sampling

Given two densities f, g with $f(x) < M \cdot g(x)$ for all x, we can generate a sample from f by

1. Draw $X \sim g$.
2. Accept X as a sample from f with probability

$$\frac{f(X)}{M \cdot g(X)},$$

otherwise go back to step 1.

For $f(x) < M \cdot g(x)$ to hold f *cannot* have heavier tails than g.

A Useful Trick

Avoiding Unknown Constants

If we know only $\tilde{f}(x)$ and $\tilde{g}(x)$, where $f(x) = C \cdot \tilde{f}(x)$, and $g(x) = D \cdot \tilde{g}(x)$we can carry out rejection sampling using acceptance probability

$$\frac{\tilde{f}(X)}{M \cdot \tilde{g}(X)}$$

provided $\tilde{f}(x) < M \cdot \tilde{g}(x)$ for all x.

Can be useful in Bayesian statistics:

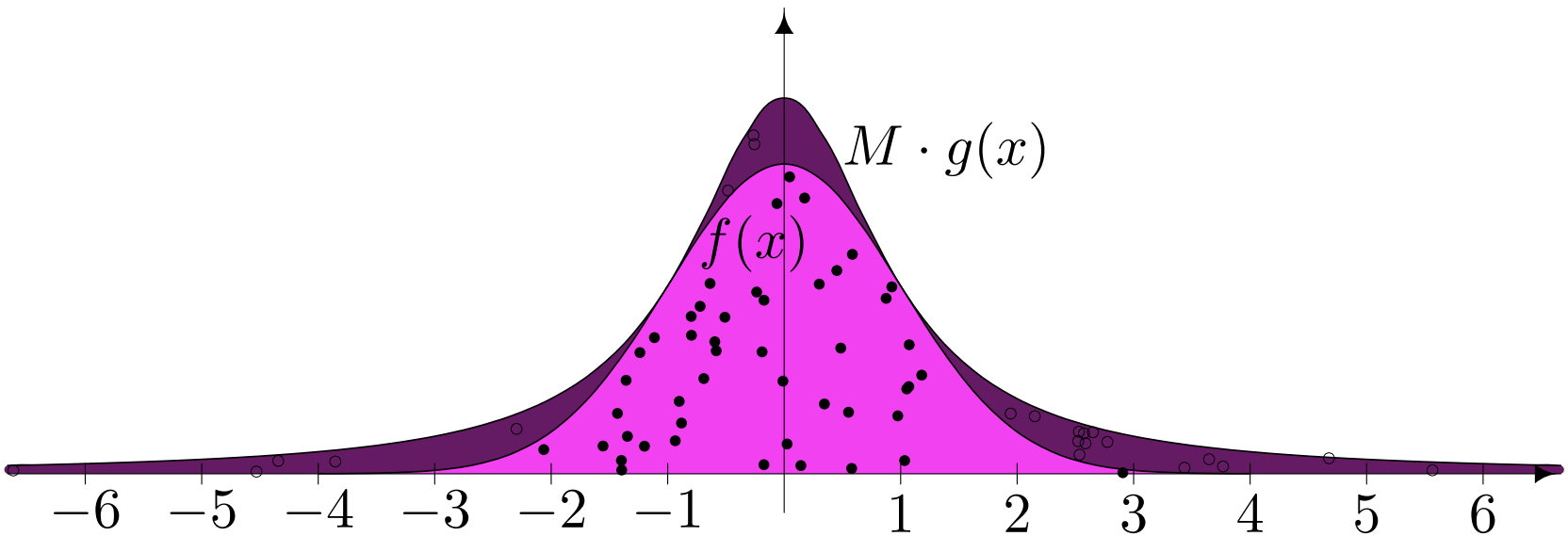
$$f^{\text{post}}(\theta) = \frac{f^{\text{prior}}(\theta) l(\mathbf{y}_1, \ldots, \mathbf{y}_n | \theta)}{\int_\Theta f^{\text{prior}}(\vartheta) l(\mathbf{y}_1, \ldots, \mathbf{y}_n | \vartheta) \, d\vartheta} = C \cdot f^{\text{prior}}(\theta) l(\mathbf{y}_1, \ldots, \mathbf{y}_n | \theta)$$

Example: Sampling from $\mathsf{N}(0,1)$

- Recall the following densities:

$$\mathsf{N}(0,1) \quad f(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) \qquad \text{Cauchy} \quad g(x) = \frac{1}{\pi(1+x^2)}$$

- For $M = \sqrt{2\pi} \cdot \exp(-1/2)$ we have that $f(x) \leq M g(x)$.
  $\rightsquigarrow$ We can use rejection sampling targetting f using g as proposal.



Non-example: Sampling from a Cauchy Distribution

- We cannot sample from a Cauchy distribution (g) using a Normal (f) as instrumental distribution.
- The Cauchy distribution has heavier tails than the Normal distribution: there is no $M \in \mathbb{R}$ such that

$$\frac{1}{\pi(1+x^2)} < M \cdot \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2}\right).$$

An Alternative to Rejection

- Rejection sampling discards many samples.
- This seems wasteful.
- Couldn't we, instead, *weight* samples based on the acceptance probability?

The fundamental identities behind importance sampling (1)

Assume that $g(x) > 0$ for (almost) all x with $f(x) > 0$:

$$\mathbb{P}(X \in \mathcal{X}) = \int_{\mathcal{X}} f(x)\,dx = \int_{\mathcal{X}} g(x) \underbrace{\frac{f(x)}{g(x)}}_{=:w(x)}\,dx = \int_{\mathcal{X}} g(x)w(x)\,dx$$

Assume that $g(x) > 0$ for (almost) all x with $f(x) \cdot \varphi(x) \neq 0$

$$\mathbb{E}_f(\varphi(X)) = \int f(x)\varphi(x)\,dx = \int g(x) \underbrace{\frac{f(x)}{g(x)}}_{=:w(x)} \varphi(x)\,dx$$

$$= \int g(x)w(x)\varphi(x)\,dx = \mathbb{E}_g(w(X) \cdot \varphi(X)),$$

The fundamental identities behind importance sampling (2)

- Consider $X_1, \ldots, X_n \sim g$ and $\mathbb{E}_g|w(X) \cdot \varphi(X)| < +\infty$. Then

$$\frac{1}{n}\sum_{i=1}^{n} w(X_i)\varphi(X_i) \overset{a.s.}{\underset{n\to\infty}{\longrightarrow}} \mathbb{E}_g(w(X) \cdot \varphi(X))$$

$$\Rightarrow \frac{1}{n}\sum_{i=1}^{n} w(X_i)\varphi(X_i) \overset{a.s.}{\underset{n\to\infty}{\longrightarrow}} \mathbb{E}_f(\varphi(X)).$$

- Thus we can estimate $\mu := \mathbb{E}_f(\varphi(X))$ by
  1. Sample $X_1, \ldots, X_n \sim g$
  2. $\tilde{\mu} := \frac{1}{n}\sum_{i=1}^{n} w(X_i)\varphi(X_i)$

The importance sampling algorithm

Algorithm: Importance Sampling

Choose g such that $\operatorname{supp}(g) \supset \operatorname{supp}(f \cdot \varphi)$.

1. For $i = 1, \ldots, n$:
   1. Generate $X_i \sim g$.
   2. Set $w(X_i) = \frac{f(X_i)}{g(X_i)}$.
2. Return

$$\tilde{\mu} = \frac{\sum_{i=1}^{n} w(W_i)\varphi(X_i)}{n}$$

as an estimate of $\mathbb{E}_f(\varphi(X))$.

- Importance sampling does not yield realisations from f,
  $\rightsquigarrow$ but a *weighted sample* (X_i, W_i),
  $\rightsquigarrow$ which can be used for estimating expectations $\mathbb{E}_f(\varphi(X))$,
  $\rightsquigarrow$ or approximating f itself.

Basic properties of the importance sampling estimate

- We have already seen that $\tilde{\mu}$ is consistent if $\text{supp}(g) \supset \text{supp}(f \cdot \varphi)$ and $\mathbb{E}_g|w(X) \cdot \varphi(X)| < +\infty$, as

$$\tilde{\mu} := \frac{1}{n} \sum_{i=1}^{n} w(X_i)\varphi(X_i) \overset{a.s.}{\underset{n\to\infty}{\longrightarrow}} \mathbb{E}_f(\varphi(X))$$

- The expected value of the weights is $\mathbb{E}_g(w(X)) = 1$.
- $\tilde{\mu}$ is unbiased (see theorem below)

Theorem 2.2: Bias and Variance of Importance Sampling

$$\begin{aligned} \mathbb{E}_g(\tilde{\mu}) &= \mu \\ \text{Var}_g(\tilde{\mu}) &= \frac{\text{Var}_g(w(X) \cdot \varphi(X))}{n} \end{aligned}$$

Optimal proposals

Theorem

Optimal proposal The proposal distribution g that minimises the variance of $\tilde{\mu}$ is

$$g^*(x) = \frac{|\varphi(x)|f(x)}{\int |\varphi(t)|f(t)\,dt}.$$

- Theorem of little practical use: the optimal proposal involves $\int |\varphi(t)|f(t)\,dt$, which is the integral we want to estimate!
- Practical relevance:
  Choose g such that it is close to $|\varphi(x)| \cdot f(x)$

Super-efficiency of importance sampling

- For the optimal g^* we have that

$$\mathrm{Var}_f\left(\frac{\varphi(X_1)+\ldots+\varphi(X_n)}{n}\right) > \mathrm{Var}_{g^\star}(\tilde{\mu}),$$

  if φ is not almost surely constant.

Superefficiency of importance sampling

The variance of the importance sampling estimate can be *less* than the variance obtained when sampling directly from the target f.

- Intuition: Importance sampling allows us to choose a g that focuses on areas which contribute most to $\int \varphi(x)f(x)\,dx$.
- Even sub-optimal proposals can be super-efficient.

Importance Sampling Example 1: Setup

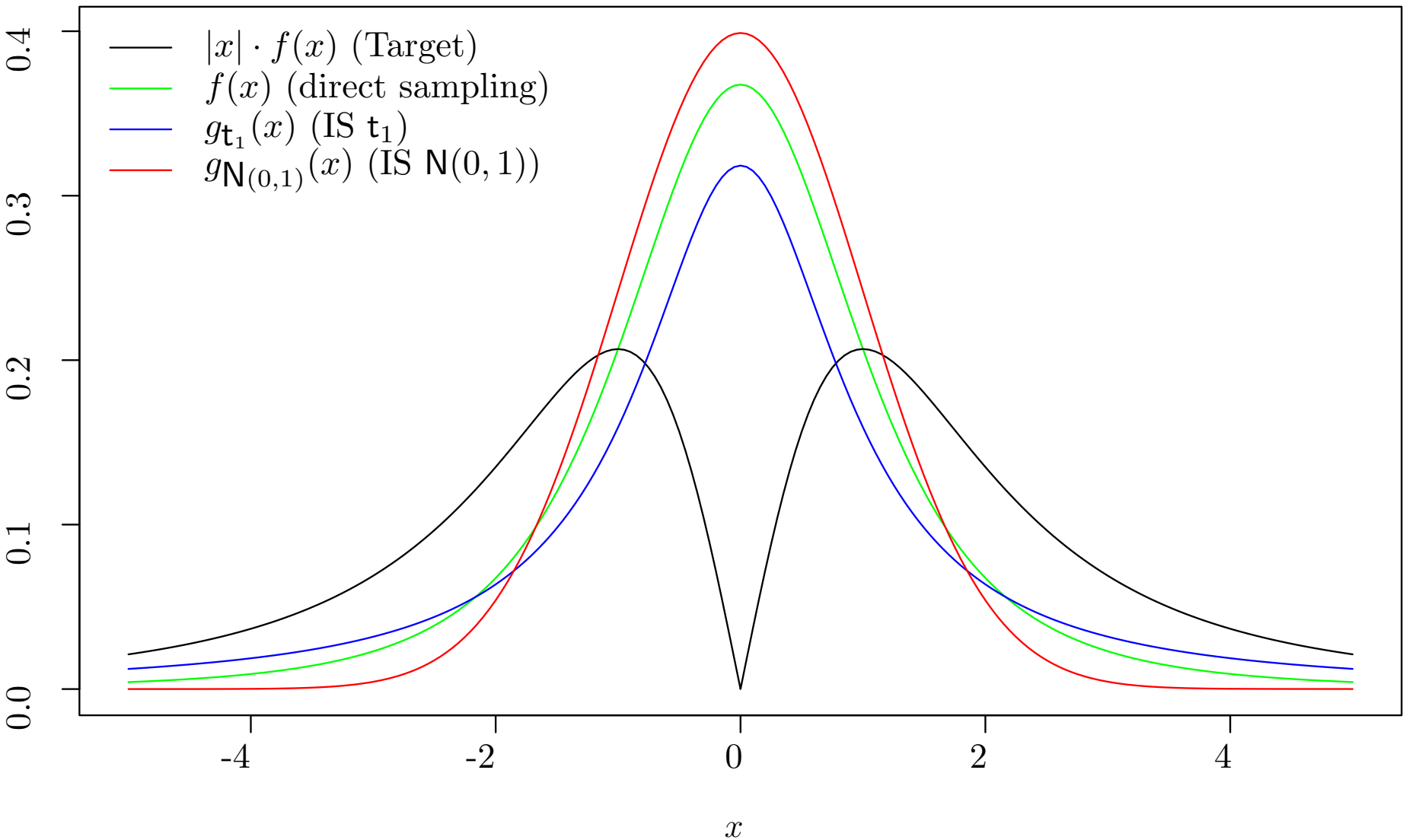
Compute $\mathbb{E}_f|X|$ for $X \sim \mathrm{t}_3$ by ...

(a) sampling directly from t_3.

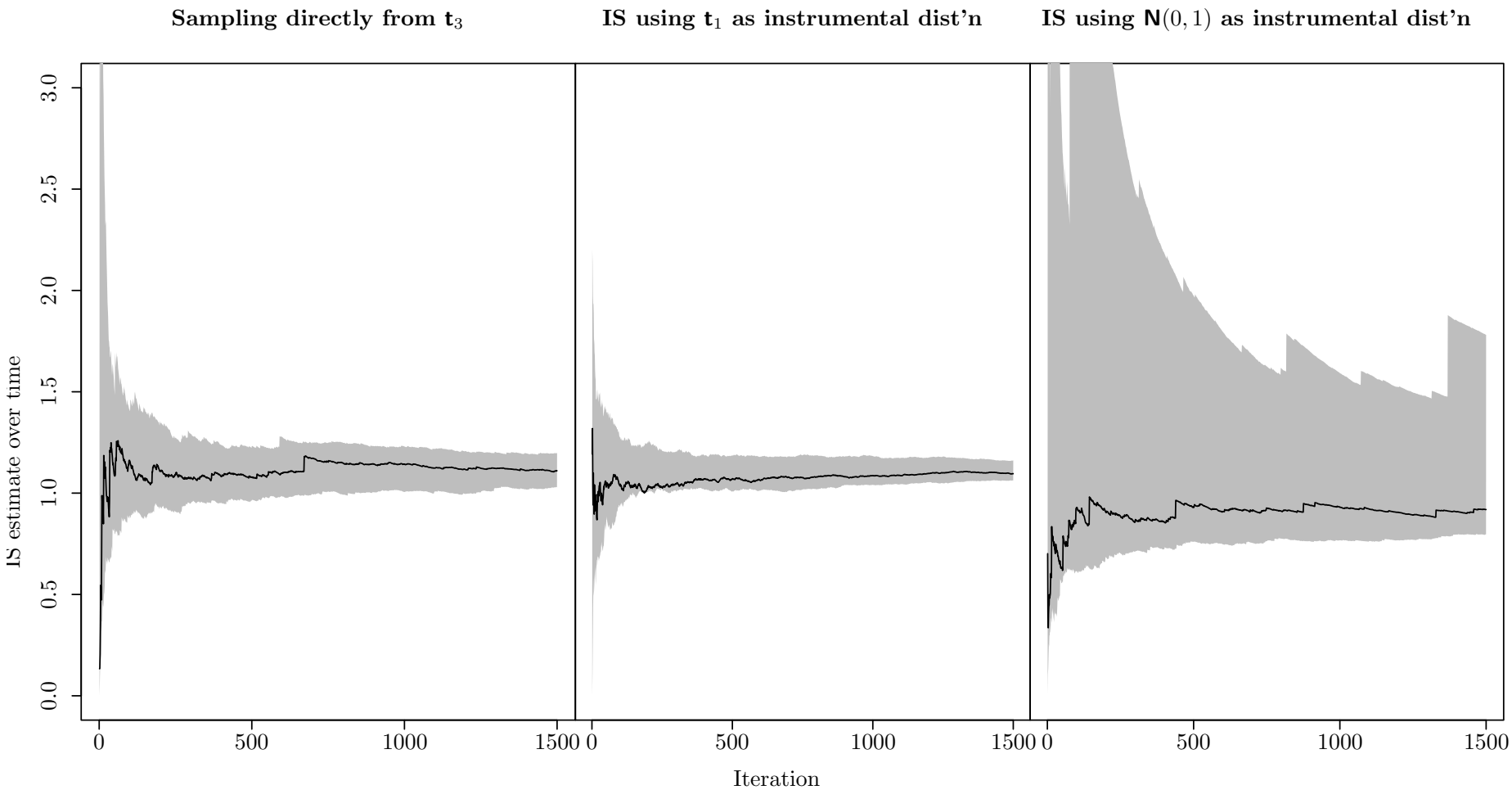
(b) using a t_1 distribution as instrumental distribution.

(c) using a $\mathrm{N}(0, 1)$ distribution as instrumental distribution.

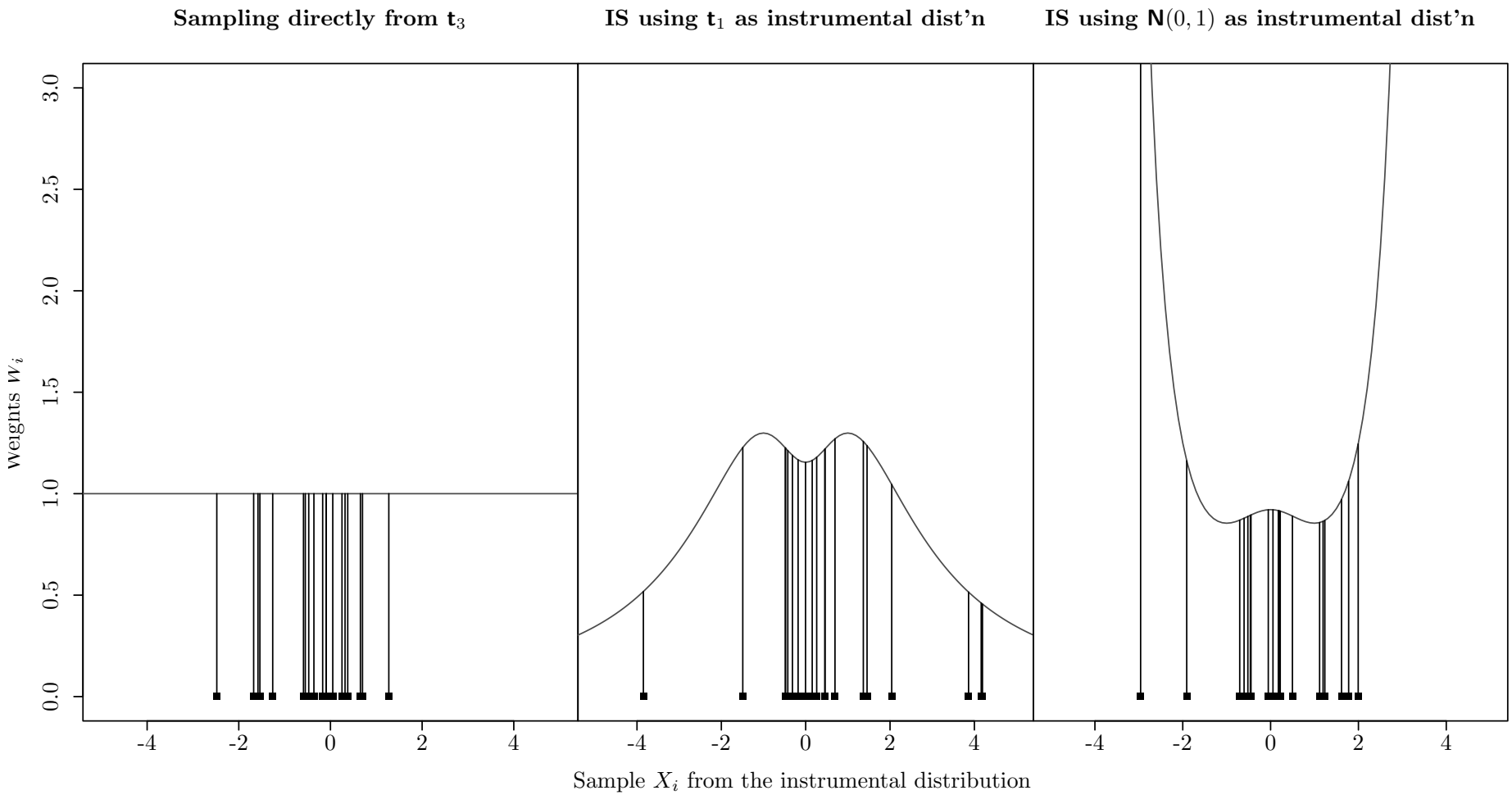
IS Example: Densities



IS Example: Estimates obtained



IS Example: Weights



Another Example: Rare Events (1)

Consider

$$f(x,y) = \mathsf{N}\left(\begin{pmatrix} x \\ y \end{pmatrix}; \mu, \Sigma\right)$$

where

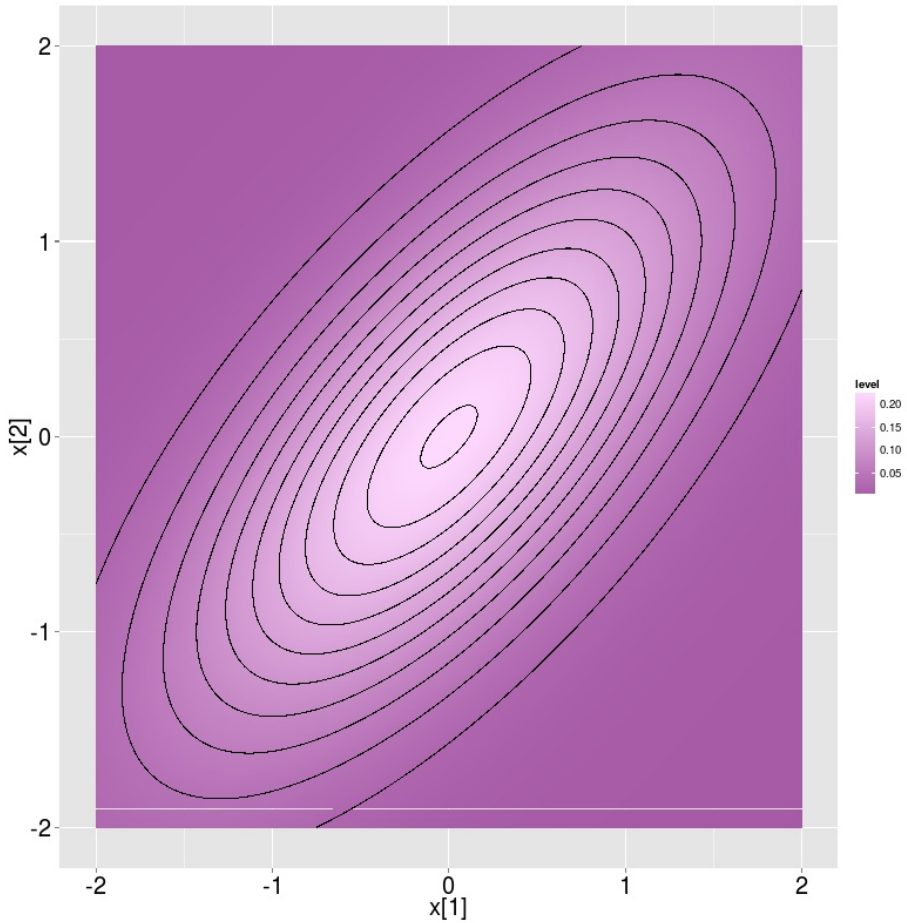
$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

and

$$\Sigma = \begin{bmatrix} 1 & 0.7 \\ 0.7 & 1 \end{bmatrix}$$

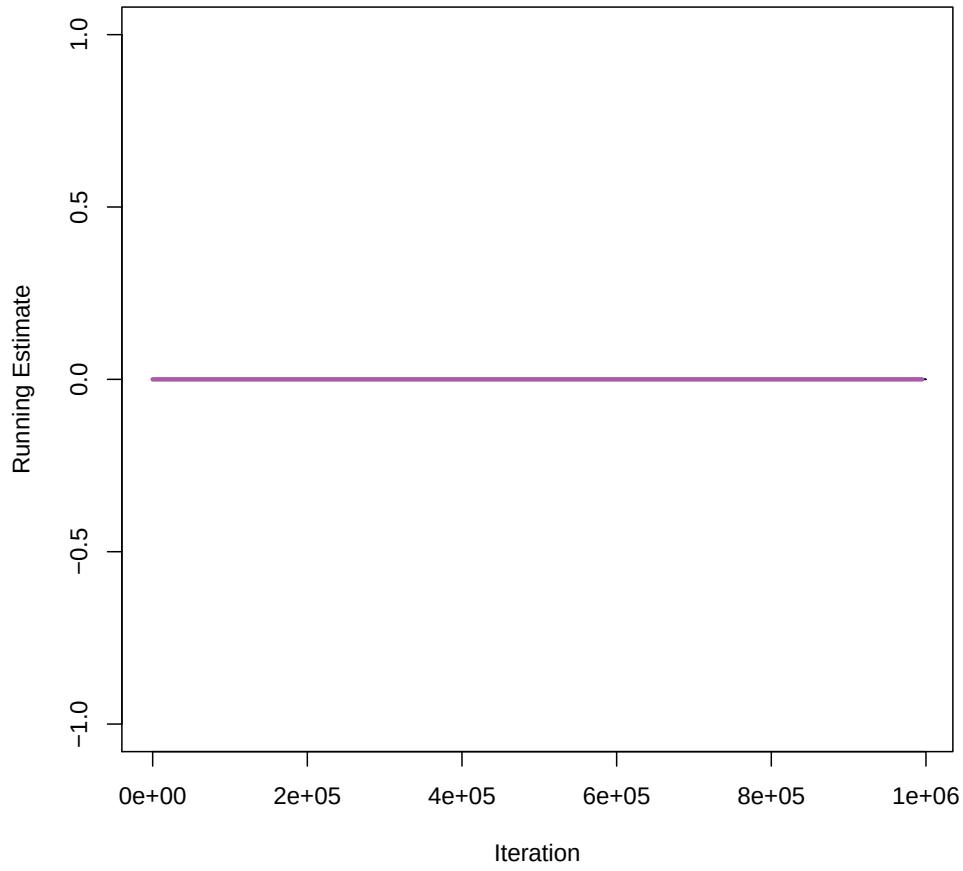
For

$$\varphi(x,y) = \mathbb{I}_{[4,\infty)}(x)\mathbb{I}_{[4,\infty)}(y)$$



Another Example: Rare Events (2)

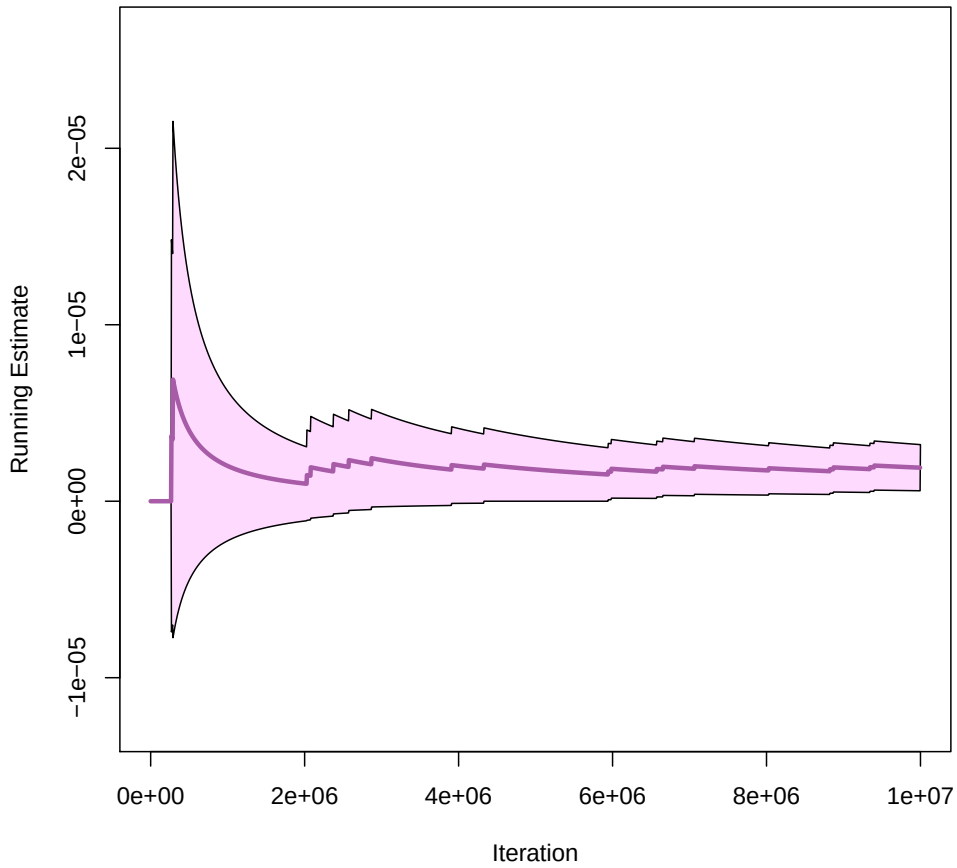
Using simple Monte Carlo with 1,000,000 samples from f:



shaded region shows *estimated* 99.7% confidence interval.

Another Example: Rare Events (3)

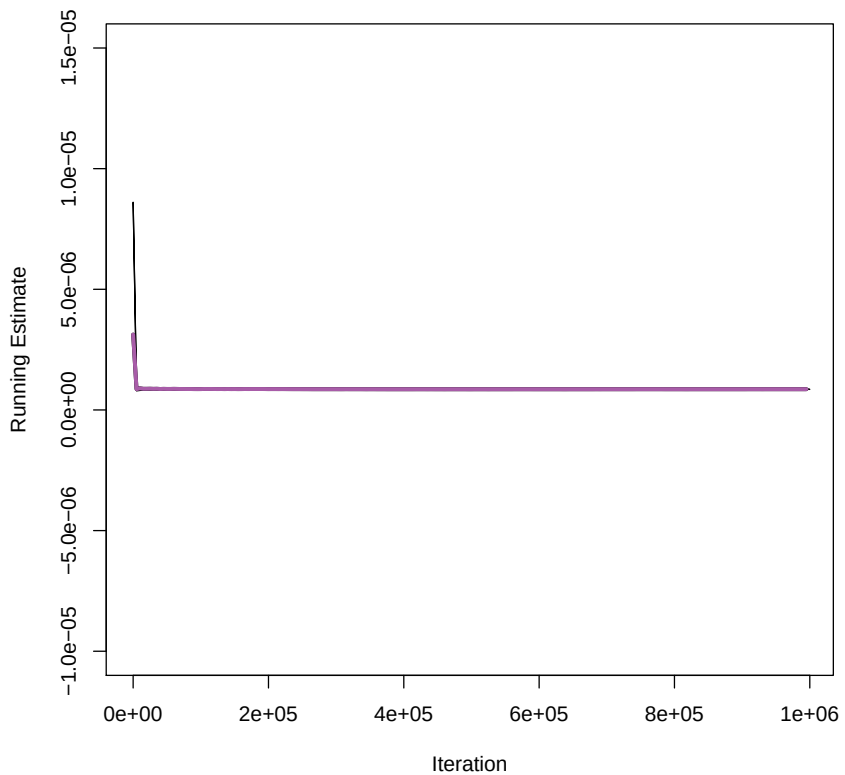
Using simple Monte Carlo with 10,000,000 samples from f:



shaded region shows *estimated* 99.7% confidence interval.

Another Example: Rare Events (4)

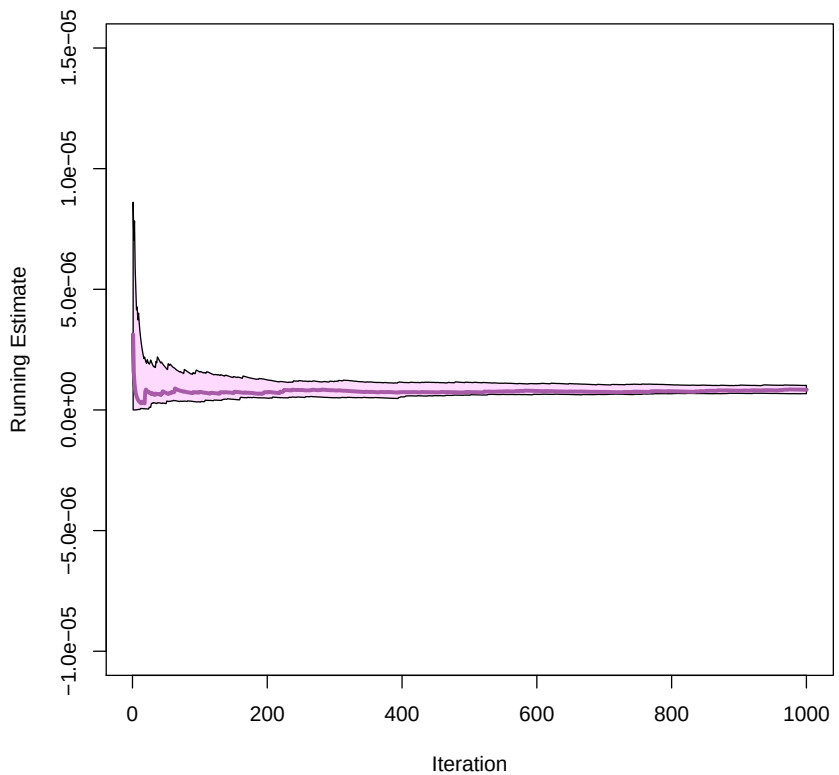
Using importance sampling with 1,000,000 samples from $g(x, y) = \exp(-(x-4)-(y-4))\mathbb{I}_{x\geq 4}\mathbb{I}_{y\geq 4}$:



shaded region shows range of 100 replications.

Another Example: Rare Events (5)

Using importance sampling with 1,000 samples from $g(x, y) = \exp(-(x-4)-(y-4))\mathbb{I}_{x\geq 4}\mathbb{I}_{y\geq 4}$:

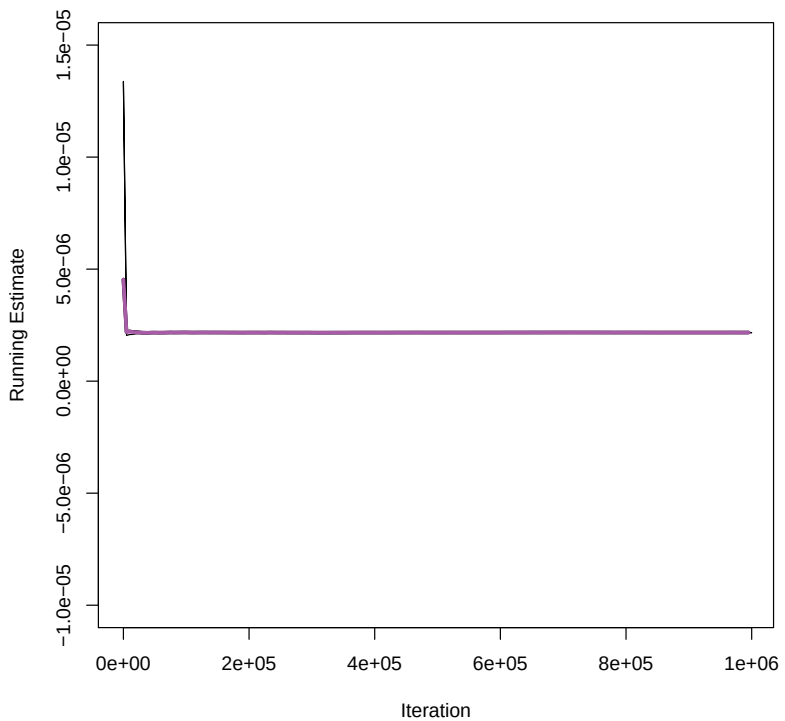


shaded region shows range of 100 replications.

Another Example: Rare Events (6)

Using importance sampling with 1,000,000 samples from

$$g(x,y) = 4\mathsf{N}\left(\begin{pmatrix} x \\ y \end{pmatrix}; \begin{pmatrix} 4 \\ 4 \end{pmatrix}, \Sigma\right) \mathbb{I}_{x\geq 4}\mathbb{I}_{y\geq 4}:$$

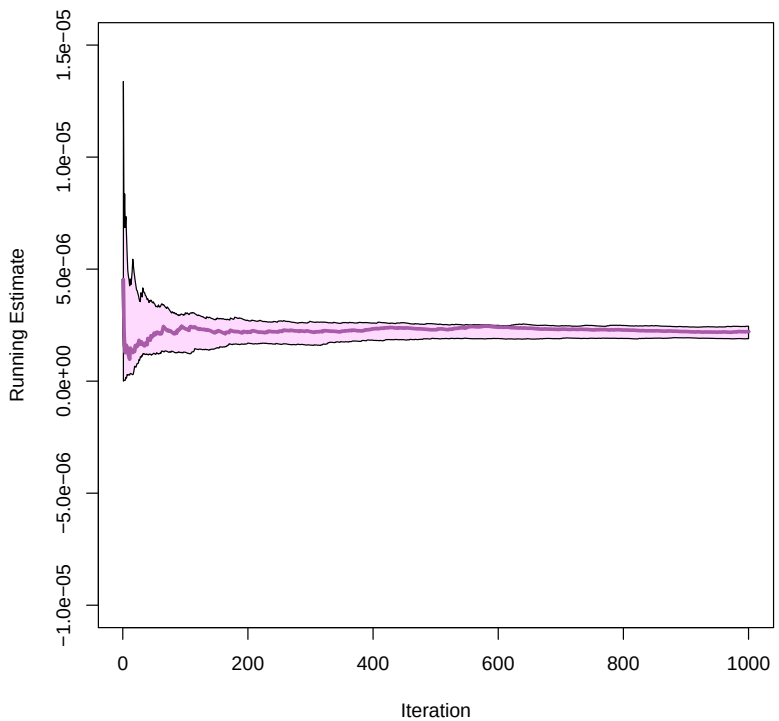


shaded region shows range of 100 replications.

Another Example: Rare Events (7)

Using importance sampling with 1,000 samples from

$$g(x,y) = 4\mathsf{N}\left(\begin{pmatrix} x \\ y \end{pmatrix}; \begin{pmatrix} 4 \\ 4 \end{pmatrix}, \Sigma\right) \mathbb{I}_{x\geq 4}\mathbb{I}_{y\geq 4}:$$



shaded region shows range of 100 replications.

We only need f up to a multiplicative constant.

- Assume $f(x) = C\tilde{f}(x)$. Then

$$\tilde{\mu} = \frac{1}{n}\sum_{i=1}^{n} w(X_i)\varphi(X_i) = \frac{1}{n}\sum_{i=1}^{n} \frac{C\tilde{f}(X_i)}{g(X_i)}\varphi(X_i)$$

  $\rightsquigarrow$ C does not cancel out $\rightsquigarrow$ knowing $\tilde{f}(\cdot)$ is not enough.
- Idea: Estimate C using the sample, via $\sum_{i=1}^{n} w(X_i)$, i.e. consider the *self-normalised estimator*

$$\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} w(X_i)\varphi(X_i) \Big/ \frac{1}{n}\sum_{i=1}^{n} w(X_i)1$$

- Now we have that

$$\hat{\mu} = \frac{\sum_{i=1}^{n} w(X_i)\varphi(X_i)}{\sum_{i=1}^{n} w(X_i)} = \frac{\sum_{i=1}^{n} \frac{\pi(X_i)}{g(X_i)}\varphi(X_i)}{\sum_{i=1}^{n} \frac{\pi(X_i)}{g(X_i)} w(X_i)},$$

  $\rightsquigarrow$ $\hat{\mu}$ does not depend on C

The importance sampling algorithm (2)

Algorithm: Importance Sampling using self-normalised weights

Choose g such that $\mathrm{supp}(g) \supset \mathrm{supp}(f)$.

1. For $i = 1, \ldots, n$:
   1. Generate $X_i \sim g$.
   2. Set $w(X_i) = \frac{f(X_i)}{g(X_i)}$.
2. Return

$$\hat{\mu} = \frac{\sum_{i=1}^{n} w(X_i)\varphi(X_i)}{\sum_{i=1}^{n} w(X_i)}$$

as an estimate of $\mathbb{E}_f(\varphi(X))$.

Basic properties of the self-normalised estimate

- $\hat{\mu}$ is consistent as

$$\hat{\mu} = \underbrace{\frac{\sum_{i=1}^{n} w(X_i)\varphi(X_i)}{n}}_{=\tilde{\mu}\longrightarrow\mathbb{E}_f(\varphi(X))} \underbrace{\frac{n}{\sum_{i=1}^{n} w(X_i)}}_{\longrightarrow 1} \overset{\substack{a.s.\\ n\to\infty}}{\longrightarrow} \mathbb{E}_f(\varphi(X)),$$

(provided $\mathrm{supp}(g) \supset \mathrm{supp}(f)$ and $\mathbb{E}_g|w(X)\cdot\varphi(X)| < +\infty$)

Theorem: Bias and Variance (ctd.)

$$\begin{aligned}
\mathbb{E}_g(\hat{\mu}) &= \mu + \frac{\mu\mathrm{Var}_g(w(X)) - \mathbb{C}ov_g\left[w(X), w(X)\cdot\varphi(X)\right]}{n} + O(n^{-2}) \\
\mathrm{Var}_g(\hat{\mu}) &= \frac{\mathrm{Var}_g(w(X)\cdot\varphi(X)) - 2\mu\mathbb{C}ov_g\left[w(X), w(X)\cdot\varphi(X)\right]}{n} \\
&\quad + \frac{\mu^2\mathrm{Var}_g(w(X))}{n} + O(n^{-2})
\end{aligned}$$

Finite variance estimators

- Importance sampling estimate consistent for large choice of g.
- More important in practice: *finite variance estimators*, i.e.

$$\mathrm{Var}(\tilde{\mu}) = \mathrm{Var}\left(\frac{\sum_{i=1}^{n} w(X_i)\varphi(X_i)}{n}\right) < +\infty$$

- Sufficient (albeit restrictive) conditions for finite variance of $\tilde{\mu}$:
  - $f(x) < M \cdot g(x)$ and $\mathrm{Var}_f(\varphi(X)) < \infty$, or
  - E is compact, f is bounded above on E, and g is bounded below on E.
- Note: If f has heavier tails then g, then the weights may have *infinite* variance!

Summary of Part 2

- Pseudorandom Number Generators (and alternatives)
- Transformation: Inversion Methods, Box-Muller
- Rejection Sampling
- Importance Sampling

Part 3

Markov chain Monte Carlo

Part 3— Section 7

Motivation and Basics

Why do we need other, more complicated methods?

- Transformation's great when it works.
- Rejection sampling's good when M is small.
- Importance sampling works well with good proposals.
- What do we do when we can't meet any of these requirements?

One Approach

Markov Chain Monte Carlo methods (MCMC)

- Key idea: Create a *dependent* sample, i.e. $X^{(t)}$ depends on the previous value $X^{(t-1)}$.
  $\rightsquigarrow$ allows for "local" updates.
- Yields an "approximate sample" from the target distribution*.
- More mathematically speaking: yields a Markov chain with the target distribution f as stationary distribution.
- Under conditions, the realised chain provides approximations of $\mathbb{E}_f[\varphi(X)]$ and of f itself.

* I don't think this is the right way to think, but it's pervasive terminology and so I mention it here.

Markov Chains

Markov Chain (NB Terminology varies)

A *discrete time* Markov process taking values in a *general space*:

$$X^{(0)} \sim \mu_0 \qquad \text{Initial Dist.}$$

$$X^{(t)} | X^{(0)} = x^{(0)}, \ldots, X^{(t-1)} = x^{(t-1)} \sim K(x^{(t-1)}, \cdot) \qquad \text{Kernel}$$

Stationary Distribution

f is a *stationary* or *invariant* distribution for a Markov Chain on E with kernel K if

$$\int_A \int_E f(x) K(x, y) dx dy = \int_A f(y) dy$$

for all measurable sets A [or $\int f(x) K(x, y) dx = f(y)$].

Heuristically Motivating MCMC

- If $X^{(0)}, \ldots$ is an f-invariant Markov chain and $X^{(t)} \sim f$ for some t then $X^{(t+s)} \sim f \quad \forall s \in \mathbb{N}$.
- So if $X^{(t)}$ is "approximately independent" of $X^{(t+s)}$ for large enough s then
  - $X^{(t)}, X^{(t+s)}, \ldots, X^{(t+ks)}, \ldots$ is approximately $\overset{\text{iid}}{\sim} f$,
  - $X^{(t+1)}, X^{(t+s+1)}, \ldots, X^{(t+ks+1)}, \ldots$ is approximately $\overset{\text{iid}}{\sim} f$,
  - $\vdots$
  - $X^{(t+s-1)}, X^{(t+2s-1)}, \ldots, X^{(t+ks-1)}, \ldots$ is approximately $\overset{\text{iid}}{\sim} f$.
- We might conjecture that for such a chain, for some large s:

$$\frac{1}{n}\sum_{k=1}^{n}\varphi(X^{(t+ks)}) \to \mathbb{E}_f\left[\varphi(X)\right] \text{ and } \frac{1}{n}\sum_{k=1}^{n}\varphi(X^{(k)}) \to \mathbb{E}_f\left[\varphi(X)\right]$$

Some Questions to Answer

- Can we formalise this heuristic argument?
  $\rightsquigarrow$ ergodic theory
- How can we construct f-invariant Markov kernels?
  $\rightsquigarrow$ various types of sampler
- What properties of these kernels are important?
  $\rightsquigarrow$ more ergodic theory
- How do we initialise the chain?
  $\rightsquigarrow$ transient phases and burning
- How do we know if it's working?
  $\rightsquigarrow$ ergodic theory and convergence diagnostics

Aperiodicity

Definition: Period

A Markov chain has a period d if there exists some partition of the state space, $E_1, \ldots, E_d$ with the properties that:

- $\forall i \neq j : E_i \cap E_j = \emptyset$
- $\bigcup_{i=1}^{d} E_i = E$
- The chain moves deterministically between elements of the partition:

$$\forall i, j, t, s : \mathbb{P}\left(X_{t+s} \in E_j | X_t \in E_i\right) = \begin{cases} 1 & j = i + s \bmod d \\ 0 & \text{otherwise.} \end{cases}$$

A Markov chain is *aperiodic* if its period is 1.

Irreducibility

Definition: Irreducibility

Given a distribution, f, over E, a Markov chain is said to be *f-irreducible* if for all points $x \in E$ and all measurable sets A such that $f(A) > 0$ there exists some t such that:

$$\int_A K^t(x, y)dy > 0.$$

If this condition holds with $t = 1$, then the chain is said to be *strongly f-irreducible*.

$$K^t(x, y) := \int K(x, z)K^{t-1}(z, y)dz \quad K^1(x, y) = K(x, y)$$

Transience and Recurrence I

Consider sets $A \subset E$ for f-irreducible Markov chains.
Let $\eta_A := \sum_{k=1}^{\infty} \mathbb{I}_A(X^{(k)})$.

Transience and Recurrence of Sets

A set A is recurrent if:

$$\forall x \in A : \mathbb{E}_x [\eta_A] = \infty.$$

A set is *uniformly transient* if there exists some $M < \infty$ such that:

$$\forall x \in A : \quad \mathbb{E}_x [\eta_A] \leq M.$$

A set, $A \subset E$, is *transient* if it may be expressed as a countable union of uniformly transient sets.

Transience and Recurrence II

Transience Recurrence of Markov Chains

A Markov chain is *recurrent* if the following hold:

- The chain is f-irreducible for some distribution f.
- For every measurable set $A \subset E$ such that $\int_A f(y)dy > 0$, $\mathbb{E}_x[\eta_A] = \infty$ for every $x \in A$.

It is *transient* if it is f-irreducible for some distribution f and the entire space is transient.

In the case of irreducible chains, transience and recurrence are properties of the chain rather than individual states.

A Motivating Convergence Result

Theorem (A Simple Ergodic Theorem)

If $(X_i)_{i\in\mathbb{N}}$ is an f-irreducible, f-invariant, recurrent $\mathbb{R}^d$-valued Markov chain then the following strong law of large numbers holds for any integrable function $\varphi : \mathbb{R}^d \to \mathbb{R}$:

$$\lim_{t\to\infty} \frac{1}{t} \sum_{i=1}^{t} \varphi(\xi_i) \overset{a.s.}{=} \int \varphi(x) f(x) dx.$$

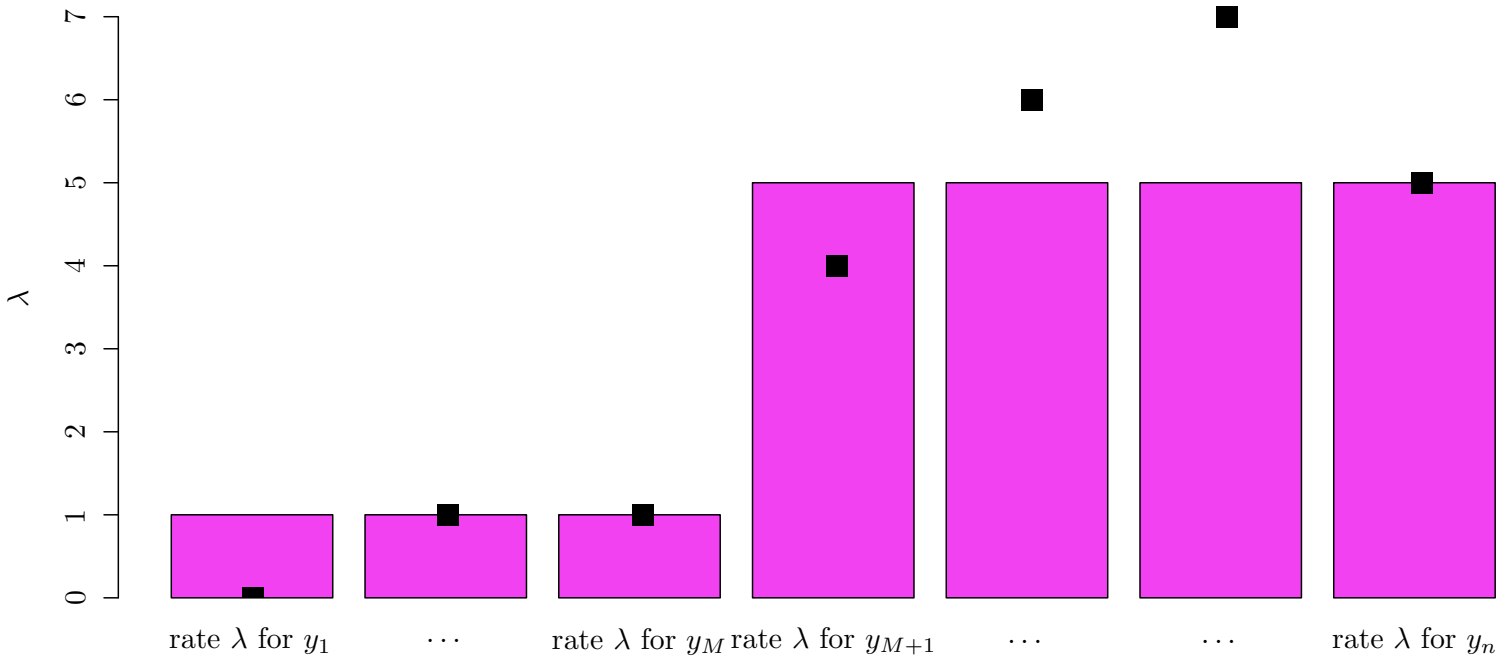
for almost every starting value x.

Note: this gives no *rate* of convergence.

Part 3— Section 8

The Gibbs Sampler

Example: Poisson change point model I



$$Y_i \sim \text{Poi}(\lambda_1) \quad \text{for} \quad i = 1, \ldots, M$$
$$Y_i \sim \text{Poi}(\lambda_2) \quad \text{for} \quad i = M+1, \ldots, n$$

Objective: (Bayesian) inference about the parameters λ_1, λ_2, and M given observed data $Y_1, \ldots, Y_n$.

Example: Poisson change point model II

- Prior distributions: $\lambda_j \sim \text{Gamma}(\alpha_j, \beta_j)$ $(j = 1, 2)$, i.e.

$$f(\lambda_j) = \frac{1}{\Gamma(\alpha_j)} \lambda_j^{\alpha_j - 1} \beta_j^{\alpha_j} \exp(-\beta_j \lambda_j).$$

  (discrete uniform prior on M, i.e. $p(M) \propto 1$).

- Likelihood: $l(y_1, \ldots, y_n | \lambda_1, \lambda_2, M)$

$$= \left(\prod_{i=1}^{M} \frac{\exp(-\lambda_1) \lambda_1^{y_i}}{y_i!} \right) \cdot \left(\prod_{i=M+1}^{n} \frac{\exp(-\lambda_2) \lambda_2^{y_i}}{y_i!} \right)$$

Example: Poisson change point model III

- Joint distribution $f(y_1, \ldots, y_n, \lambda_1, \lambda_2, M)$

$$
\begin{aligned}
&= l(y_1, \ldots, y_n | \lambda_1, \lambda_2, M) \cdot f(\lambda_1) \cdot f(\lambda_2) \cdot p(M) \\
&\propto \left(\prod_{i=1}^{M} \frac{\exp(-\lambda_1)\lambda_1^{y_i}}{y_i!} \right) \cdot \left(\prod_{i=M+1}^{n} \frac{\exp(-\lambda_2)\lambda_2^{y_i}}{y_i!} \right) \\
&\quad \cdot \frac{1}{\Gamma(\alpha_1)} \lambda_1^{\alpha_1 - 1} \beta_1^{\alpha_1} \exp(-\beta_1 \lambda_1) \cdot \frac{1}{\Gamma(\alpha_2)} \lambda_2^{\alpha_2 - 1} \beta_2^{\alpha_2} \exp(-\beta_2 \lambda_2)
\end{aligned}
$$

- Joint posterior distribution $f(\lambda_1, \lambda_2, M | y_1, \ldots, y_n)$

$$
\begin{aligned}
&\propto \lambda_1^{\alpha_1 - 1 + \sum_{i=1}^{M} y_i} \exp(-(\beta_1 + M)\lambda_1) \\
&\qquad \cdot \lambda_2^{\alpha_2 - 1 + \sum_{i=M+1}^{n} y_i} \exp(-(\beta_2 + n - M)\lambda_2)
\end{aligned}
$$

Example: Poisson change point model IV

- Conditional on M (i.e. if M was known) we have

$$f(\lambda_1|y_1,\ldots,y_n,M) \propto \lambda_1^{\alpha_1-1+\sum_{i=1}^{M} y_i} \exp(-(\beta_1+M)\lambda_1),$$

i.e.

$$\begin{aligned}
\lambda_1|Y_1,\ldots Y_n,M &\sim \text{Gamma}\left(\alpha_1+\sum_{i=1}^{M} y_i, \beta_1+M\right)\\
\lambda_2|Y_1,\ldots Y_n,M &\sim \text{Gamma}\left(\alpha_2+\sum_{i=M+1}^{n} y_i, \beta_2+n-M\right).
\end{aligned}$$

- $p(M|\ldots) \propto \lambda_1^{\sum_{i=1}^{M} y_i} \cdot \lambda_2^{\sum_{i=M+1}^{n} y_i} \cdot \exp((\lambda_2-\lambda_1)\cdot M)$

Example: Poisson change point model V

This suggests an iterative algorithm:

1. Draw λ_1 from $\lambda_1|Y_1, \ldots, Y_n, M$, i.e. draw

$$\lambda_1 \sim \text{Gamma}\left(\alpha_1 + \sum_{i=1}^{M} y_i, \beta_1 + M\right)$$

2. Draw λ_2 from $\lambda_2|Y_1, \ldots, Y_n, M$, i.e. draw

$$\lambda_2 \sim \text{Gamma}\left(\alpha_2 + \sum_{i=M+1}^{n} y_i, \beta_2 + n - M\right)$$

3. Draw M from $M|Y_1, \ldots, Y_n, \lambda_1, \lambda_2$, i.e. draw

$$p(M) \propto \lambda_1^{\sum_{i=1}^{M} y_i} \cdot \lambda_2^{\sum_{i=M+1}^{n} y_i} \cdot \exp((\lambda_2 - \lambda_1) \cdot M)$$

The systematic scan Gibbs sampler

Algorithm: (Systematic scan) Gibbs sampler

Starting with $(X_1^{(0)}, \ldots, X_p^{(0)})$ iterate for $t = 1, 2, \ldots$

1. Draw $X_1^{(t)} \sim f_{X_1|X_{-1}}(\cdot|X_2^{(t-1)}, \ldots, X_p^{(t-1)})$.

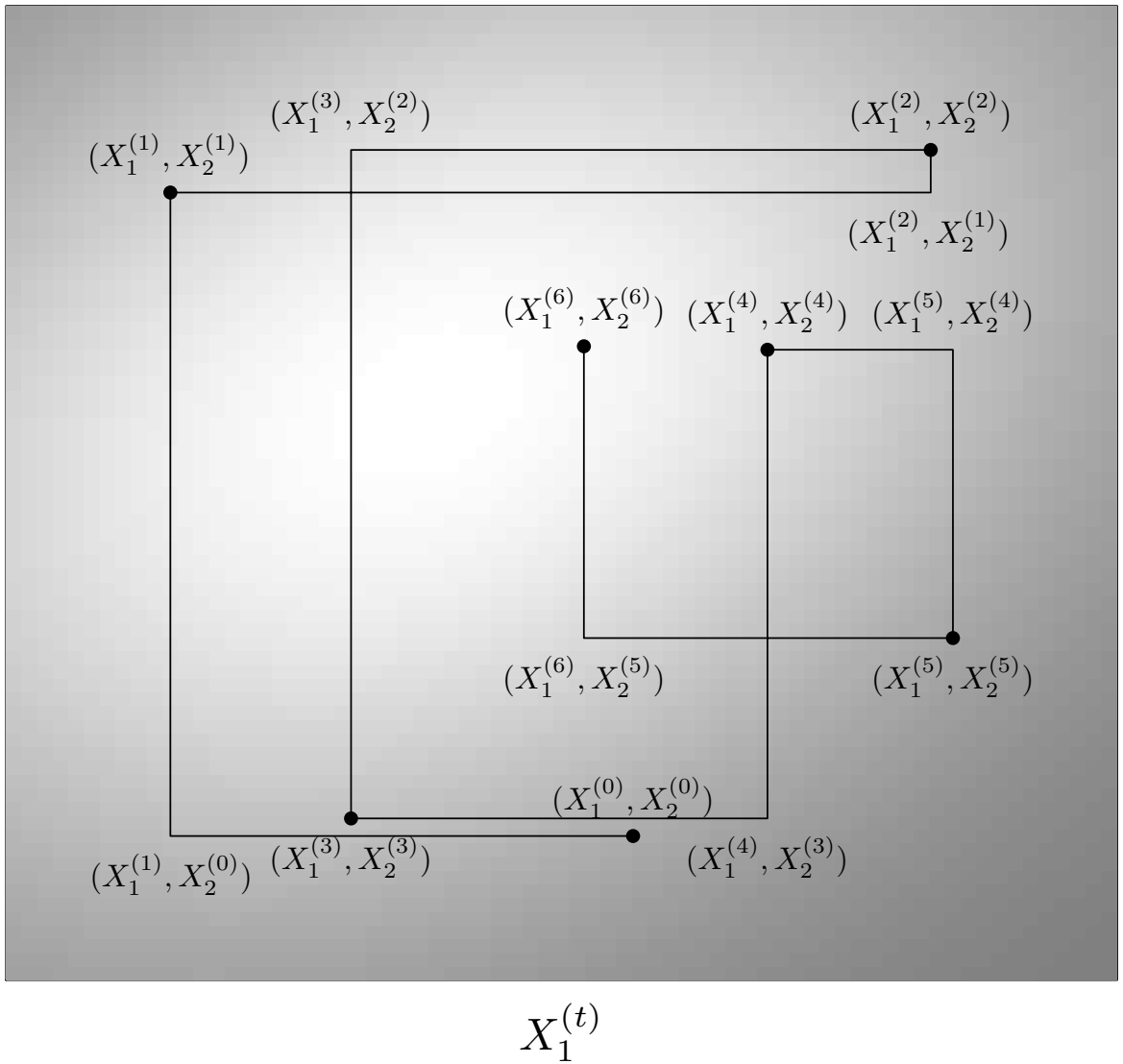
...

j. Draw $X_j^{(t)} \sim f_{X_j|X_{-j}}(\cdot|X_1^{(t)}, \ldots, X_{j-1}^{(t)}, X_{j+1}^{(t-1)}, \ldots, X_p^{(t-1)})$.

...

p. Draw $X_p^{(t)} \sim f_{X_p|X_{-p}}(\cdot|X_1^{(t)}, \ldots, X_{p-1}^{(t)})$.

Illustration of the systematic scan Gibbs sampler



The random scan Gibbs sampler

Algorithm: (Random scan) Gibbs sampler

Starting with $(X_1^{(0)}, \ldots, X_p^{(0)})$ iterate for $t = 1, 2, \ldots$

1. Draw an index j from a distribution on $\{1, \ldots, p\}$ (e.g. uniform)
2. Draw $X_j^{(t)} \sim f_{X_j|X_{-j}}(\cdot|X_1^{(t-1)}, \ldots, X_{j-1}^{(t-1)}, X_{j+1}^{(t-1)}, \ldots, X_p^{(t-1)})$, and set $X_\iota^{(t)} := X_\iota^{(t-1)}$ for all $\iota \neq j$.

Invariant distribution

Lemma (Kernel)

The transition kernel of the systematic scan Gibbs sampler is

$$\begin{aligned} K(\mathbf{x}^{(t-1)}, \mathbf{x}^{(t)}) &= f_{X_1|X_{-1}}(x_1^{(t)}|x_2^{(t-1)}, \ldots, x_p^{(t-1)}) \\ &\quad \cdot f_{X_2|X_{-2}}(x_2^{(t)}|x_1^{(t)}, x_3^{(t-1)}, \ldots, x_p^{(t-1)}) \\ &\quad \cdot \ldots \\ &\quad \cdot f_{X_p|X_{-p}}(x_p^{(t)}|x_1^{(t)}, \ldots, x_{p-1}^{(t)}) \end{aligned}$$

Proposition (Invariance)

The joint distribution $f(x_1, \ldots, x_p)$ is indeed the invariant distribution of the Markov chain $(\mathbf{X}^{(0)}, \mathbf{X}^{(1)}, \ldots)$ generated by the Gibbs sampler.

Proof (outline) I

Assume that $\mathbf{X}^{(t-1)} \sim f$, then

$$\mathbb{P}(\mathbf{X}^{(t)} \in \mathcal{X}) = \int_{\mathcal{X}} \int f(\mathbf{x}^{(t-1)}) K(\mathbf{x}^{(t-1)}, \mathbf{x}^{(t)}) \, d\mathbf{x}^{(t-1)} \, d\mathbf{x}^{(t)}$$

We can expand the $K(\mathbf{x}^{(t-1)}, \mathbf{x}^{(t)})$ of the integrand, and compute the $x_1^{(t-1)}$-integral:

$$\underbrace{\underbrace{\int f(x_1^{(t-1)}, \ldots, x_p^{(t-1)}) \, dx_1^{(t-1)}}_{= f(x_2^{(t-1)}, \ldots, x_p^{(t-1)})} f_{X_1|X_{-1}}(x_1^{(t)} | x_2^{(t-1)}, \ldots, x_p^{(t-1)}) \cdot}_{= f(x_1^{(t)}, x_2^{(t-1)}, \ldots, x_p^{(t-1)})}$$
$$f_{X_2|X_{-2}}(x_2^{(t)} | x_1^{(t)}, \ldots, x_p^{(t-1)}) \cdots f_{X_p|X_{-p}}(x_p^{(t)} | x_1^{(t)}, \ldots, x_{p-1}^{(t)})$$

Proof (outline) II

And we can then compute the $x_2^{(t-1)}$ integral:

$$\underbrace{\int \underbrace{\int f(x_1^{(t)}, x_2^{(t-1)}, \ldots, x_p^{(t-1)})\, dx_2^{(t-1)}}_{=f(x_1^{(t)}, x_3^{(t-1)}, \ldots, x_p^{(t-1)})} f_{X_2|X_{-2}}(x_2^{(t)}|x_1^{(t)}, x_3^{(t-1)}, \ldots, x_p^{(t-1)})}_{=f(x_1^{(t)}, x_2^{(t)}, x_3^{(t-1)}, \ldots, x_p^{(t-1)})}$$
$$f_{X_3|X_{-3}}(x_3^{(t)}|x_1^{(t)}, \ldots, x_p^{(t-1)}) \cdots f_{X_p|X_{-p}}(x_p^{(t)}|x_1^{(t)}, \ldots, x_{p-1}^{(t)})$$

And so on until the $x_p^{(t-1)}$-integral:

$$\underbrace{\underbrace{\int f(x_1^{(t)}, \ldots, x_{p-1}^{(t)}, x_p^{(t-1)})\, dx_p^{(t-1)}}_{=f(x_1^{(t)}, \ldots, x_{p-1}^{(t)})} f_{X_p|X_{-p}}(x_p^{(t)}|x_1^{(t)}, \ldots, x_{p-1}^{(t)})}_{=f(x_1^{(t)}, \ldots, x_p^{(t)})}$$

Proof (outline) III

This just leaves the $\mathbf{x}^{(t)}$-integrals:

$$\mathbb{P}(\mathbf{X}^{(t)} \in \mathcal{X}) = \int_{\mathcal{X}} f(x_1^{(t)}, \ldots, x_p^{(t)}) \, d\mathbf{x}^{(t)}$$

Thus f is the density of $\mathbf{X}^{(t)}$ (if $\mathbf{X}^{(t-1)} \sim f$).

Recall our Poisson Changepoint Model

- Joint posterior distribution $f(\lambda_1, \lambda_2, M|y_1, \ldots, y_n)$

$$\begin{aligned} \propto \quad & \lambda_1^{\alpha_1 - 1 + \sum_{i=1}^{M} y_i} \exp(-(\beta_1 + M)\lambda_1) \\ & \cdot \lambda_2^{\alpha_2 - 1 + \sum_{i=M+1}^{n} y_i} \exp(-(\beta_2 + n - M)\lambda_2) \end{aligned}$$

- Full Posterior Distributions

$$\lambda_1|Y_1, \ldots Y_n, M \quad \sim \quad \text{Gamma}\left(\alpha_1 + \sum_{i=1}^{M} y_i, \beta_1 + M\right)$$

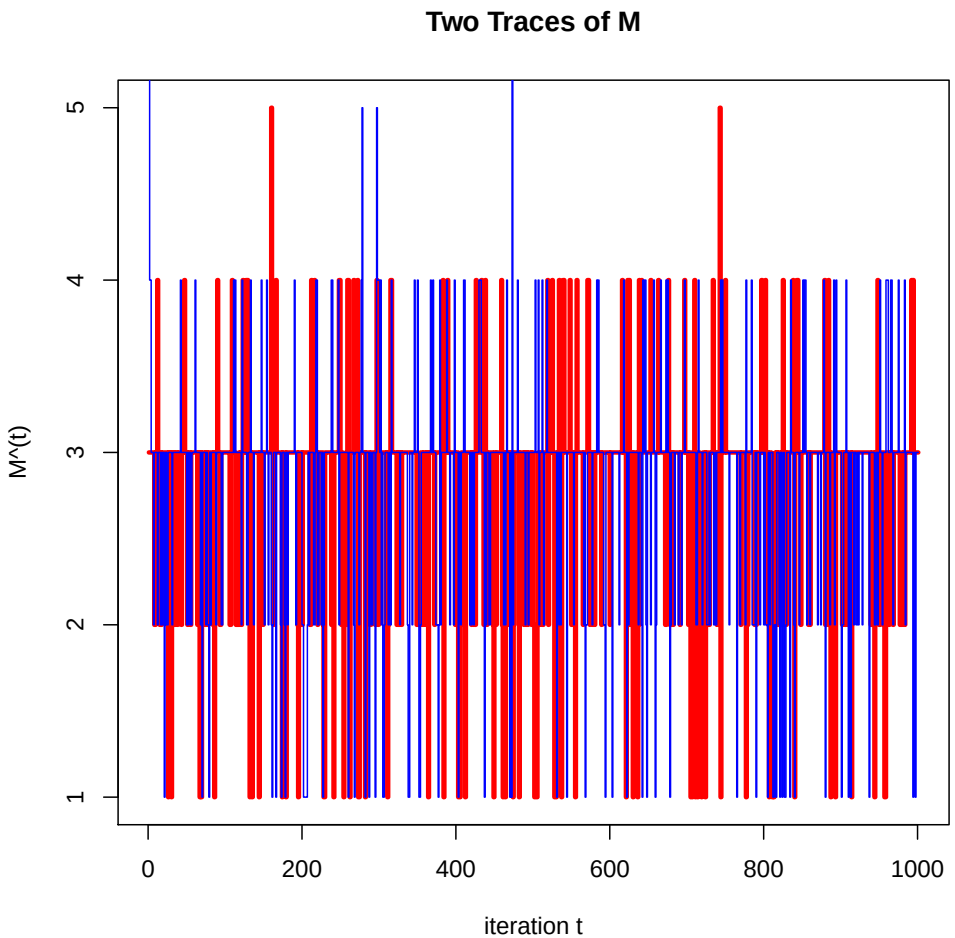
$$\lambda_2|Y_1, \ldots Y_n, M \quad \sim \quad \text{Gamma}\left(\alpha_2 + \sum_{i=M+1}^{n} y_i, \beta_2 + n - M\right).$$

- and $p(M|\ldots) \propto \lambda_1^{\sum_{i=1}^{M} y_i} \cdot \lambda_2^{\sum_{i=M+1}^{n} y_i} \cdot \exp((\lambda_2 - \lambda_1) \cdot M)$

An R Implementation

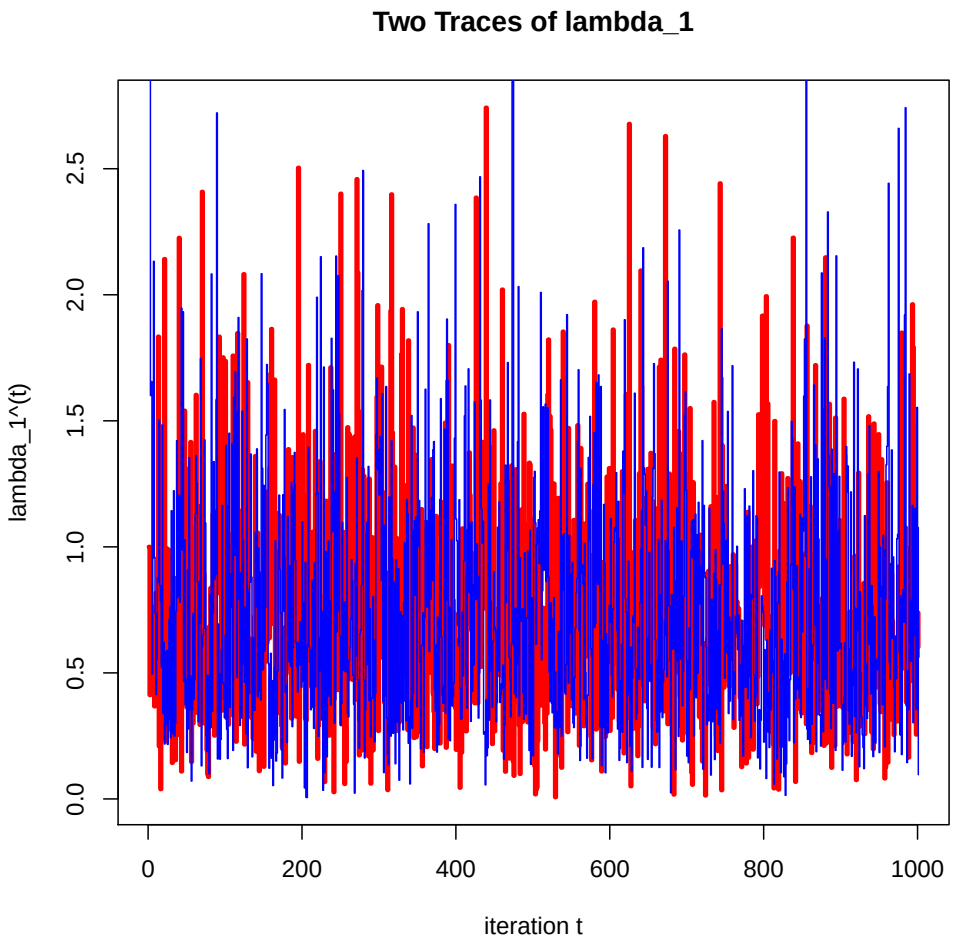
```
cdist.M <- function(lambda1,lambda2) {
    dist.M.log <- cumsum(y[1:n-1]) * log(lambda1) +
        (sum(y)-cumsum(y[1:n-1]))*log(lambda2) +
        (lambda2-lambda1) * (1:(n-1))
    dist.M <- exp(dist.M.log - mean(dist.M.log))
    dist.M <- dist.M / sum(dist.M)
}

pmix.gibbs <- function(M,lambda1,lambda2,t) {
 r <- array(NA,c(t+1,3))
 r[1,] <- c(M,lambda1,lambda2)
 for (i in 1:t) {
  #lambda1
  r[i+1,2] <- rgamma(1,a1+sum(y[1:r[i,1]]), b1+r[i,1])
  #lambda2
  r[i+1,3] <- rgamma(1,a2+sum(y[(r[i,1]+1):n]), b2+n-r[i,1])
  #M
  r[i+1,1] <- sample.int(n-1,1,prob=cdist.M(r[i+1,2],r[i+1,3]))
 }
 r
}
```

Traces and Estimates: M



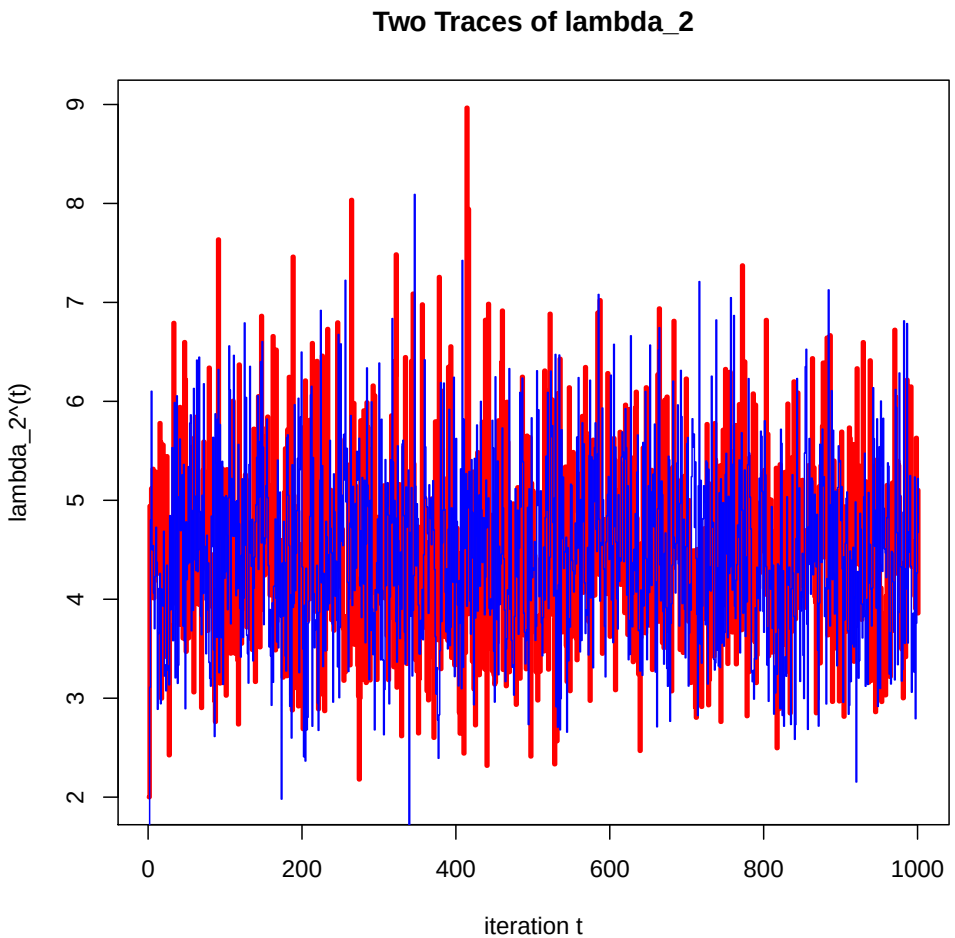
Consider two differently-initialised chains.
Chain 1:
$(M, \lambda_1, \lambda_2)^{(0)} = (3, 1, 2)$
Chain 2:
$(M, \lambda_1, \lambda_2)^{(0)} = (6, 4, \frac{1}{2})$
Estimated Posterior *Modes*:
Chain 1: 3
Chain 2: 3

Traces and Estimates: λ_1



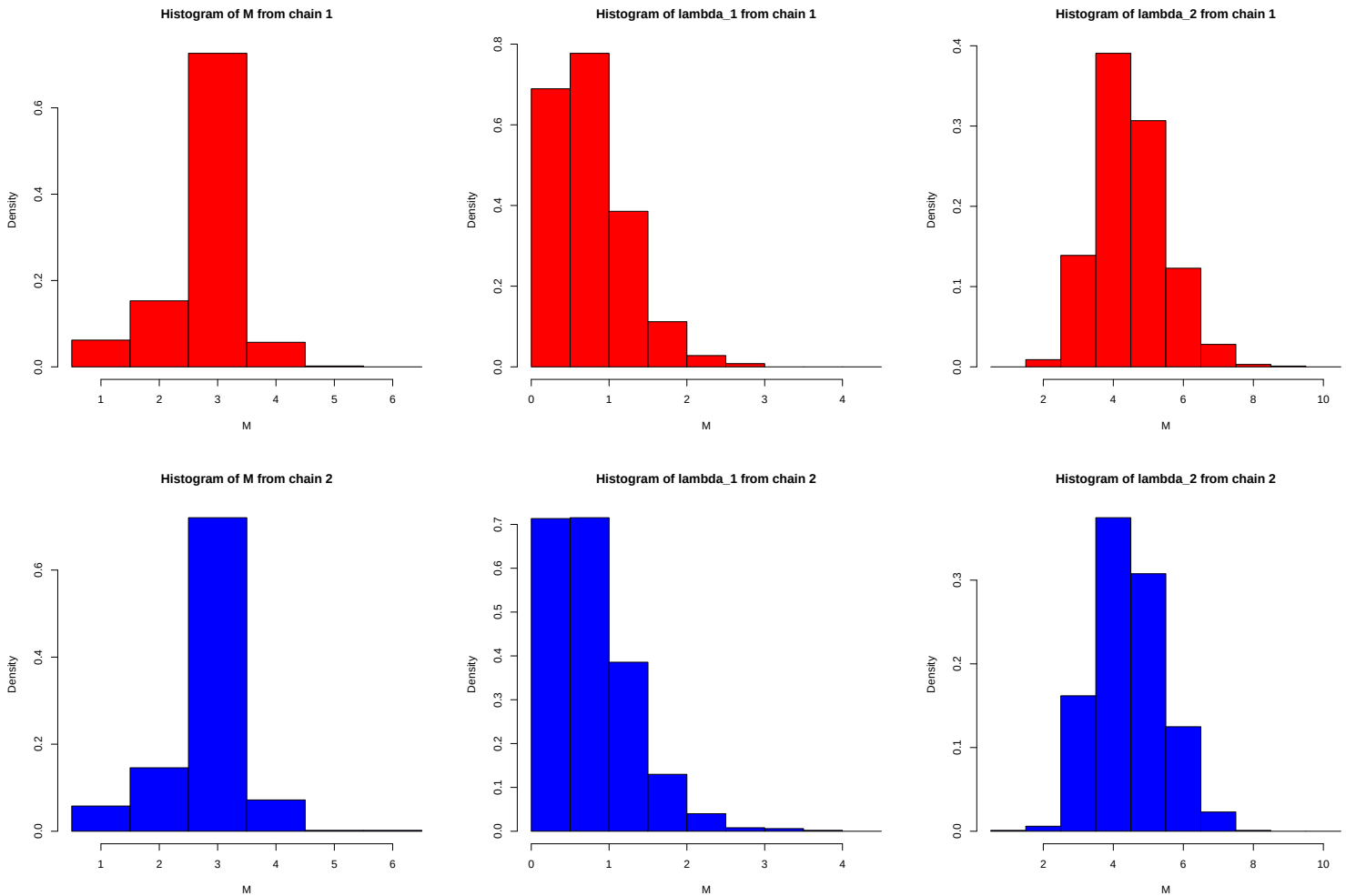
Estimated Posterior *Means*:
Chain 1: 0.76
Chain 2: 0.78

Traces and Estimates: λ_2



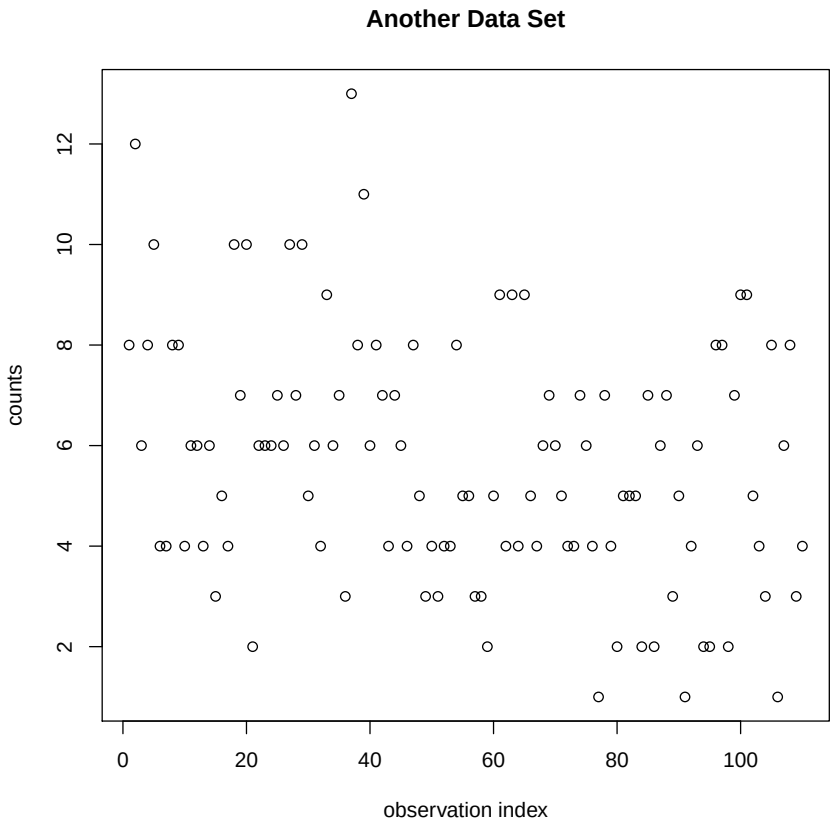
Estimated Posterior *Means*:
Chain 1: 4.51
Chain 2: 4.47

Histograms: Approximations of the Posterior



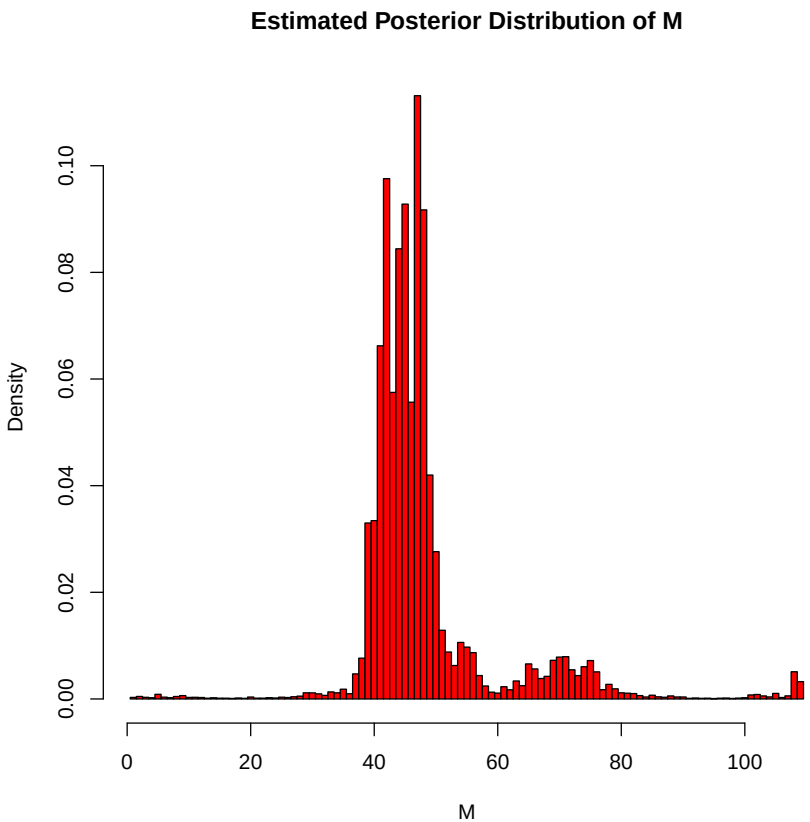
Poisson Change-Point Model: More Challenging Data I

Consider the more realistic data:



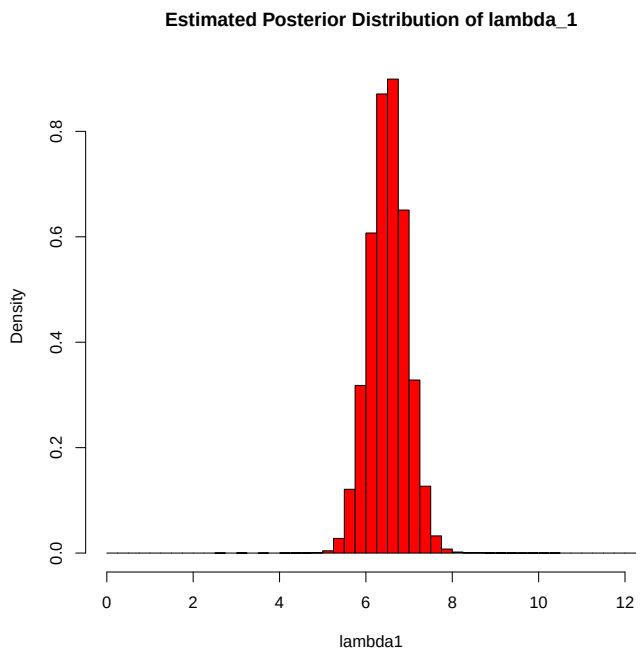
Poisson Change-Point Model: More Challenging Data II

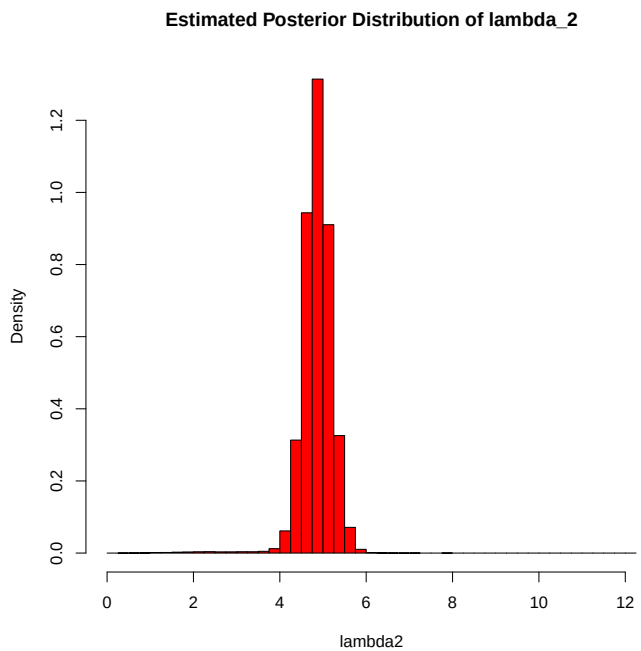
From a chain of length 100,000 we obtain the following histograms:



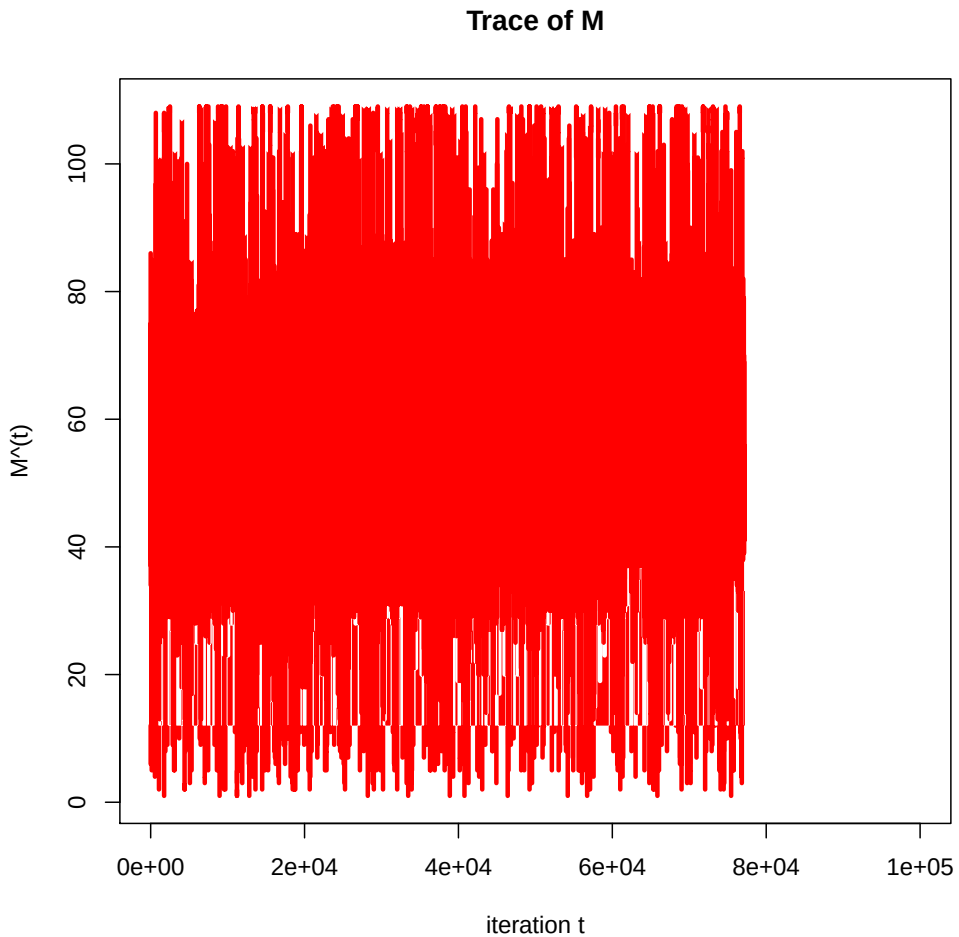
Data was generated with: `y <- c(rpois(40,7),rpois(70,5))`

Poisson Change-Point Model: More Challenging Data III

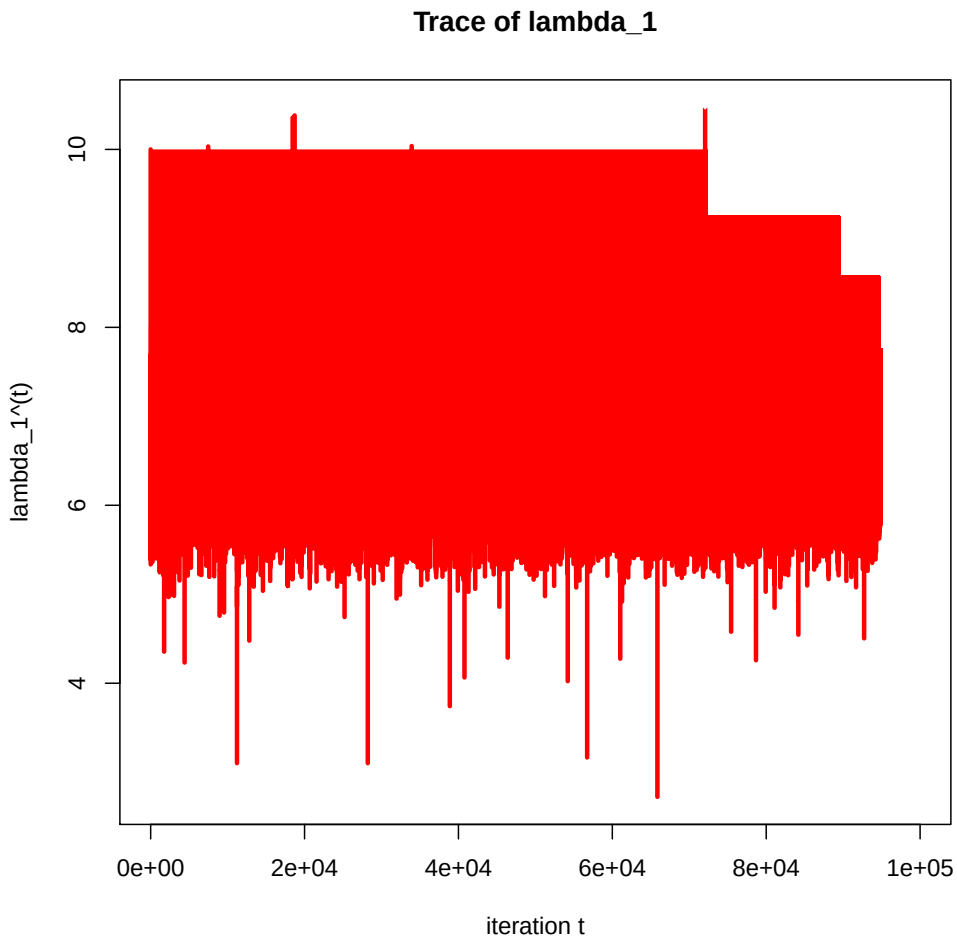




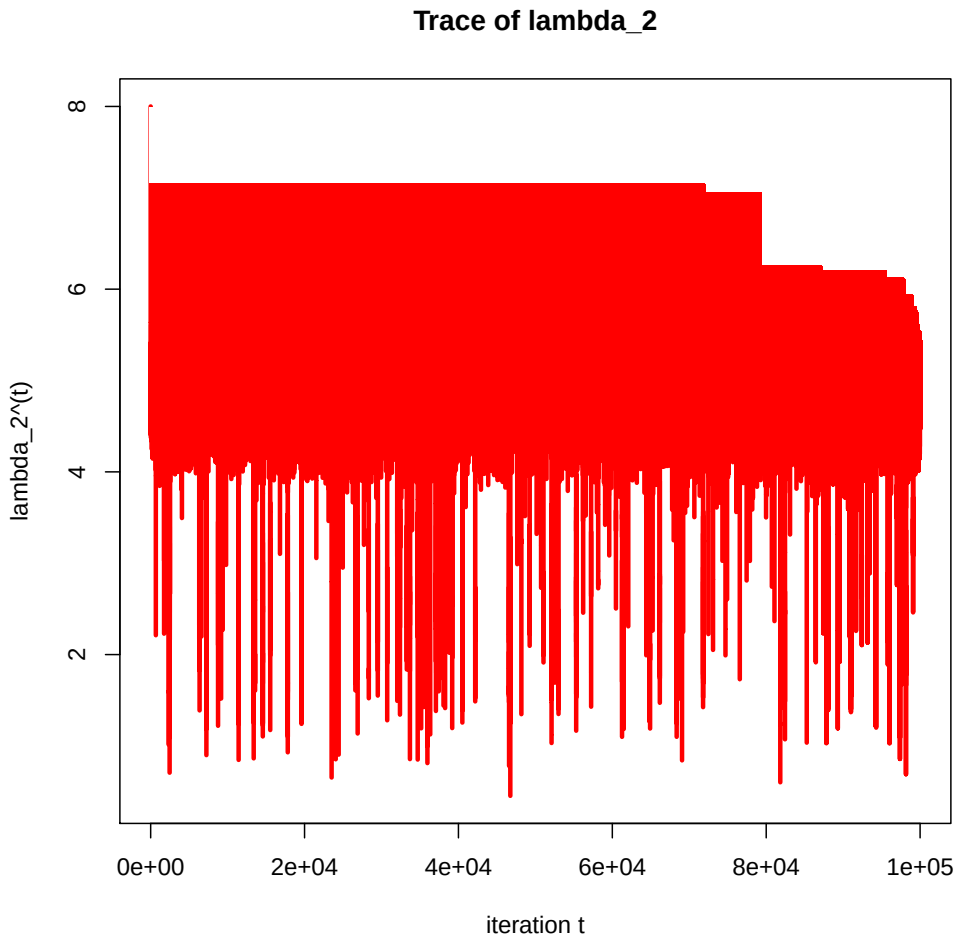
Poisson Change-Point Model: More Challenging Data IV



Poisson Change-Point Model: More Challenging Data V

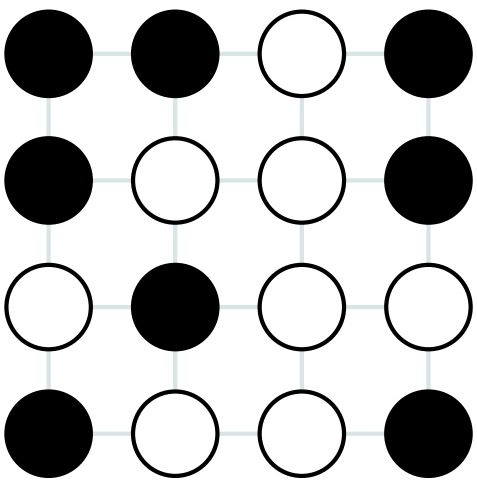


Poisson Change-Point Model: More Challenging Data VI



The Ising Model

The Ising model on $(\mathcal{V}, \mathcal{E})$ each $v_i \in \mathcal{V}$ has an associated x_i:



$$\begin{aligned}
&\pi(x_1, \ldots, x_m) \\
=&\frac{1}{Z} \exp\left(J \sum_{(i,j)\in\mathcal{E}} x_i, x_j \right) \\
=&\frac{1}{Z} \exp(-J|\mathcal{E}|) \exp\left(2J \sum_{(i,j)\in\mathcal{E}} \mathbb{I}(x_i = x_j) \right) \\
=&\frac{1}{Z'} \exp\left(2J \sum_{(i,j)\in\mathcal{E}} \mathbb{I}(x_i = x_j) \right)
\end{aligned}$$

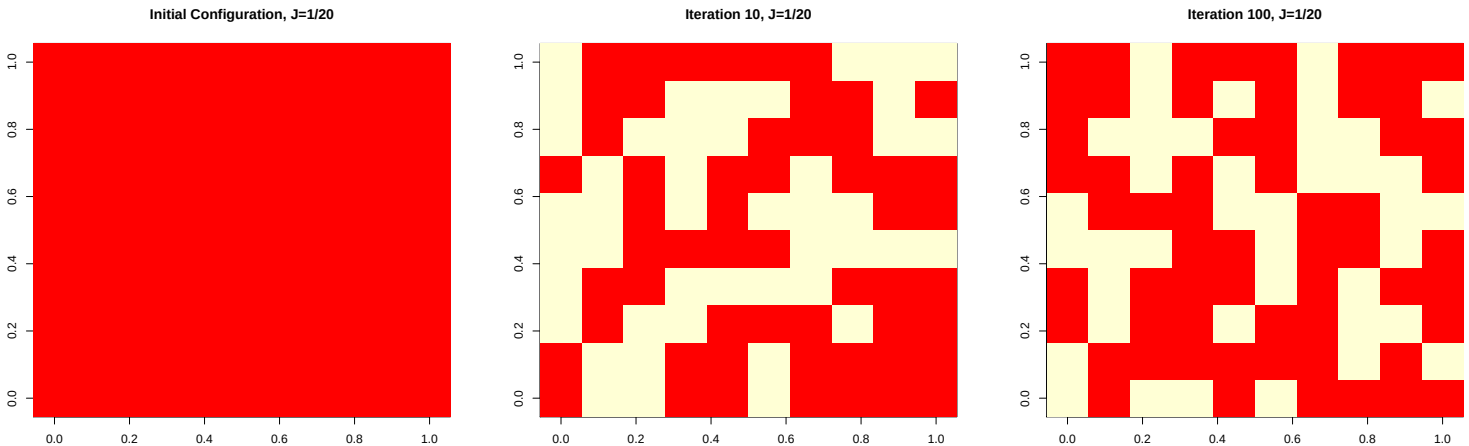
$$\pi(x_j | x_{-j}) = \exp\left(J \sum_{i\sim j} x_i x_j \right) \Big/ \left[\exp\left(-J \sum_{i\sim j} x_i \right) + \exp\left(J \sum_{i\sim j} x_i \right) \right]$$

The Core Logic in R

```
tr <- list()
tr[[1]] <- x <- array(0,c(m,n))

for (t in 1:100) {
    for(i in 1:m) {
        for(j in 1:n) {
            ns <- neighbours(m,n,i,j)
            p1 <- 0
            for(k in 1:length(ns)) {
                p1 <- p1 + x[(ns[[k]])[1],(ns[[k]])[2]]
            }
            p0 <- length(ns) - p1
            pp <- c(exp(J*p0),exp(J*p1))
            pp <- pp / sum(pp)
            x[i,j] <- sample(c(0,1),1,prob=pp)
        }
    }
    tr[[t+1]] <- x
}
```

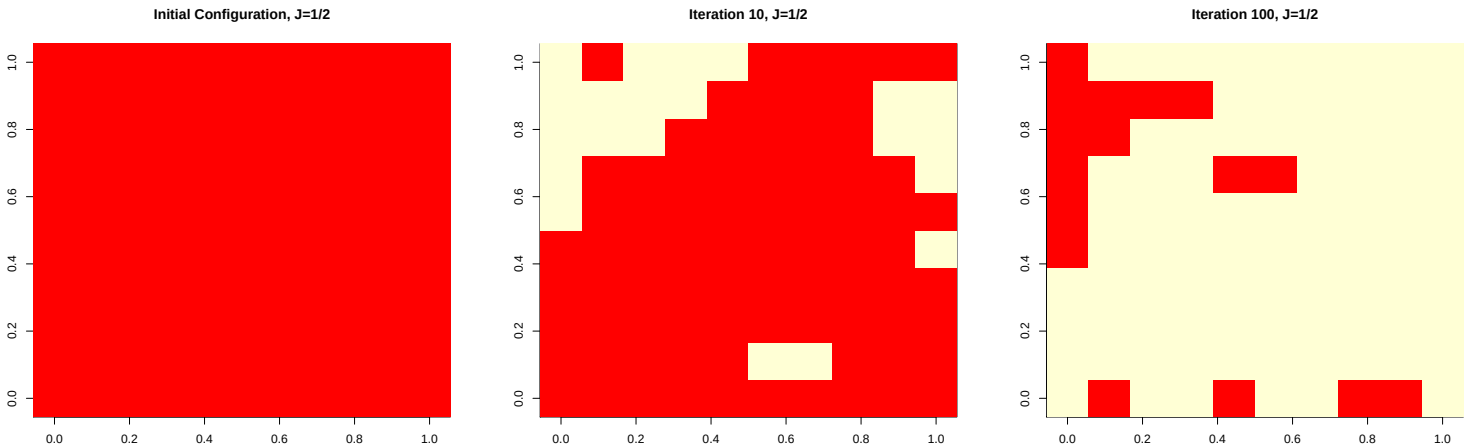
The Gibbs Sampler for Ising Models I

Samples 1, 10 and 100 with $J = 0.05$:



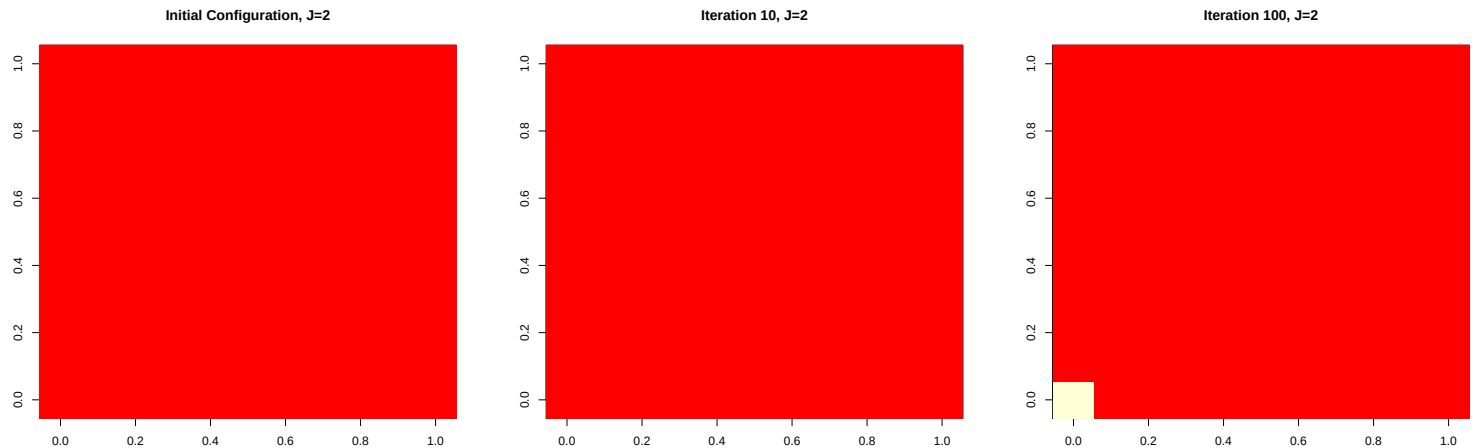
The Gibbs Sampler for Ising Models II

Samples 1, 10 and 100 with $J = 0.50$:



The Gibbs Sampler for Ising Models III

Samples 1, 10 and 100 with $J = 1.00$:



Solutions include the *Swendsen-Wang* algorithm (cf. assessment) or *perfect simulation*...

The Ising Model and Image Reconstruction

The Ising Model is widely used in statistics as a prior distribution.

- Consider image denoising: x an $m \times n$ image on $\mathcal{V} \subset \mathbb{Z}^2$ with obvious neighbourhood structure $\mathcal{E}$:
- Observe y where $y_v = x_v$ wp 1-ϵ.
- Prior: $X \sim \text{Ising}(J, \mathcal{V}, \mathcal{E})$.
- Likelihood: $l(y; x) = \prod_{v \in \mathcal{V}} [(1-\epsilon)\mathbb{I}\{y_v = x_v\} + \epsilon \mathbb{I}\{y_v \neq x_v\}]$
- Posterior:

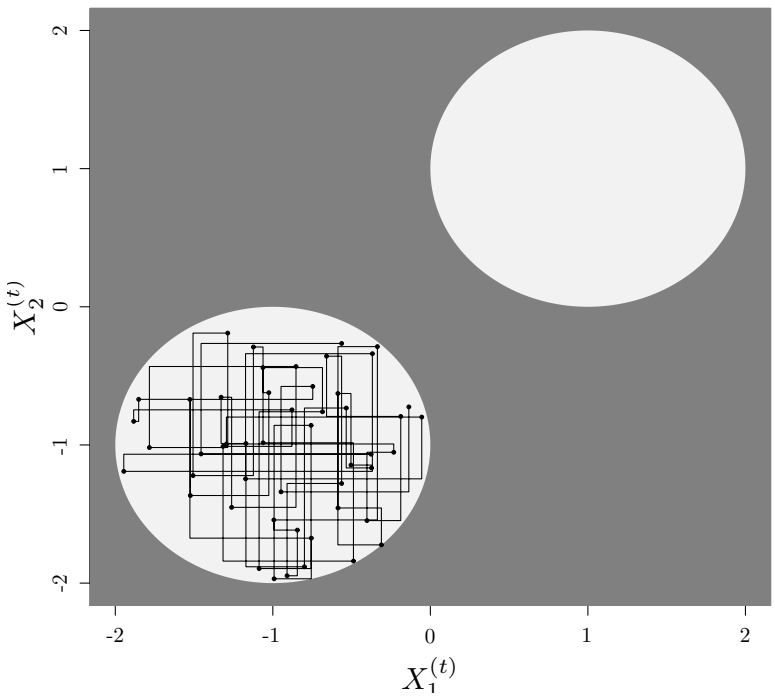
$$p(x|y) \propto \exp\left(2J \sum_{(i,j)\in\mathcal{E}} \mathbb{I}(x_i = x_j)\right) \cdot \prod_{v \in \mathcal{V}} [(1-\epsilon)\mathbb{I}\{y_v = x_v\} + \epsilon \mathbb{I}\{y_v \neq x_v\}]$$

A Pathological Example: The Reducible Gibbs sampler

Consider Gibbs sampling from the uniform distribution

$$f(x_1, x_2) = \frac{1}{2\pi} \mathbb{I}_{C_1 \cup C_2}(x_1, x_2),$$

$$\begin{aligned} C_1 &:= \{(x_1, x_2) : \|(x_1, x_2) - (1, 1)\| \leq 1\} \\ C_2 &:= \{(x_1, x_2) : \|(x_1, x_2) + (1, 1)\| \leq 1\} \end{aligned}$$



The resulting Markov chain is *reducible*:

It stays forever in either C_1 or C_2.

Part 3— Section 9

The Metropolis-Hastings Algorithm

The Metropolis-Hastings algorithm

Algorithm: Metropolis-Hastings

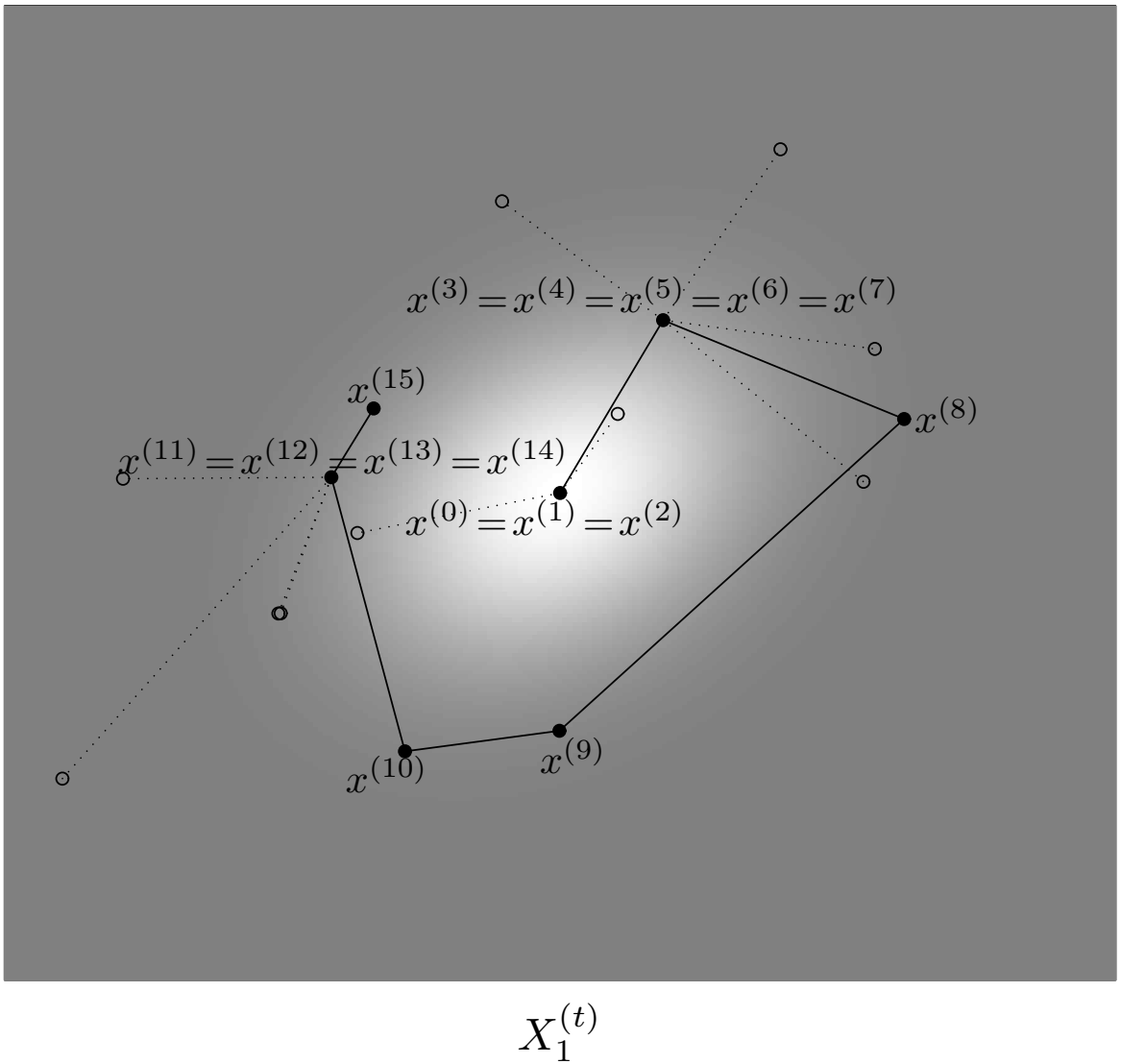
Starting with $\mathbf{X}^{(0)} := (X_1^{(0)}, \ldots, X_p^{(0)})$ iterate for $t = 1, 2, \ldots$

1. Draw $\mathbf{X} \sim q(\cdot|\mathbf{X}^{(t-1)})$.
2. Compute

$$\alpha(\mathbf{X}|\mathbf{X}^{(t-1)}) = \min\left\{1, \frac{f(\mathbf{X}) \cdot q(\mathbf{X}^{(t-1)}|\mathbf{X})}{f(\mathbf{X}^{(t-1)}) \cdot q(\mathbf{X}|\mathbf{X}^{(t-1)})}\right\}.$$

3. With probability $\alpha(\mathbf{X}|\mathbf{X}^{(t-1)})$ set $\mathbf{X}^{(t)} = \mathbf{X}$, otherwise set $\mathbf{X}^{(t)} = \mathbf{X}^{(t-1)}$.

Illustration of the Metropolis-Hastings method



Basic properties of the Metropolis-Hastings algorithm

- The probability that a newly proposed value is accepted given $\mathbf{X}^{(t-1)} = \mathbf{x}^{(t-1)}$ is

$$a(\mathbf{x}^{(t-1)}) = \int \alpha(\mathbf{x}|\mathbf{x}^{(t-1)}) q(\mathbf{x}|\mathbf{x}^{(t-1)}) \, d\mathbf{x}.$$

- The probability of remaining in state $\mathbf{X}^{(t-1)}$ is

$$\mathbb{P}(\mathbf{X}^{(t)} = \mathbf{X}^{(t-1)} | \mathbf{X}^{(t-1)} = \mathbf{x}^{(t-1)}) = 1 - a(\mathbf{x}^{(t-1)}).$$

- The probability of acceptance does not depend on the normalisation constant:
  If $f(\mathbf{x}) = C \cdot \tilde{f}(\mathbf{x})$, then

$$\alpha(\mathbf{X}|\mathbf{X}^{(t-1)}) = \min\left(1, \frac{\tilde{f}(\mathbf{X}) \cdot q(\mathbf{X}^{(t-1)}|\mathbf{X})}{\tilde{f}(\mathbf{X}^{(t-1)}) \cdot q(\mathbf{X}|\mathbf{X}^{(t-1)})}\right)$$

Transition Kernel

Lemma (Transition Kernel of Metropolis-Hastings)

The transition kernel of the Metropolis-Hastings algorithm is

$$\begin{aligned} K(\mathbf{x}^{(t-1)}, \mathbf{x}^{(t)}) &= \alpha(\mathbf{x}^{(t)}|\mathbf{x}^{(t-1)})q(\mathbf{x}^{(t)}|\mathbf{x}^{(t-1)}) \\ &\quad +(1 - a(\mathbf{x}^{(t-1)}))\delta_{\mathbf{x}^{(t-1)}}(\mathbf{x}^{(t)}), \end{aligned}$$

Lemma (Detailed Balance and Metropolis Hastings)

The Metropolis-Hastings kernel satisfies the detailed balance condition

$$K(\mathbf{x}^{(t-1)}, \mathbf{x}^{(t)})f(\mathbf{x}^{(t-1)}) = K(\mathbf{x}^{(t)}, \mathbf{x}^{(t-1)})f(\mathbf{x}^{(t)}).$$

f-invariance of Metropolis-Hastings

Proposition (Detailed Balanced implies Invariance)

Any K which satisfies the detailed balance condition with respect to f,

$$K(\mathbf{x}^{(t-1)}, \mathbf{x}^{(t)}) f(\mathbf{x}^{(t-1)}) = K(\mathbf{x}^{(t)}, \mathbf{x}^{(t-1)}) f(\mathbf{x}^{(t)}),$$

is f-invariant.

Proof

Integrate both sides wrt $\mathbf{x}^{(t-1)}$.

Hence the Metropolis-Hastings algorithm is f-invariant.

Random-walk Metropolis: Idea

- In the Metropolis-Hastings algorithm the proposal is from $\mathbf{X} \sim q(\cdot|\mathbf{X}^{(t-1)})$.
- A popular choice for the proposal is $q(\mathbf{x}|\mathbf{x}^{(t-1)}) = g(\mathbf{x} - \mathbf{x}^{(t-1)})$ with g being a *symmetric* distribution, thus

$$\mathbf{X} = \mathbf{X}^{(t-1)} + \varepsilon, \qquad \varepsilon \sim g.$$

- Probability of acceptance becomes

$$\min\left\{1, \frac{f(\mathbf{X}) \cdot g(\mathbf{X} - \mathbf{X}^{(t-1)})}{f(\mathbf{X}^{(t-1)}) \cdot g(\mathbf{X}^{(t-1)} - \mathbf{X})}\right\} = \min\left\{1, \frac{f(\mathbf{X})}{f(\mathbf{X}^{(t-1)})}\right\},$$

- We accept ...
  - every move to a more probable state with probability 1.
  - moves to less probable states with a probability $f(\mathbf{X})/f(\mathbf{x}^{(t-1)}) < 1$.

Random-walk Metropolis: Algorithm

Random-Walk Metropolis

Starting with $\mathbf{X}^{(0)} := (X_1^{(0)}, \ldots, X_p^{(0)})$ and using a symmetric random walk proposal g, iterate for $t = 1, 2, \ldots$

1. Draw $\boldsymbol{\varepsilon} \sim g$ and set $\mathbf{X} = \mathbf{X}^{(t-1)} + \boldsymbol{\varepsilon}$.
2. Compute

$$\alpha(\mathbf{X}|\mathbf{X}^{(t-1)}) = \min\left\{1, \frac{f(\mathbf{X})}{f(\mathbf{X}^{(t-1)})}\right\}.$$

3. With probability $\alpha(\mathbf{X}|\mathbf{X}^{(t-1)})$ set $\mathbf{X}^{(t)} = \mathbf{X}$, otherwise set $\mathbf{X}^{(t)} = \mathbf{X}^{(t-1)}$.

Popular choices for g are (multivariate) Gaussians or t-distributions (the latter having heavier tails)

Example 5.2: Bayesian probit model (1)

- Medical study on infections resulting from birth by Cæsarean section
- 3 influence factors:
  - indicator whether the Cæsarian was planned or not (z_{i1}),
  - indicator of whether additional risk factors were present at the time of birth (z_{i2}), and
  - indicator of whether antibiotics were given as a prophylaxis (z_{i3}).
- Response variable: number of infections Y_i that were observed amongst n_i patients having the same covariates.

# births		planned	risk factors	antibiotics
infection	total			
y_i	n_i	z_{i1}	z_{i2}	z_{i3}
11	98	1	1	1
1	18	0	1	1
0	2	0	0	1
23	26	1	1	0
28	58	0	1	0
0	9	1	0	0
8	40	0	0	0

Example 5.2: Bayesian probit model (2)

- Model for Y_i:

$$Y_i \sim \text{Bin}(n_i, \pi_i), \qquad \pi = \Phi(\mathbf{z}_i'\boldsymbol{\beta}),$$

  where $\mathbf{z}_i = (1, z_{i1}, z_{i2}, z_{i3})$ and $\Phi(\cdot)$ being the CDF of a $\text{N}(0, 1)$.
- Prior on the parameter of interest $\boldsymbol{\beta}$: $\boldsymbol{\beta} \sim N(\mathbf{0}, \mathbb{I}/\lambda)$.
- The posterior density of $\boldsymbol{\beta}$ is

$$f(\boldsymbol{\beta}|y_1, \ldots, y_n) \propto \left(\prod_{i=1}^{N} \Phi(\mathbf{z}_i'\boldsymbol{\beta})^{y_i} \cdot (1 - \Phi(\mathbf{z}_i'\boldsymbol{\beta}))^{n_i - y_i} \right) \cdot \exp\left(-\frac{\lambda}{2} \sum_{j=0}^{3} \beta_j^2 \right)$$

Example 5.2: Bayesian probit model (3)

Use the following "random walk Metropolis" algorithm. Starting with any $\boldsymbol{\beta}^{(0)}$ iterate for $t = 1, 2, \ldots$:

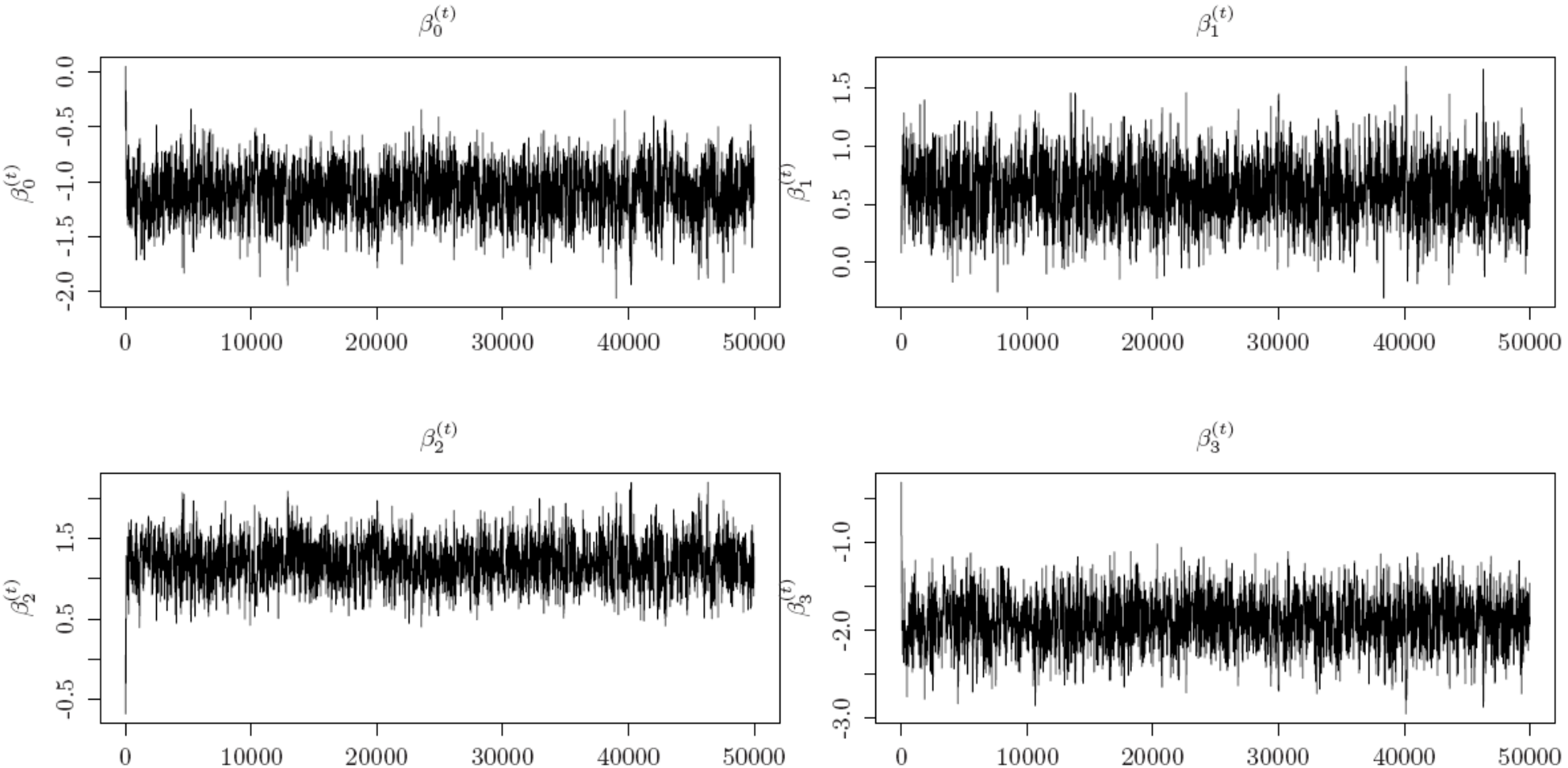
1. Draw $\boldsymbol{\varepsilon} \sim N(\mathbf{0}, \boldsymbol{\Sigma})$ and set $\boldsymbol{\beta} = \boldsymbol{\beta}^{(t-1)} + \boldsymbol{\varepsilon}$.
2. Compute

$$\alpha(\boldsymbol{\beta}|\boldsymbol{\beta}^{(t-1)}) = \min\left\{1, \frac{f(\boldsymbol{\beta}|Y_1, \ldots, Y_n)}{f(\boldsymbol{\beta}^{(t-1)}|Y_1, \ldots, Y_n)}\right\}.$$

3. With probability $\alpha(\boldsymbol{\beta}|\boldsymbol{\beta}^{(t-1)})$ set $\boldsymbol{\beta}^{(t)} = \boldsymbol{\beta}$, otherwise set $\boldsymbol{\beta}^{(t)} = \boldsymbol{\beta}^{(t-1)}$.

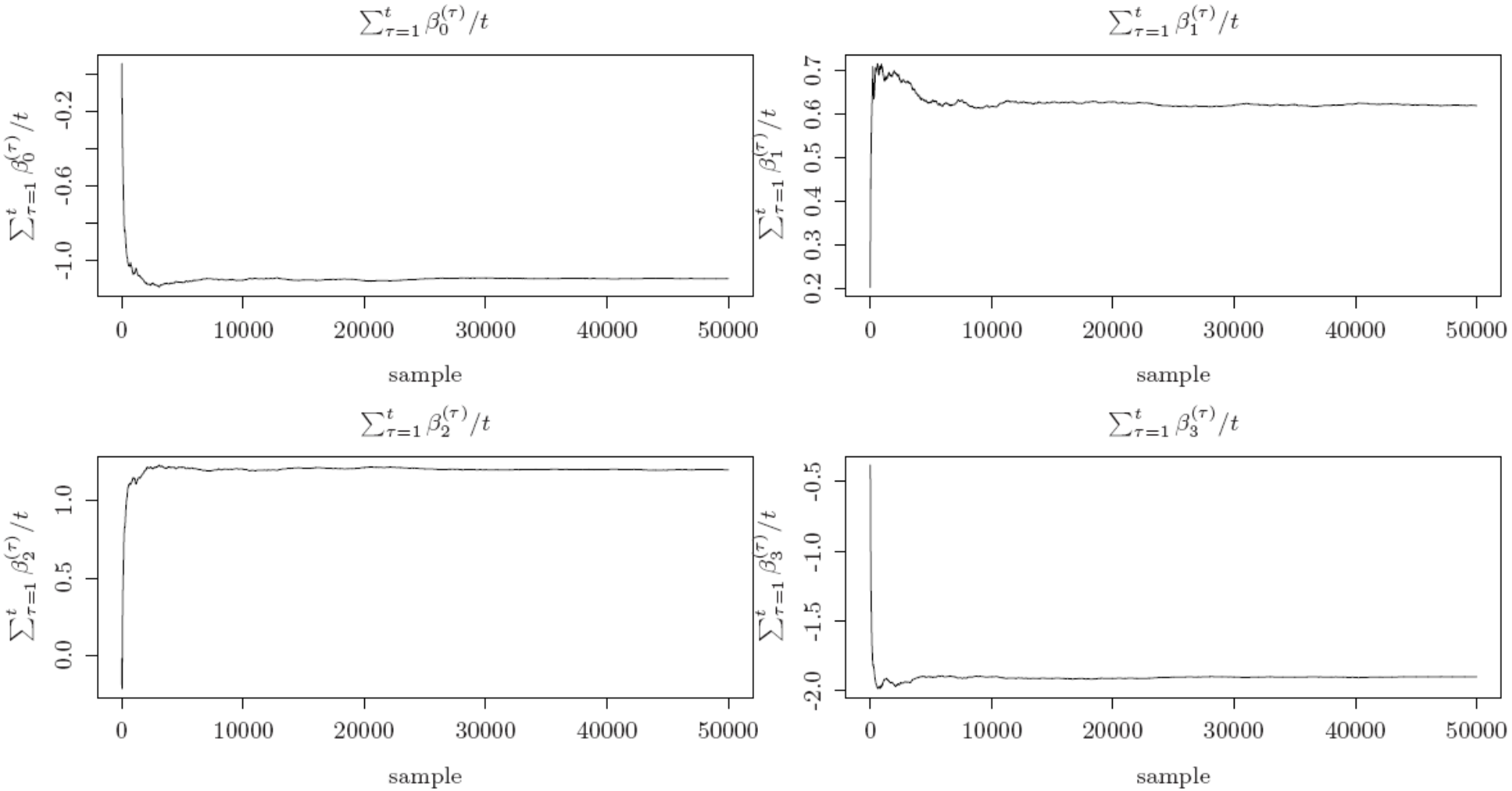
(for the moment we use $\boldsymbol{\Sigma} = 0.08 \cdot \mathbb{I}$, and $\lambda = 10$).

Example 5.2: Bayesian probit model (4)



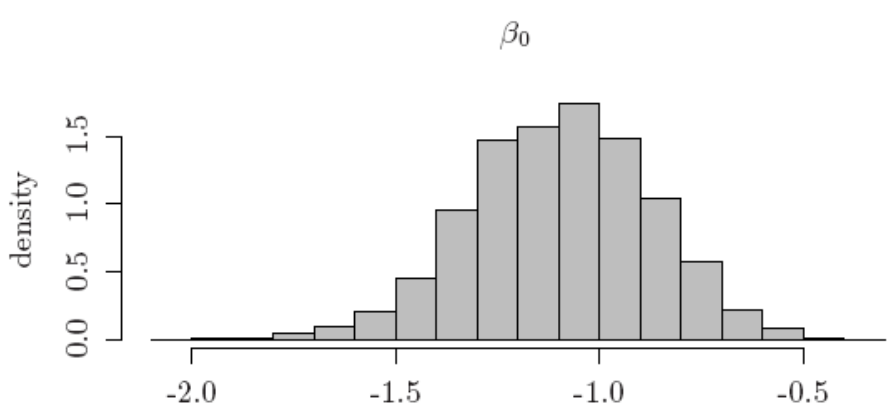
Convergence of the $\beta_j^{(t)}$ is to a distribution, not a value!

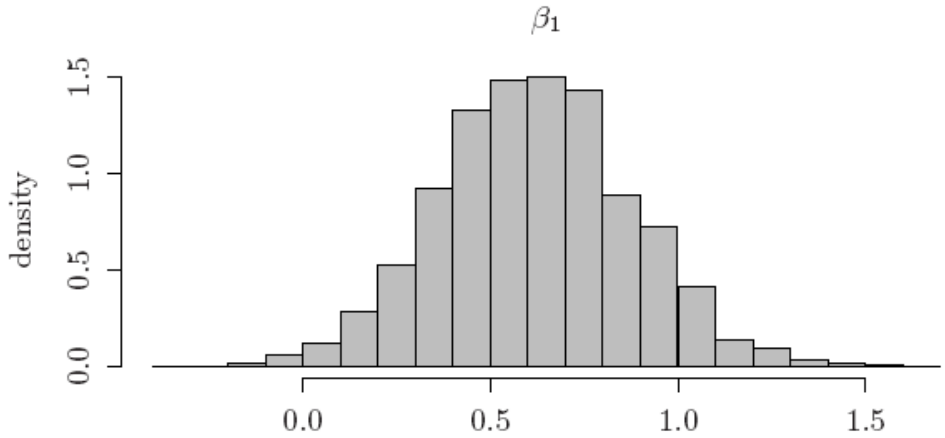
Example 5.2: Bayesian probit model (5)

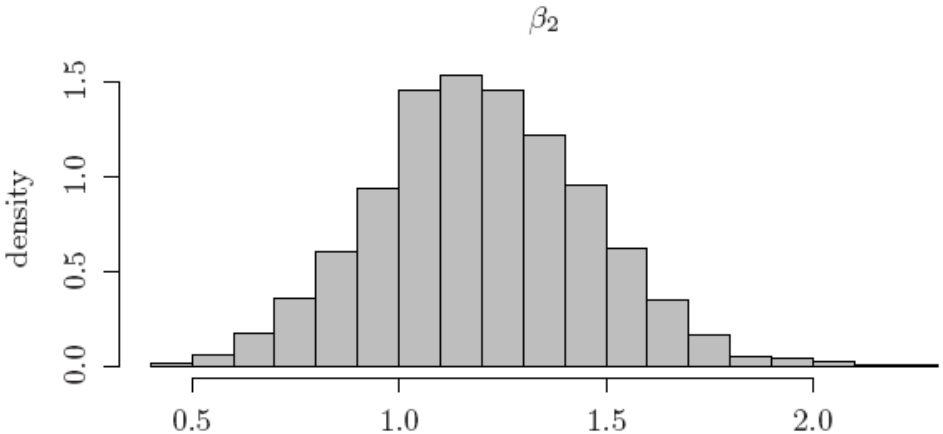


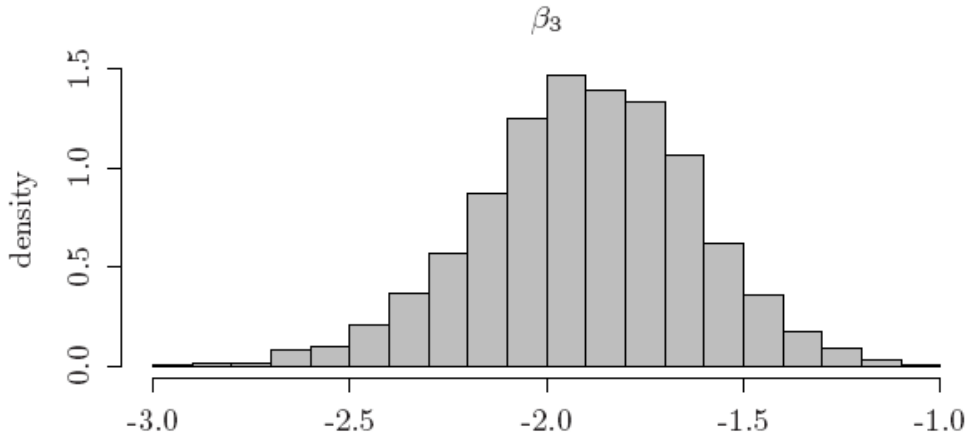
Convergence of cumulative averages $\sum_{\tau=1}^{t} \beta_j^{(\tau)}/t$ is to a value.

Example 5.2: Bayesian probit model (6)









Example 5.2: Bayesian probit model (7)

		Posterior mean	95% credible interval	
intercept	β_0	-1.0952	-1.4646	-0.7333
planned	β_1	0.6201	0.2029	1.0413
risk factors	β_2	1.2000	0.7783	1.6296
antibiotics	β_3	-1.8993	-2.3636	-1.471

Choosing a good proposal distribution

- Ideally: Markov chain with small correlation $\rho(\mathbf{X}^{(t-1)}, \mathbf{X}^{(t)})$ between subsequent values.
  $\rightsquigarrow$ fast exploration of the support of the target f.
- Two sources for this correlation:
  - the correlation between the current state $\mathbf{X}^{(t-1)}$ and the newly proposed value $\mathbf{X} \sim q(\cdot|\mathbf{X}^{(t-1)})$
    (can be reduced using a proposal with high variance)
  - the correlation introduced by retaining a value $\mathbf{X}^{(t)} = \mathbf{X}^{(t-1)}$ because the newly generated value $\mathbf{X}$ has been rejected
    (can be reduced using a proposal with small variance)
- Trade-off for finding the ideal compromise between:
  - fast exploration of the space (good mixing behaviour)
  - obtaining a large probability of acceptance
- For multivariate distributions: covariance of proposal should reflect the covariance structure of the target.

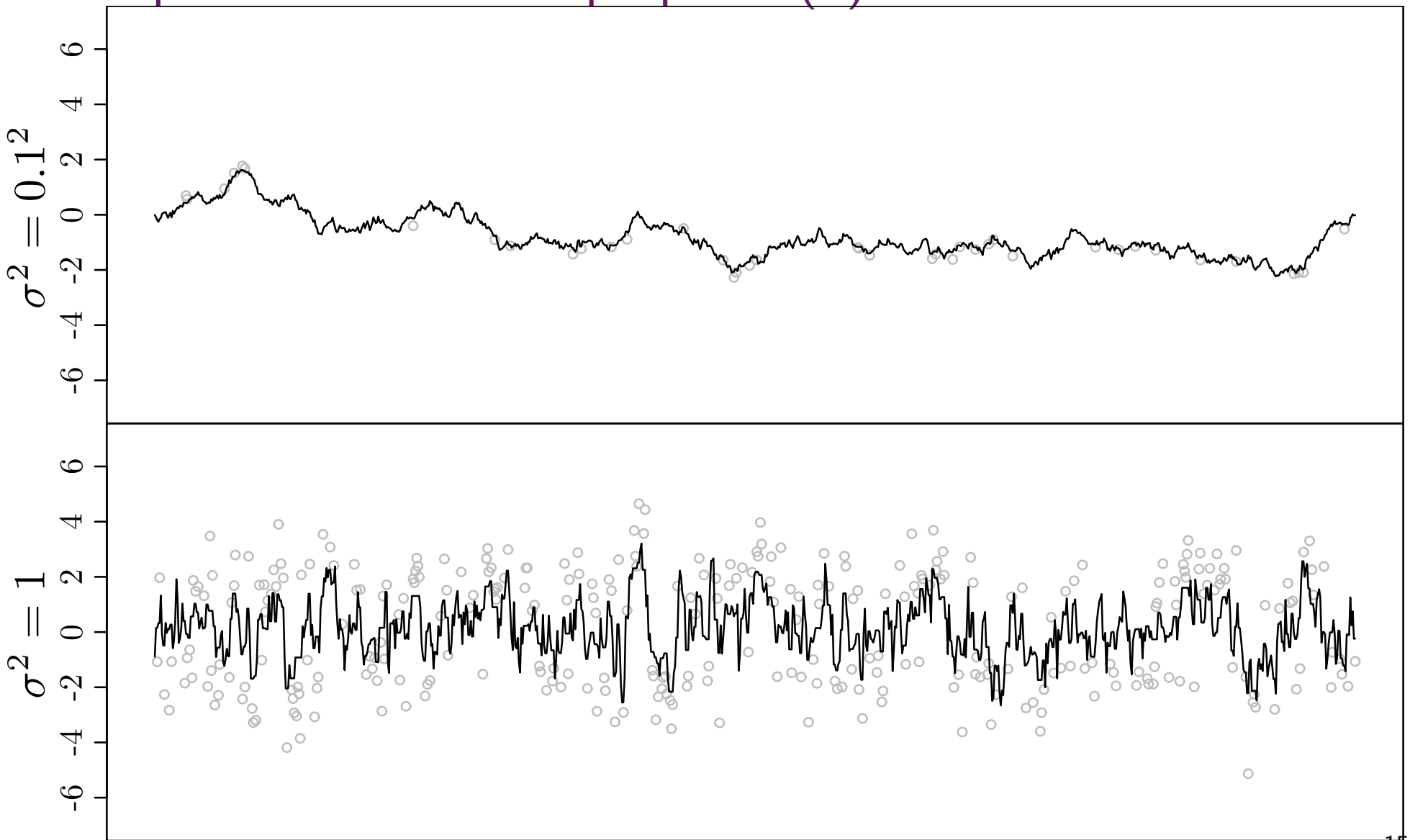
Example: Choice of proposal (1)

- Target distribution, we want to sample from: $\mathsf{N}(0,1)$ (i.e. $f(\cdot) = \phi_{(0,1)}(\cdot)$)
- We want to use a random walk Metropolis algorithm with

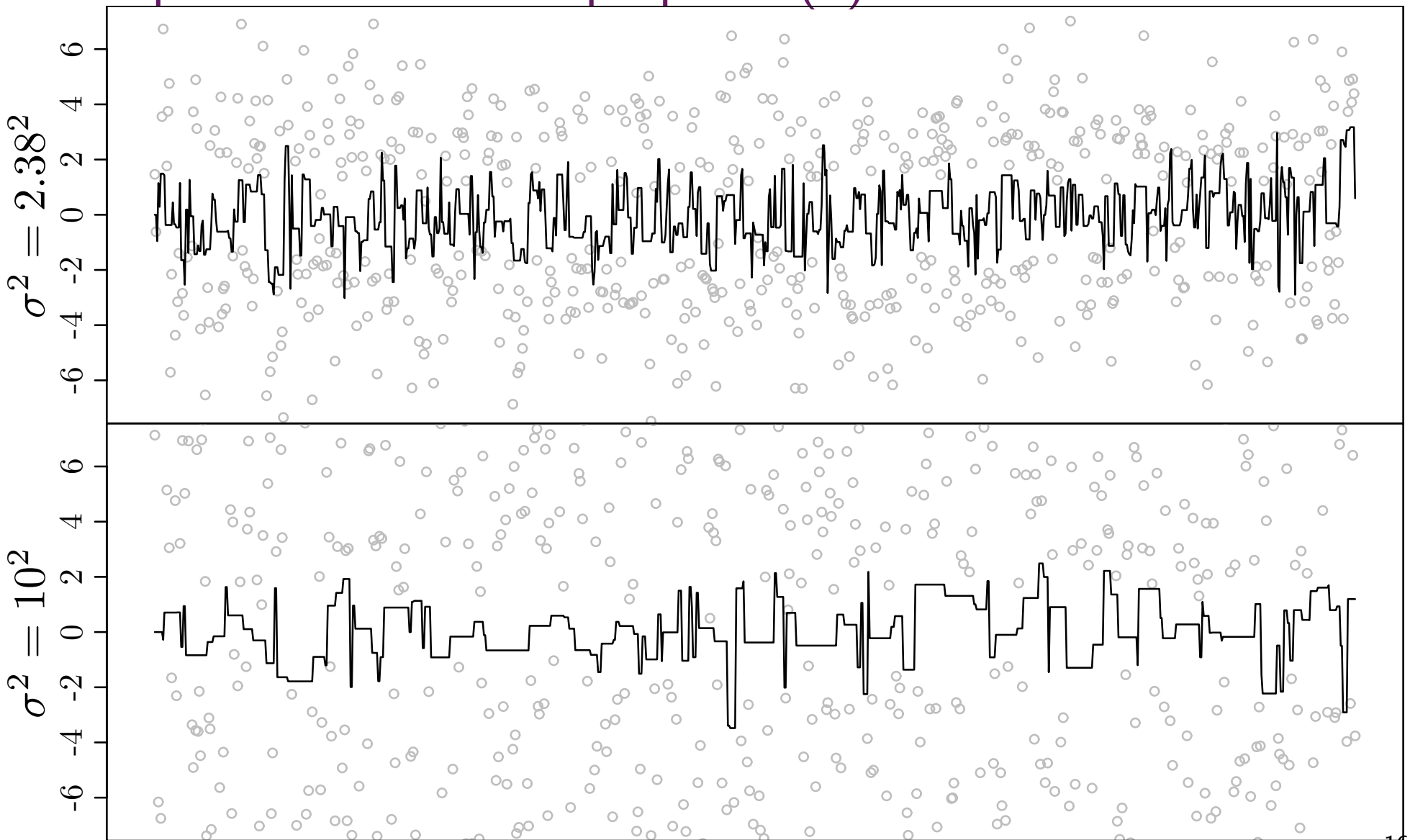
$$\varepsilon \sim \mathsf{N}(0, \sigma^2)$$

- What is the optimal choice of σ^2?
- We consider four choices $\sigma^2 = 0.1^2, 1, 2.38^2, 10^2$.

Example 5.3: Choice of proposal (2)



Example 5.3: Choice of proposal (3)



Example 5.3: Choice of proposal (4)

	Autocorrelation $\rho(X^{(t-1)}, X^{(t)})$		Probability of acceptance $\alpha(X, X^{(t-1)})$	
	Mean	95% CI	Mean	95% CI
$\sigma^2 = 0.1^2$	0.9901	(0.9891,0.9910)	0.9694	(0.9677,0.9710)
$\sigma^2 = 1$	0.7733	(0.7676,0.7791)	0.7038	(0.7014,0.7061)
$\sigma^2 = 2.38^2$	0.6225	(0.6162,0.6289)	0.4426	(0.4401,0.4452)
$\sigma^2 = 10^2$	0.8360	(0.8303,0.8418)	0.1255	(0.1237,0.1274)

Suggests: Optimal choice is $2.38^2 > 1$.

Example 5.4: Bayesian probit model (revisited)

- So far we used: $\mathrm{Var}(\boldsymbol{\varepsilon}) = 0.08 \cdot \mathbb{I}$).
- Better choice: Let $\mathrm{Var}(\boldsymbol{\varepsilon})$ reflect the covariance structure
- Frequentist asymptotic theory: $\mathrm{Var}(\hat{\boldsymbol{\beta}}^{\mathrm{m.l.e}}) = (\mathbf{Z}'\mathbf{D}\mathbf{Z})^{-1}$
  $\mathbf{D}$ is a suitable diagonal matrix
- Better choice: $\mathrm{Var}(\boldsymbol{\varepsilon}) = 2 \cdot (\mathbf{Z}'\mathbf{D}\mathbf{Z})^{-1}$
- Increases rate of acceptance from 13.9% to 20.0% and reduces autocorrelation:

$\boldsymbol{\Sigma} = 0.08 \cdot \mathbf{I}$	β_0	β_1	β_2	β_3
Autocorrelation $\rho(\beta_j^{(t-1)}, \beta_j^{(t)})$	0.9496	0.9503	0.9562	0.9532
$\boldsymbol{\Sigma} = 2 \cdot (\mathbf{Z}'\mathbf{D}\mathbf{Z})^{-1}$	β_0	β_1	β_2	β_3
Autocorrelation $\rho(\beta_j^{(t-1)}, \beta_j^{(t)})$	0.8726	0.8765	0.8741	0.8792

(in this example $\det(0.08 \cdot \mathbb{I}) = \det(2 \cdot (\mathbf{Z}'\mathbf{D}\mathbf{Z})^{-1})$)

Positron Emission Tomography I

Positron Emission Tomography

- Inject radioactive tracer into subject's bloodstream.
- Record tracer concentration in blood (at high speed).
- Record numbers of emissions from each volume element (voxel).
- Reconstruct brain activity from measurements.

Compartmental Modelling of Each Voxel Model each site as:

- A system of compartments...
- into which tracer flows from the blood
- between which tracer flows
- and from which tracer can flow back into the blood.

Positron Emission Tomography II

Consider a linear m-compartment model.

Vector $\boldsymbol{f}(t)$: element i element corresponds to concentration in compartment i at time t.

Similarly, $\boldsymbol{b}(t)$ describe all flow into the system from outside.

These models yields a set of ODEs:

$$\dot{\boldsymbol{f}}(t) = \boldsymbol{A}\boldsymbol{f}(t) + \boldsymbol{b}(t),$$
$$\boldsymbol{f}(0) = \boldsymbol{\xi},$$

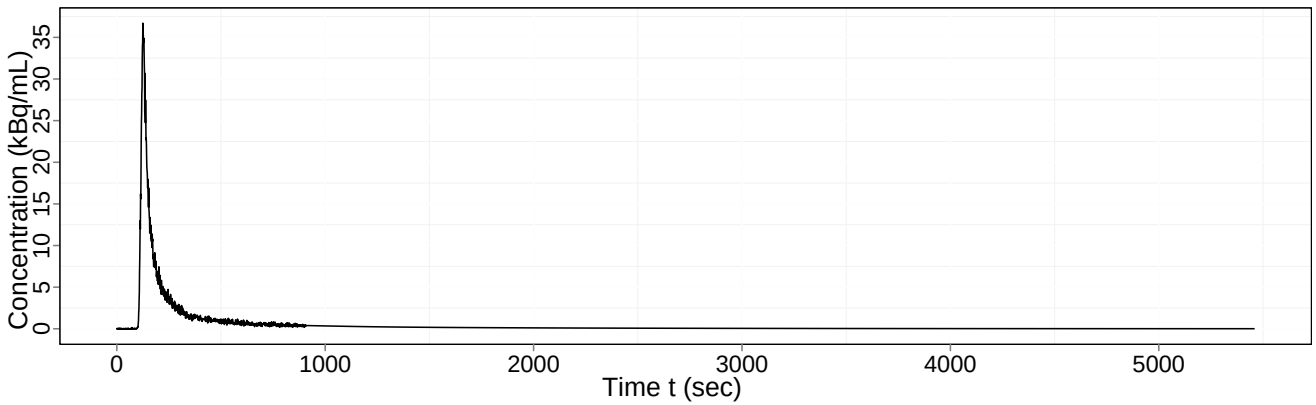
where $\boldsymbol{\xi}$ is the vector of initial concentrations and $\dot{\boldsymbol{f}}$ denotes the time derivative of $\boldsymbol{f}$.

The solution is:

$$\boldsymbol{f}(t) = e^{\boldsymbol{A}t}\boldsymbol{\xi} + \int_0^t e^{\boldsymbol{A}(t-s)}\boldsymbol{b}(s)ds,$$

Positron Emission Tomography III

We also have the measure *input* signal:



A plasma input model with m tissue compartments:

$$\dot{\boldsymbol{C}}_{\boldsymbol{T}}(t) = \boldsymbol{A}\boldsymbol{C}_{\boldsymbol{T}}(t) + \boldsymbol{b}C_P(t) \qquad \boldsymbol{C}_{\boldsymbol{T}}(0) = \mathbf{0},$$
$$C_T(t) = \mathbf{1}^T \boldsymbol{C}_{\boldsymbol{T}}(t)$$

where:

Positron Emission Tomography IV

- $\boldsymbol{C_T}(t)$ are the compartmental "activities"
- $C_P(t)$ is the input signal
- $\boldsymbol{A}$ is an $m \times m$ rate matrix
- $\boldsymbol{b} = (K_1, 0, \ldots, 0)^T$
- $\mathbf{1}$ and $\mathbf{0}$ are m-vectors of ones and zeroes.

The solution to this set of ODES is:

$$C_T(t) = \int_0^t C_P(t-s) H_{TP}(s) ds$$

$$H_{TP}(t) = \sum_{i=1}^{m} \phi_i e^{-\theta_i t},$$

where the ϕ_i and θ_i parameters are functions of the rate constants.

Positron Emission Tomography V

The macro parameter of interest is the *volume of distribution*,

$$V_D := \int_0^\infty H_{TP}(t)dt = \sum_{i=1}^m \frac{\phi_i}{\theta_i}.$$

Combining this deterministic model with a measurement model:

$$C_T(t_j; \phi_{1:m}, \theta_{1:m}) = \sum_{i=1}^m \phi_i \int_0^{t_j} C_P(s) e^{-\theta_i(t_j - s)} ds$$

$$y_j = C_T(t_j; \phi_{1:m}, \theta_{1:m}) + \sqrt{\frac{C_T(t_j; \phi_{1:m}, \theta_{1:m})}{t_j - t_{j-1}}} \varepsilon_j,$$

With normally-distributed errors, choosing an inverse gamma prior for σ^2 and uniform priors for the other parameters:

Positron Emission Tomography VI

$$p(\phi_{1:m}, \theta_{1:m}, \lambda|\boldsymbol{y}) \propto \prod_{j=1}^{n} \sqrt{\lambda} \exp\left\{ -\frac{\lambda}{2} \left[\frac{t_j - t_{j-1}}{C_T(t_j; \phi_{1:m}, \theta_{1:m})} \right] \right.$$
$$\left. (y_j - C_T(t_j; \phi_{1:m}, \theta_{1:m}))^2 \right\}$$
$$\times \lambda^{\alpha-1} e^{-\beta\lambda} \times \prod_{i=1}^{m} I_{[\phi_i^a, \phi_i^b]}(\phi_i) I_{[\theta_i^a, \theta_i^b]}(\theta_i),$$

Positron Emission Tomography VII

Some information is available from biology and physics: the following prior distributions are used to encode this information:

$$\phi_1 \sim \underset{[10^{-5},.01]}{\mathcal{TN}}\left(\cdot; 3\times 10^{-3}, 10^{-3}\right) \qquad \theta_1|\phi_1 \sim \underset{[2\times 10^{-4},.01]}{\mathcal{TN}}\left(\cdot; \frac{\phi_1}{15}, .01\right)$$

$$\phi_2 \sim \underset{[10^{-5},.01]}{\mathcal{TN}}\left(\cdot; 10^{-3}, 10^{-3}\right) \qquad \theta_2|\phi_2,\theta_1 \sim \underset{[\theta_1,6\times .01]}{\mathcal{TN}}\left(\cdot; \frac{\phi_2}{4}, .01\right)$$

$$\phi_3 \sim \underset{[10^{-5},.01]}{\mathcal{TN}}\left(\cdot; 10^{-3}, 10^{-3}\right) \qquad \theta_1|\phi_3,\theta_2 \sim \underset{[\theta_2,6\times .01]}{\mathcal{TN}}\left(\cdot; \phi_3, .01\right).\lambda \qquad \sim$$

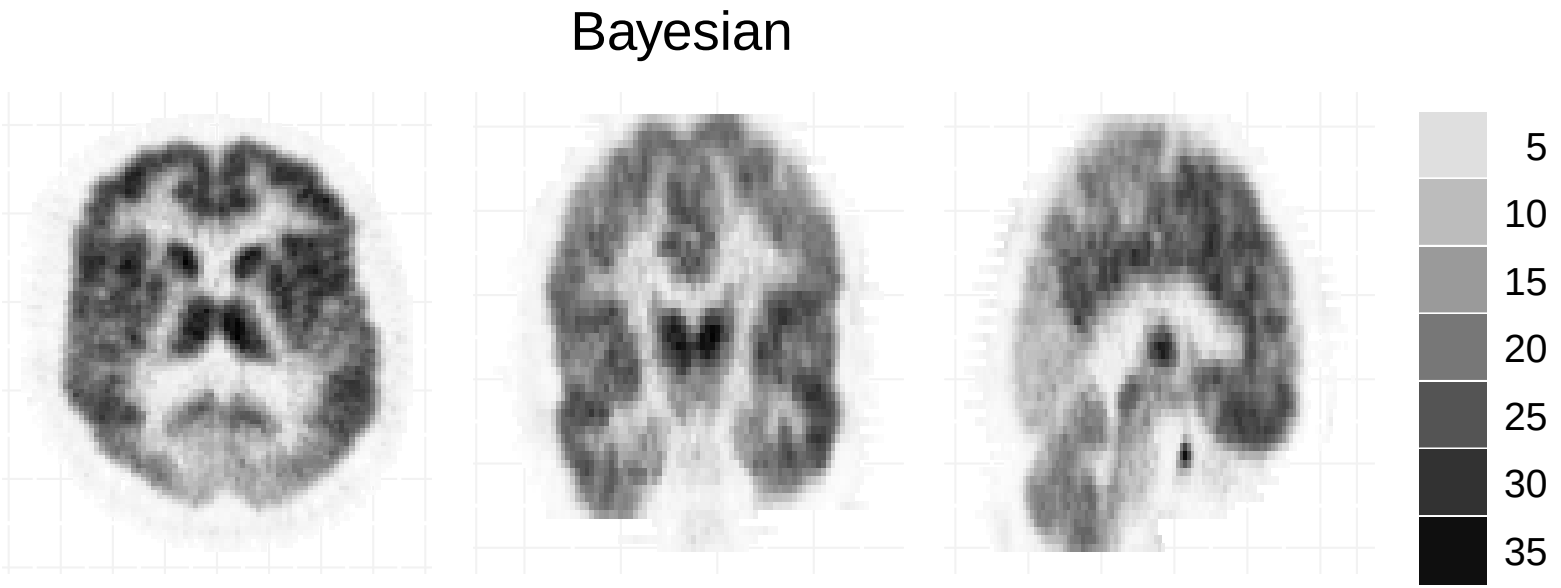
Positron Emission Tomography VIII

Algorithmically, a valid procedure is simply, let $\boldsymbol{\psi} = (\phi_1, \ldots, \phi_3, \theta_1, \ldots, \theta_3, \lambda)$:

1. Initialize $\boldsymbol{\psi}$ with $\boldsymbol{\psi}^{(0)} = \boldsymbol{\psi}_0$, set $t = 0$. $\boldsymbol{\psi}_0$ can be any value within the boundaries of the priors.
2. Generate $\boldsymbol{U}_t$ according to p-dimensional uniform random distribution on $\prod_{i=1}^{p}[-s_i, s_i]$. Where s_i is the step size for ψ_i. Set $\boldsymbol{\eta}_t = \boldsymbol{\psi}^{(t)} + \boldsymbol{U}_t$.
3. Calculate $r_t = f(\boldsymbol{\eta}_t)/f(\boldsymbol{\psi}^{(t)})$. Generate u_t according to uniform distribution on $[0, 1]$. If $u_t \leq r_t$, Set $\boldsymbol{\psi}^{(t+1)} = \boldsymbol{\eta}_t$, otherwise set $\boldsymbol{\psi}^{(t+1)} = \boldsymbol{\psi}^{(t)}$. Increment t. If $t < N$ for some preset positive integer N, go to step (b), otherwise stop.

Positron Emission Tomography IX

The following estimates of V_D were obtained using MCMC (three slices through the brain volume are shown):



See: Y. Zhou, J. A. D. Aston, and A. M. Johansen. Bayesian model comparison for compartmental models with applications in positron emission tomography. Journal of Applied Statistics, 40(5):993–1016, May 2013.

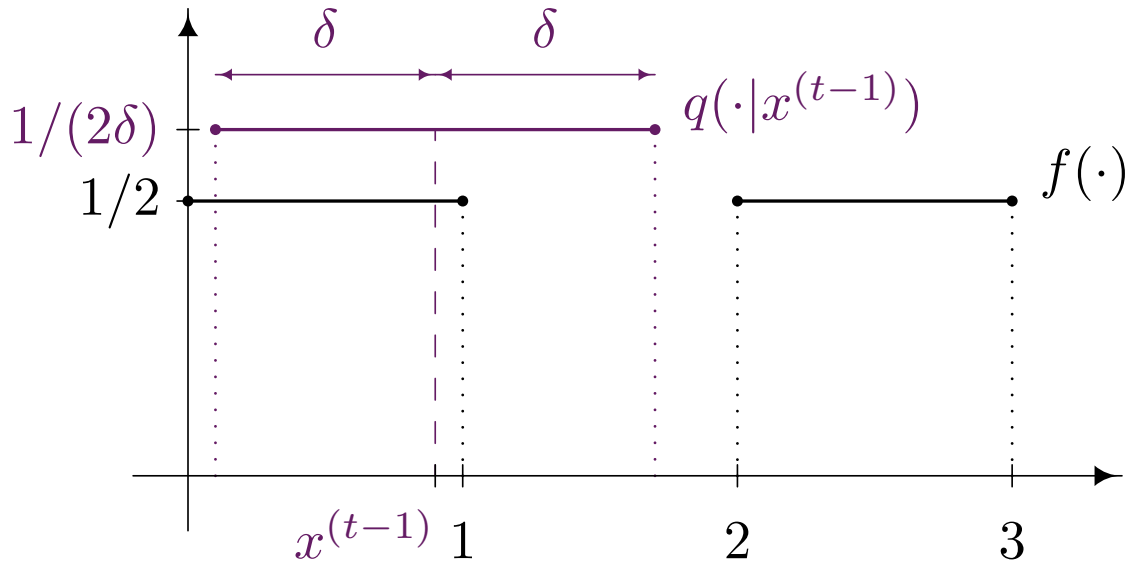
Pathological Example: Reducible Metropolis-Hastings

Consider the target distribution

$$f(x) = (\mathbb{I}_{[0,1]}(x) + \mathbb{I}_{[2,3]}(x))/2.$$

and the proposal distribution $q(\cdot|\mathbf{x}^{(t-1)})$:

$$X|X^{(t-1)} = x^{(t-1)} \sim \mathsf{U}[x^{(t-1)} - \delta, x^{(t-1)} + \delta]$$



Reducible if $\delta \leq 1$: the chain stays either in $[0, 1]$ or $[2, 3]$.

The Metropolis-Adjusted Langevin Algorithm

- Based on the Langevin diffusion:

$$d\mathbf{X}_t = -\frac{1}{2}\nabla \log(f(\mathbf{X}_t))dt + d\mathbf{B}_t$$

  which is f-invariant *in continuous time*.
- Given target f the MALA proposal mechanism samples:

$$\mathbf{X} \leftarrow \mathbf{X}^{(t-1)} + \epsilon$$
$$\epsilon \sim \mathrm{N}\left(-\frac{\sigma^2}{2}\nabla \log f(\mathbf{X}^{(t-1)}), \sigma^2 I_p\right)$$

  at time t.
- Accepts X with the usual MH acceptance probability.

The Metropolised Independence Sampler

Independent proposals: choose $q(\cdot|x) = q(\cdot)$.

Algorithm 5.3 The Independence Sampler

Starting with $\mathbf{X}^{(0)} := (X_1^{(0)}, \ldots, X_p^{(0)})$ iterate for $t = 1, 2, \ldots$

1. Draw $\mathbf{X} \sim q(\cdot)$.
2. Compute

$$\alpha(\mathbf{X}|\mathbf{X}^{(t-1)}) = \min\left\{1, \frac{f(\mathbf{X}) \cdot q(\mathbf{X}^{(t-1)})}{f(\mathbf{X}^{(t-1)}) \cdot q(\mathbf{X})}\right\}.$$

3. With probability $\alpha(\mathbf{X}|\mathbf{X}^{(t-1)})$ set $\mathbf{X}^{(t)} = \mathbf{X}$, otherwise set $\mathbf{X}^{(t)} = \mathbf{X}^{(t-1)}$.

Acceptance Rate

Proposition (Acceptance Rate of Independence Sampler)

If $f(x)/q(x) \leq M < \infty$ the acceptance rate of the independence sampler is at least as high as that of the corresponding rejection sampler.

Gibbs Samplers Revisited

What about full conditionals as MH proposals?

- For $\mathbf{X} = (X_1, \ldots, X_p)$:
- Consider $q(\mathbf{X}|\mathbf{x}^{(t-1)}) = \delta_{x_{-p}^{(t-1)}}(X_{-p}) f_{X_p|X_{-p}}(X_p|X_{-p})$.

Remark

A Gibbs sampler step is a special case of the Metropolis-Hastings algorithm.

Part 3— Section 10

Simulated Annealing

Finding the mode of a distribution

- Our objective so far: estimate $\mathbb{E}(h(\mathbf{X}))$.
- A new objective: estimate (global) mode(s) of a distribution:

$$\{\boldsymbol{\xi} : \ f(\boldsymbol{\xi}) \geq f(\mathbf{x}) \ \forall \mathbf{x}\}$$

- Naïvely: Choose the $\mathbf{X}^{(t)}$ with maximal density $f(\mathbf{X}^{(t)})$.

Example: Naïvely Finding The Mode of a Normal Density

- Consider $f(\mathbf{x}) = \phi(\mathbf{x})$
- Use a Random Walk proposal $\mathbf{X} \sim \mathrm{N}(\mathbf{X}^{(t-1)}, \sigma^2)$ with $\sigma^2 = 0.1^2, 1, 2.38^2, 10^2$.
- Run chains for various T, and pick for each: $\mathbf{X}^{\max} = \arg\max_{\mathbf{X} \in (X^{(t)})_{t=1}^{T}} f(\mathbf{X})$

$N \vert \sigma^2$	0.1^2	1.0^2	2.38^2	10^2
10	0.906	0.091	0.609	0.623
100	0.315	0.020	-0.063	-0.033
100b	-0.033	0.007	0.065	0.005
1000	0.001	0.001	-0.002	-0.002
1000b	0.015	0.001	-0.001	-0.001

- This approach seems to work here...

More Efficiently Finding the Mode

- Idea: Transform distribution such that it is more concentrated around the mode(s).
- Consider

$$f_{(\beta)}(x) \propto (f(x))^{\beta}$$

  for very large values of β.
- For $\beta \to +\infty$ the distribution $f_{(\beta)}(\cdot)$ will be concentrated on the (global) modes.

Example: Normal distribution (1)

- Consider the $\mathrm{N}(\mu, \sigma^2)$ distribution with density

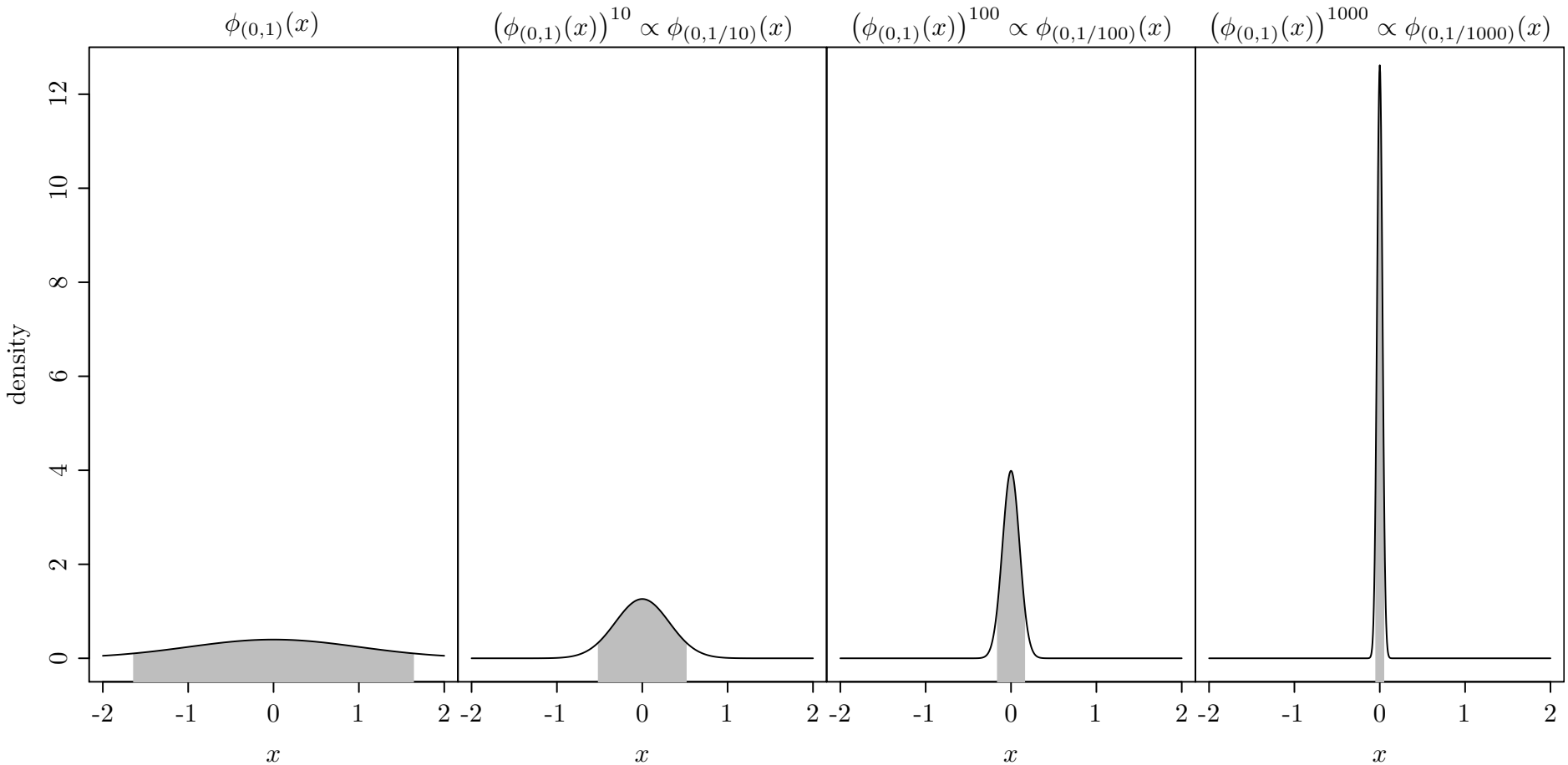
$$f_{(\mu,\sigma^2)}(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \propto \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right).$$

- Mode of the $\mathrm{N}(\mu, \sigma^2)$ distribution is μ.
- For increasing β the distribution is more and more concentrated around its mode μ, as

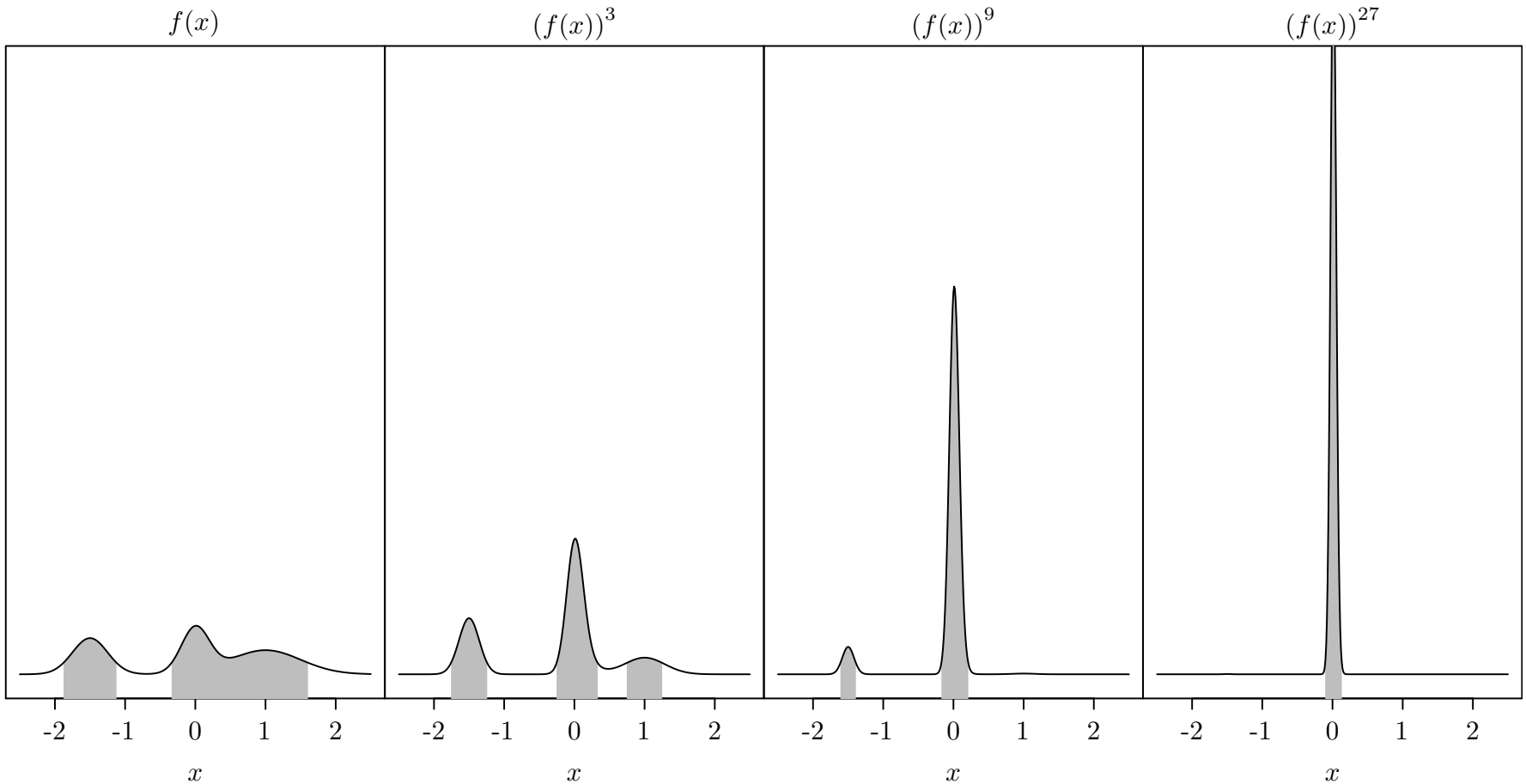
$$\begin{aligned} \left(f_{(\mu,\sigma^2)}(x)\right)^\beta &\propto \left(\exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)\right)^\beta \\ &= \exp\left(-\frac{(x-\mu)^2}{2\sigma^2/\beta}\right) \propto f_{(\mu,\sigma^2/\beta)}(x). \end{aligned}$$

- Increasing β corresponds to reducing the variance.

Example: Normal distribution (2)



Another example



Sampling from $f_{(\beta)}(\cdot)$

- We can sample from $f_{(\beta)}(\cdot)$ using a random walk Metropolis algorithm.
- Probability of acceptance becomes

$$\min\left\{1, \frac{f_{(\beta)}(\mathbf{X})}{f_{(\beta)}(\mathbf{X}^{(t-1)})}\right\} = \min\left\{1, \left(\frac{f(\mathbf{X})}{f(\mathbf{X}^{(t-1)})}\right)^{\beta}\right\}.$$

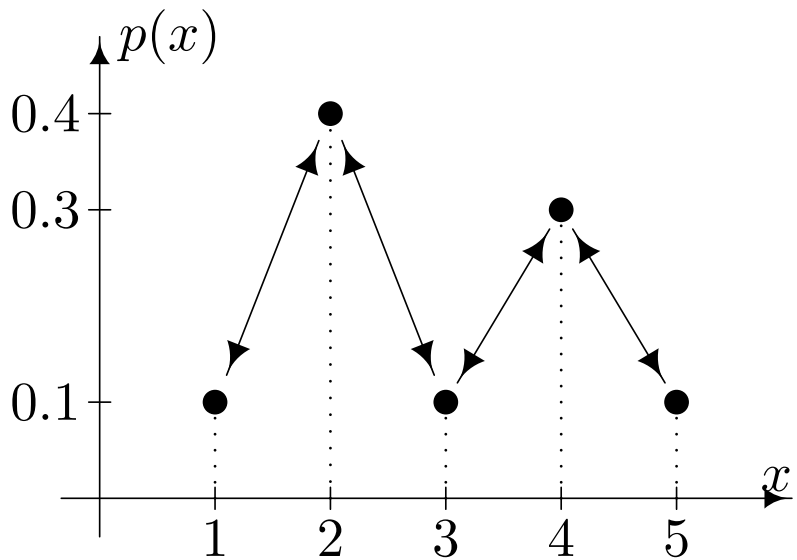
- For $\beta \to +\infty$ the probability of acceptance converges to ...
  - 1 if $f(\mathbf{X}) \geq f(\mathbf{X}^{(t-1)})$, and
  - 0 if $f(\mathbf{X}) < f(\mathbf{X}^{(t-1)})$.
- For large β the chain $(\mathbf{X}^{(t)})_t$ converges to a local maximum of $f(\cdot)$.
- Whether the chain can escape from local maxima of the density depends on whether it can reach the (global) mode within a single step.

Another Example

Assume we want to find the mode of

$$p(x) = \begin{cases} 0.4 & \text{for } x = 2 \\ 0.3 & \text{for } x = 4 \\ 0.1 & \text{for } x = 1, 3, 5. \end{cases}$$

using a random walk Metropolis algorithm that can only move one to the left or one to the right.



For $\beta \to +\infty$ the probability for accepting a move from 4 to 3 converges to 0, as $p(4) > p(3)$, thus the chain cannot escape from the local maximum at 4.

Sampling from $f_{(\beta)}(\cdot)$ is difficult

- For large β the distribution $f_{(\beta)}(\cdot)$ is increasingly concentrated around its modes.
- For large β sampling from $f_{(\beta)}$ gets increasingly difficult.

- Remedy: Start with a small β_0 and let β_t slowly increase.
- The sequence β_t determines whether local extrema are escaped.

Simulated Annealing: Minimising an arbitrary function

- More general objective: find global minima of a function $H : E \to \mathbb{R}_+$.
- Idea: Consider a distribution

$$f(x) \propto \exp(-H(x)) \text{ for } x \in E,$$

yielding

$$f_{(\beta_t)}(x) = (f(x))^{\beta_t} \propto \exp(-\beta_t \cdot H(x)) \text{ for } x \in E.$$

$\rightsquigarrow$ back to the framework of the previous slides.

- In this context β_t is often referred to as *inverse temperature*.

Simulated Annealing: Algorithm

Algorithm: Simulated Annealing

Starting with $\mathbf{X}^{(0)} := (X_1^{(0)}, \ldots, X_p^{(0)})$ and $\beta^{(0)} > 0$ iterate for $t = 1, 2, \ldots$

1. Increase β_{t-1} to β_t (see below for different annealing schedules)
2. Draw $\mathbf{X} \sim q(\cdot|\mathbf{X}^{(t-1)})$.
3. Compute

$$\alpha(\mathbf{X}|\mathbf{X}^{(t-1)}) = \min\left\{1, \exp\left(-\beta_t(H(\mathbf{X}^{(t-1)}) - H(\mathbf{X})\right) \cdot \frac{q(\mathbf{X}^{(t-1)}|\mathbf{X})}{q(\mathbf{X}|\mathbf{X}^{(t-1)})}\right\}.$$

4. With probability $\alpha(\mathbf{X}|\mathbf{X}^{(t-1)})$ set $\mathbf{X}^{(t)} = \mathbf{X}$, otherwise set $\mathbf{X}^{(t)} = \mathbf{X}^{(t-1)}$.

Annealing schedules

- As before $\mathbf{X}^{(t)}$ converges for $\beta_t \to \infty$ to a *local* minimum of $H(\cdot)$.
- Convergence to a *global* minimum depends on annealing schedule:

  Logarithmic tempering $\beta_t = \frac{\log(1+t)}{\beta_0}$.
  Good theoretical properties; practically irrelevant.

  Geometric tempering $\beta_t = \alpha^t \cdot \beta_0$ for some $\alpha > 1$. Popular choice, no theoretical convergence results.
- In practise: expect simulated annealing to find a "good" *local* minimum, but don't expect it to find the *global* minimum!

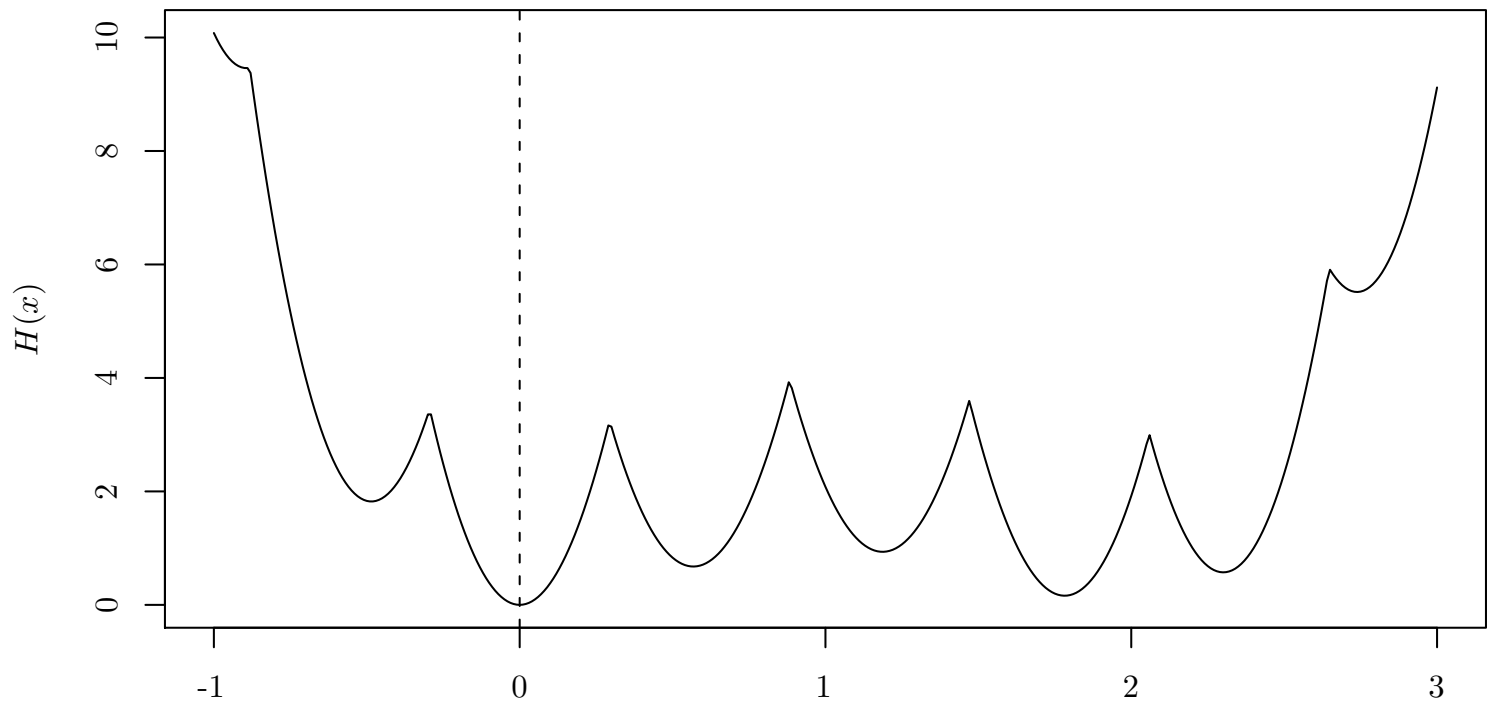
SA Example (1)

Minimise

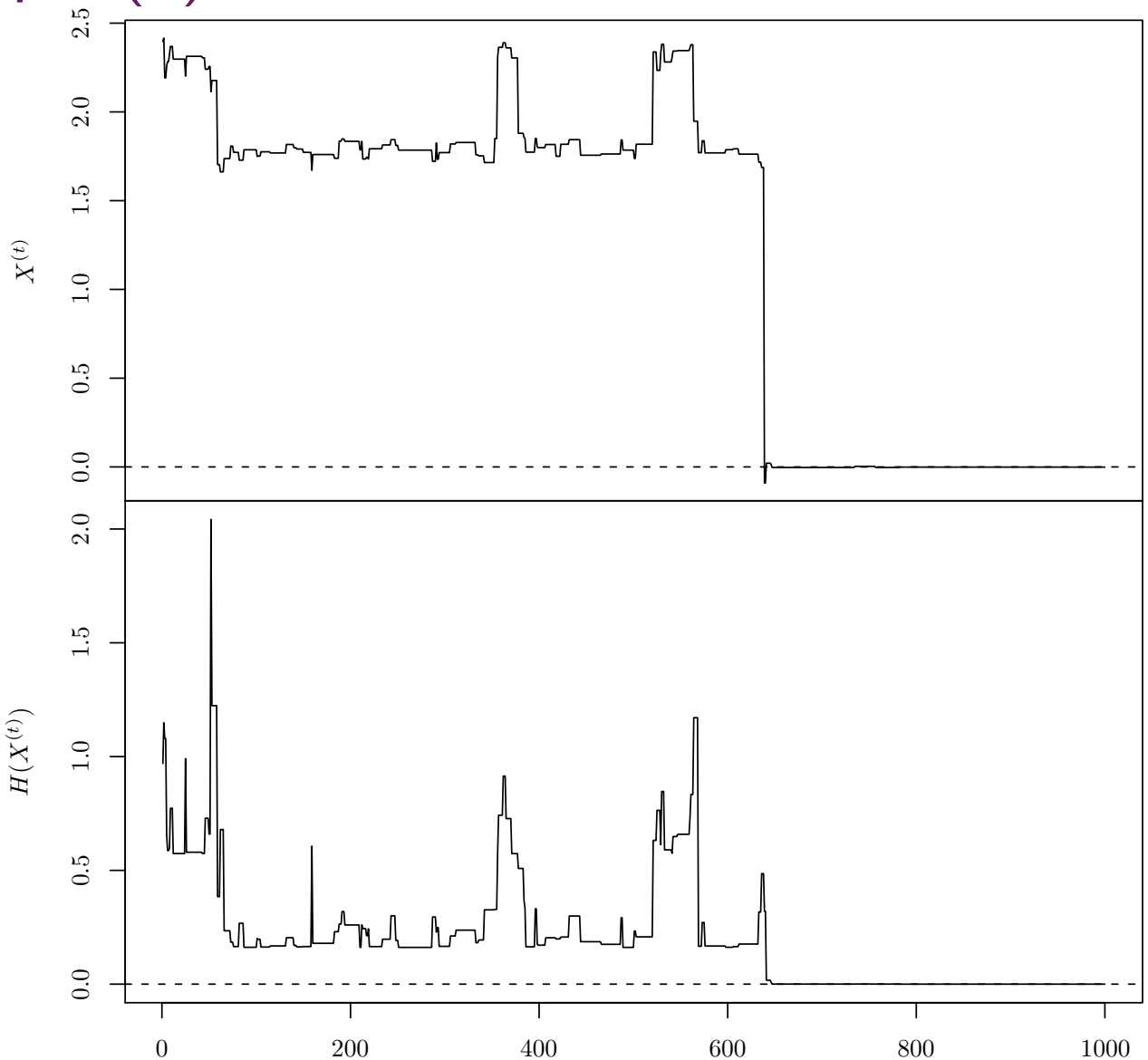
$$H(x) = \left((x-1)^2 - 1\right)^2 + 3 \cdot s(11.56 \cdot x^2)$$

with

$$s(x) = \begin{cases} |x| \mod 2 & \text{for } 2k \leq |x| \leq 2k+1,\ k \in \mathbb{N}_0 \\ 2 - |x| \mod 2 & \text{for } 2k+1 \leq |x| \leq 2(k+1),\ k \in \mathbb{N}_0 \end{cases}$$



SA Example (2)



Summary of Part 3

- Motivation
- MCMC
- Gibbs Samplers
- Metropolis-Hastings-type Algorithms
- Simulated Annealing

Part 4

Augmentation

Augmentation

- "Making the *space* bigger to make the problem easier."
- To target a distribution $f_X(\mathbf{x})$:
  - Construct some $f_{X,Z}(\mathbf{x}, \mathbf{z})$ on $\mathcal{X} \otimes \mathcal{Z}$
  - such that
$$f_X(\mathbf{x}) = \int_{\mathcal{Z}} f_{X,Z}(\mathbf{x}, \mathbf{z}) d\mathbf{z}$$
  - and $f_{X,Z}$ is easy to sample from (when f_X is not).
- Versatile technique with many applications.

Part 4— Section 11

Composition Sampling

Composition Sampling

- Given a *mixture distribution*,

$$f_{\mathbf{X}}(\mathbf{x}) = \sum_{i=1}^{n} w_i f_i(\mathbf{x})$$

- Define

$$f_{\mathbf{X},Z}(\mathbf{x}, z) = w_z \cdot f_z(\mathbf{x})$$

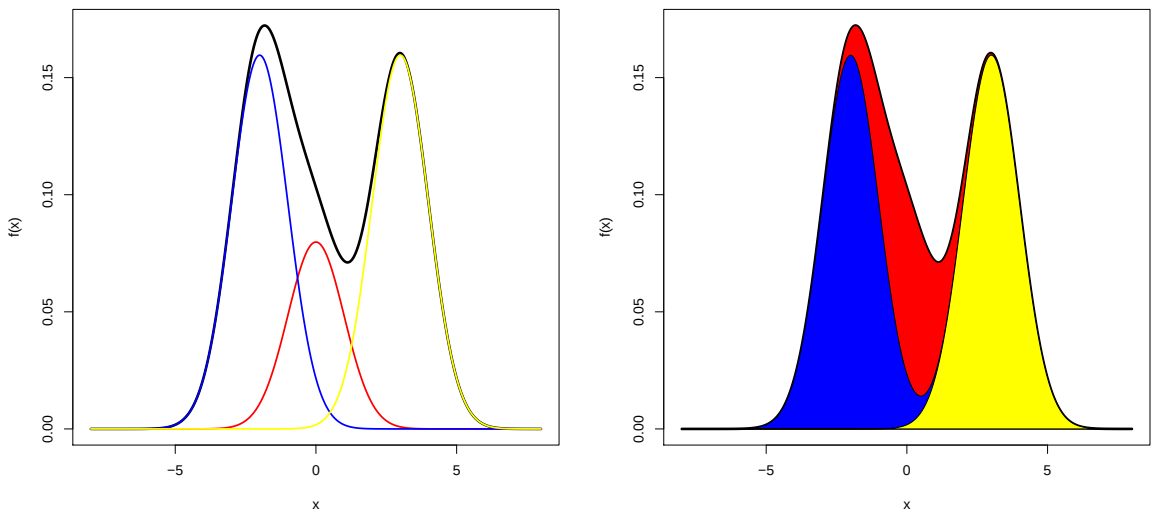
  on $\mathcal{X} \otimes \{1, \ldots, n\}$.
- Sample $Z \sim \sum_{i=1}^{n} w_i \delta_{\{i\}}(\cdot)$
- Sample $X \sim f_Z(\cdot)$

Normal Mixture: Composition Sampling in Detail I

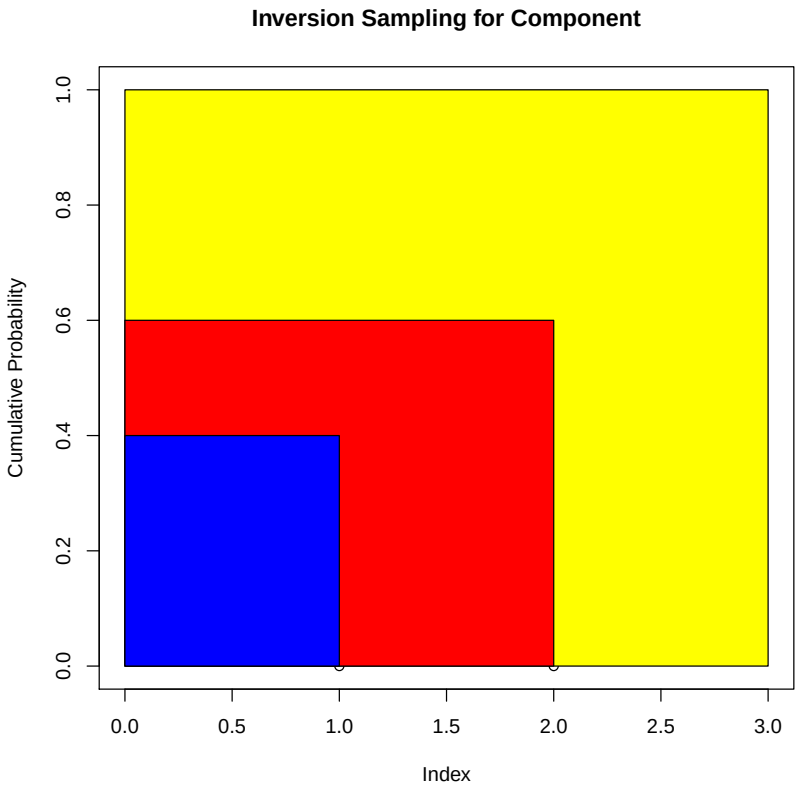
Example of Composition Sampling: Normal Mixture

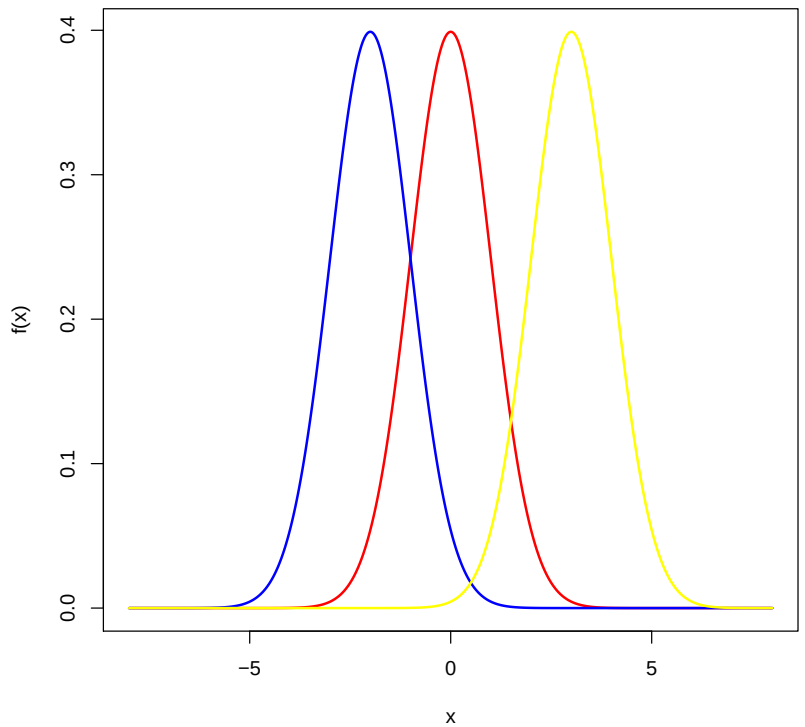
- For $f(x) = 0.4\mathsf{N}(x; -2, 1) + 0.2\mathsf{N}(x; 0, 1) + 0.4\mathsf{N}(x; 3, 1)$
- Sample $U \sim \mathsf{U}[0, 1]$; set $I = 1$ if $U < 0.4$, $I = 2$ if $U \in [0.4, 0.6)$ $I = 3$ otherwise.
- Sample $X \sim f_I$ where $f_I = \mathsf{N}(\mu_I, 1)$ and $\boldsymbol{\mu} = \{-2, 0, 3\}$.

Normal Mixture: Composition Sampling in Detail II



Normal Mixture: Composition Sampling in Detail III





Part 4— Section 12

Rejection Revisited

A Generic Augmentation Scheme

- Given any density $f(\mathbf{x})$, define

$$\bar{f}(\mathbf{x}, u) := f(\mathbf{x}) \cdot \bar{f}_{U|\mathbf{X}}(u|\mathbf{x})$$

- with

$$\bar{f}_{U|\mathbf{X}}(u|\mathbf{x}) = \frac{1}{f(\mathbf{x})} \mathbb{I}_{[0, f(\mathbf{x})]}(u)$$

- Then

$$\bar{f}(\mathbf{x}, u) = \mathbb{I}_{[0, f(\mathbf{x})]}(u).$$

Rejection Sampling Revisited I

Rejection Sampling Revisited II

Proposition (Rejection Sampling Estimators are Equivalent to Importance Sampling Estimators)

- *Given* $f(\mathbf{x})$*, define*

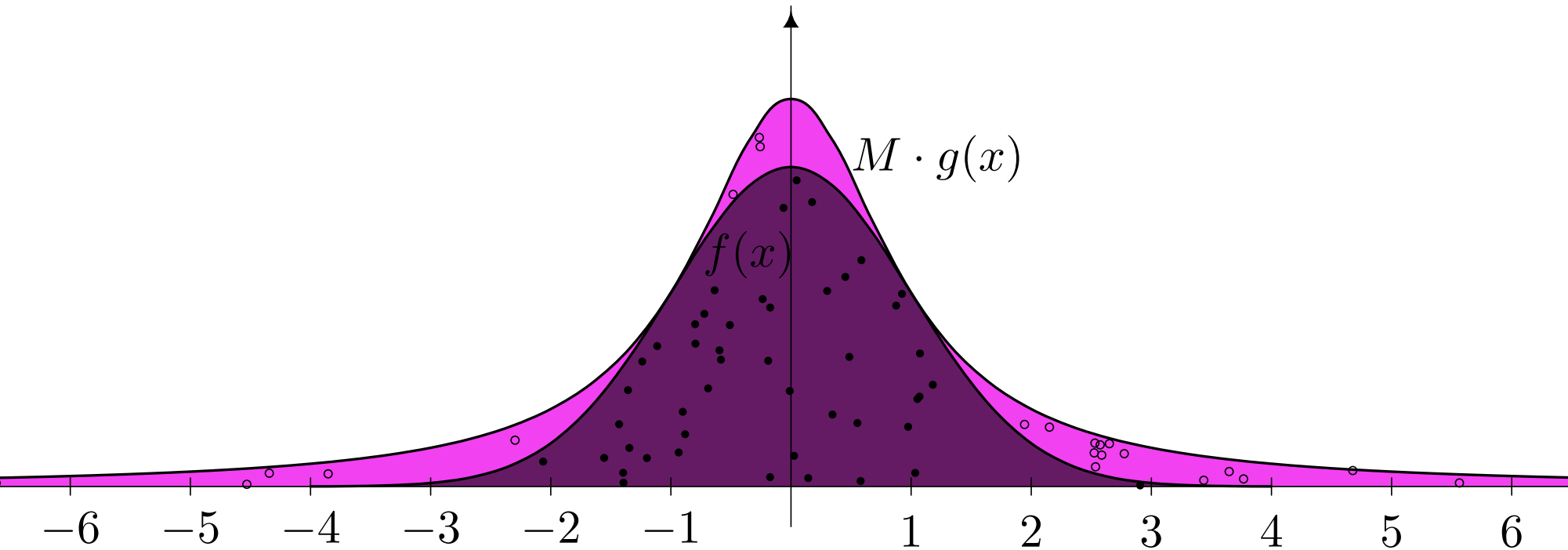
$$\bar{f}(\mathbf{x}, u) = \mathbb{I}_{[0, f(\mathbf{x})]}(u).$$

- *Given proposal* $g(\mathbf{x})$ *and* $M \geq \sup_{\mathbf{x}} f(\mathbf{x})/g(\mathbf{x})$*, define*

$$\bar{g}(\mathbf{x}, u) = \frac{1}{M} \mathbb{I}_{[0, M \cdot g(\mathbf{x})]}.$$

- *Let* $w(\mathbf{x}, u) = c \cdot \bar{f}(\mathbf{x}, u)/\bar{g}(\mathbf{x}, u)$
- *The associated self-normalised importance sampling estimator of* $\mathbb{E}_{\bar{f}}[\varphi(\mathbf{X})] \equiv \mathbb{E}_f[\varphi(\mathbf{X})]$ *is the rejection sampling estimator.*

Rejection Sampling Again



Sample uniformly and weight. . .

Slice Sampling

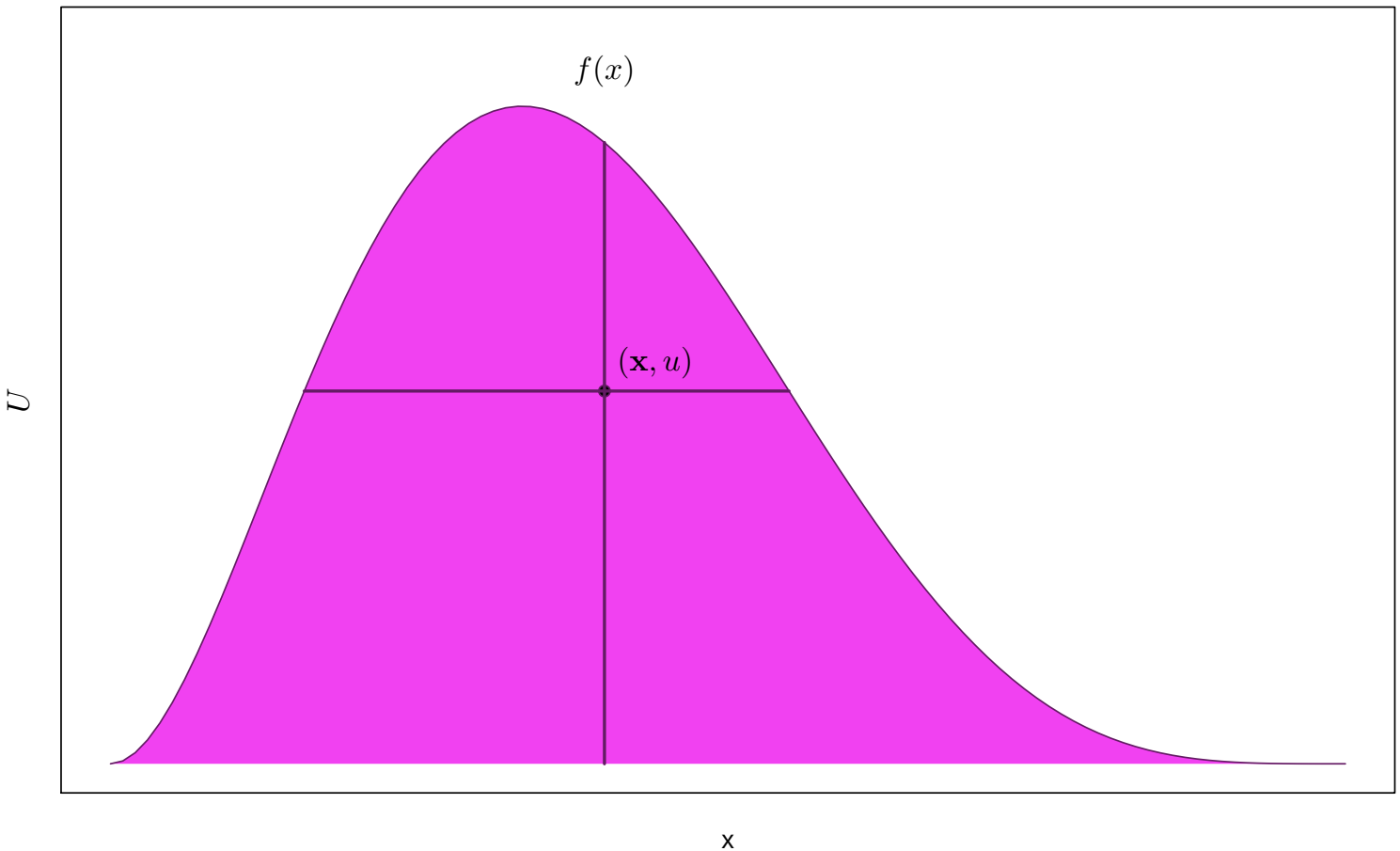
- Rejection sampling can be viewed as importance sampling with an extended distribution...
- so can we apply other algorithms to that extended distribution?

Algorithm: The Slice Sampler

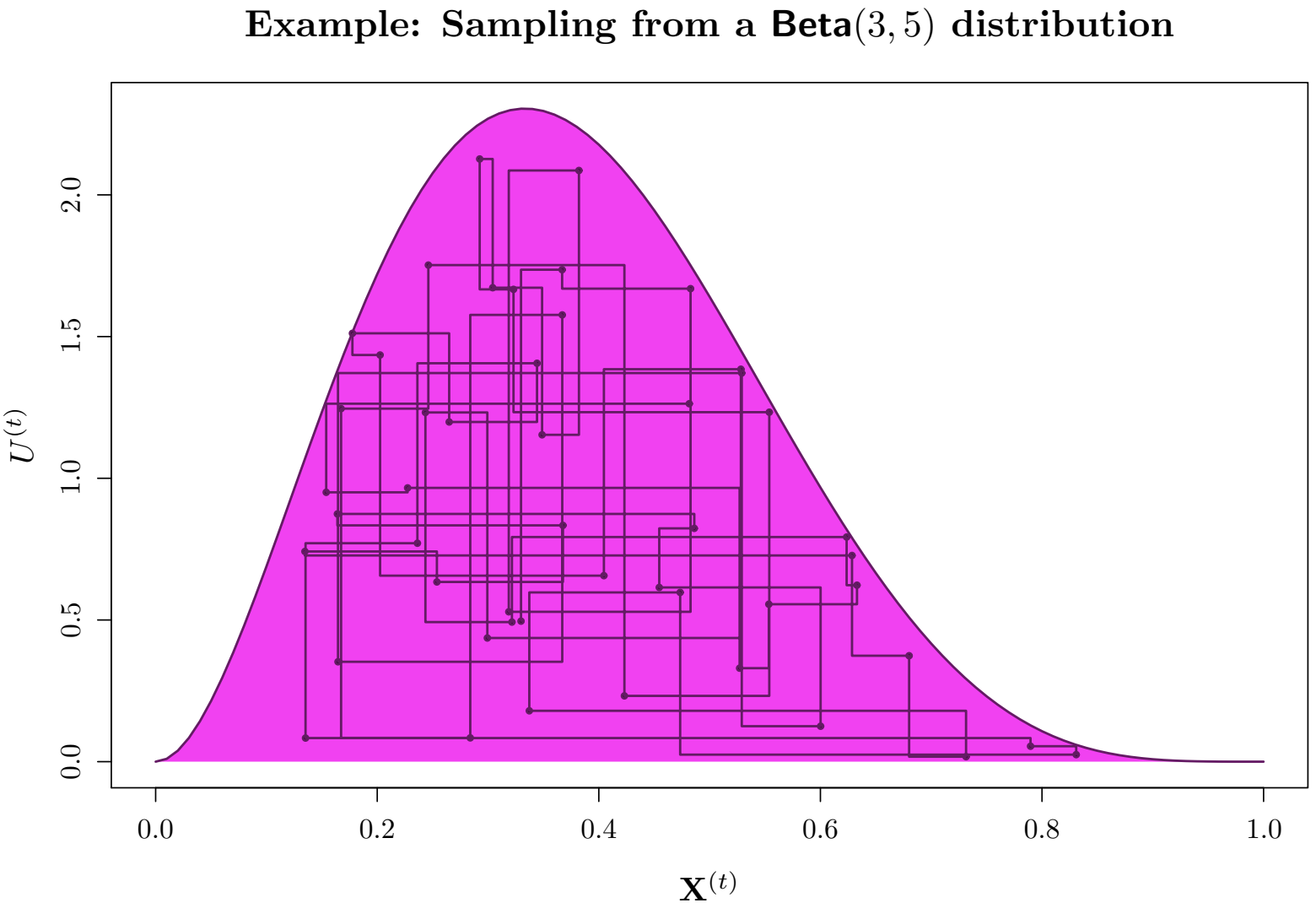
Starting with $(\mathbf{X}^{(0)}, U^{(0)})$ iterate for $t = 1, 2, \ldots$

1. Draw $\mathbf{X}^{(t)} \sim \bar{f}_{\mathbf{X}|U}(\cdot|U^{(t-1)})$.
2. Draw $U^{(t)} \sim \bar{f}_{U|\mathbf{X}}(\cdot|\mathbf{X}^{(t)})$.

An Illustration of the Conditional Distributions



A Slice-Sampler Trajectory



How Practical Is This?

- Sampling $U \sim \mathsf{U}[0, f(\mathbf{X})]$ is *easy*.
- Sampling $\mathbf{X} \sim \mathsf{U}(L(U))$ where

$$L(u) := \{\mathbf{x} : f(\mathbf{x}) \geq u\}$$

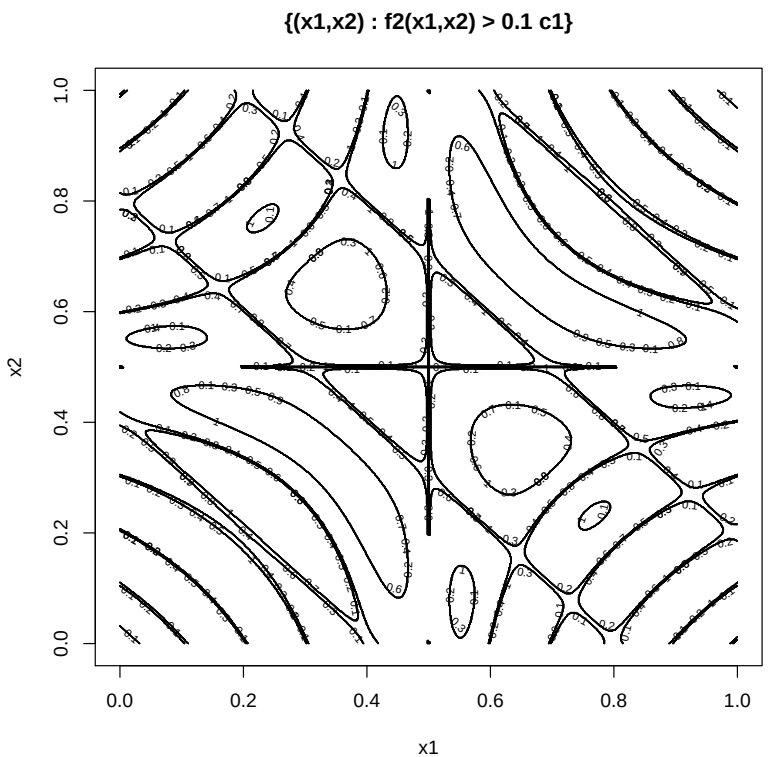
  can be easy...
- but it might not be.
- Consider the bivariate density:

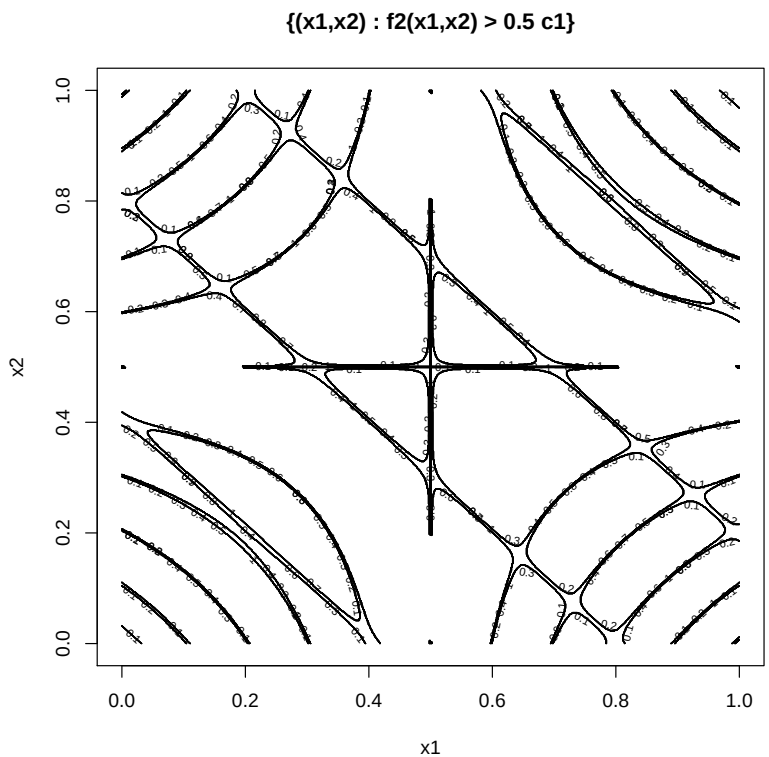
$$f_2(x_1, x_2) = c_1 \cdot \sin^2(x_1 \cdot x_2) \cdot \cos^2(x_1 + x_2) \cdot \exp(-\frac{1}{2}(|x_1| + |x_2|))$$

The Trouble with Slice Sampling

Level sets of:

$$f_2(x_1, x_2) = c_1 \cdot \sin^2(x_1 \cdot x_2) \cdot \cos^2(x_1 + x_2) \cdot \exp(-\frac{1}{2}(|x_1| + |x_2|))$$





here we could use rejection.

Algorithm: The Co-ordinate-wise Slice Sampler

Starting with $(X_1^{(0)}, \ldots, X_p^{(0)}, U^{(0)})$ iterate for $t = 1, 2, \ldots$

1. Draw $X_1^{(t)} \sim \bar{f}_{X_1|X_{-1},U}(\cdot|X_{-1}^{(t-1)}, U^{(t-1)})$.
2. Draw $X_2^{(t)} \sim \bar{f}_{X_2|X_{-2},U}(\cdot|X_1^{(t)}, X_3^{(t-1)}, \ldots, X_p^{(t-1)}, U^{(t-1)})$.

$\vdots$

p. Draw $X_p^{(t)} \sim \bar{f}_{X_p|X_{-p},U}(\cdot|X_{-p}^{(t)}, U^{(t-1)})$.

p+1. Draw $U^{(t)} \sim \bar{f}_{U|\mathbf{X}}(\cdot|\mathbf{X}^{(t)})$.

Algorithm: The Metropolised Slice Sampler

Starting with $(\mathbf{X}^{(0)}, U^{(0)})$ iterate for $t = 1, 2, \ldots$

1. Draw $\mathbf{X} \sim \bar{q}(\cdot|\mathbf{X}^{(t-1)}, U^{(t-1)})$.
2. With probability

$$\min\left(1, \frac{\bar{f}(\mathbf{X}, U^{(t-1)})q(\mathbf{X}^{(t-1)}|\mathbf{X}, U^{(t-1)})}{\bar{f}(\mathbf{X}^{(t-1)}, U^{(t-1)})q(\mathbf{X}|\mathbf{X}^{(t-1)}, U^{(t-1)})}\right)$$

accept and set $\mathbf{X}^{(t)} = \mathbf{X}$.
Otherwise, set $\mathbf{X}^{(t)} = \mathbf{X}^{(t-1)}$.

2. Draw $U^{(t)} \sim \bar{f}_{U|\mathbf{x}}(\cdot|\mathbf{X}^{(t)})$.

Part 4— Section 13

Data Augmentation

Data Augmentation I

- *Latent variable models* are common: statistical models with:
  - parameters θ,
  - observations $\mathbf{y}$, and
  - latent variables, $\mathbf{z}$.
- Typically, the joint distribution, $f_{\mathbf{Y},\mathbf{Z},\theta}$, is known,
- but integrating out the latent variables in not feasible.
- Without $f_{\mathbf{Y},\theta}$ we can't implement an MCMC algorithm targetting $f_{\theta|\mathbf{Y}}$.
- The basis of data augmentation is to *augment* θ with $\mathbf{z}$ and to run an MCMC algorithm which targets $f_{\theta,\mathbf{Z}|\mathbf{Y}}$.
- This distribution has the correct marginal in θ.

Data Augmentation and Gibbs Samplers

- Gibbs sampling is only feasible when we can sample easily from the full conditionals.
- A technique that can help achieving full conditionals that are easy to sample from is *demarginalisation*:
  Introduce a set of auxiliary random variables $Z_1, \ldots, Z_r$ such that f is the marginal density of $(X_1, \ldots, X_p, Z_1, \ldots, Z_r)$, i.e.

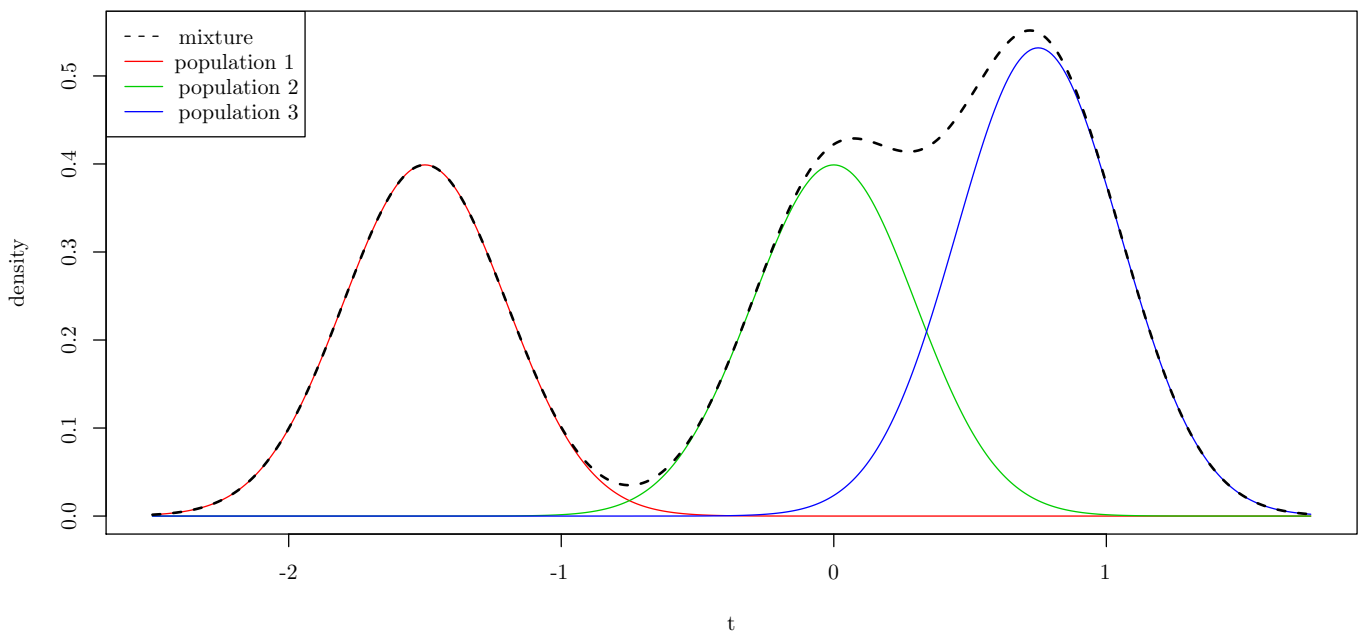
$$f(x_1, \ldots, x_p) = \int f(x_1, \ldots, x_n, z_1, \ldots, z_r)\, d(z_1, \ldots, z_r).$$

- In many cases there is a "natural choice" of the *completion* $(Z_1, \ldots, Z_r)$.

Example: Mixture of Gaussians — Model

Consider the following K population mixture model for data $Y_1, \ldots, Y_n$:

$$f(y_i) = \sum_{k=1}^{K} \pi_k \phi_{(\mu_k, 1/\tau)}(y_i)$$



Objective: Bayesian inference for the parameters $(\pi_1, \ldots, \pi_K, \mu_1, \ldots, \mu_K)$.

Example: Mixture of Gaussians — Priors

- The number of components K is assumed to be known.
- The variance parameter τ is assumed to be known.
- $(\pi_1, \ldots, \pi_K) \sim \text{Dirichlet}(\alpha_1, \ldots, \alpha_K)$, i.e.

$$f_{(\alpha_1,\ldots,\alpha_K)}(\pi_1, \ldots, \pi_K) = \frac{\Gamma(\sum_{k=1}^K \alpha_k)}{\prod_{k=1}^K \Gamma(\alpha_k)} \prod_{k=1}^K \pi_k^{\alpha_k - 1}$$

- $(\mu_1, \ldots, \mu_K) \sim \text{N}(\mu_0, 1/\tau_0)$, i.e.

$$f_{(\mu_0,\tau_0)}(\mu_k) \propto \exp\left(-\tau_0(\mu_k - \mu_0)^2/2\right)$$

Example: Mixture of Gaussians — Joint distribution

$$f(\mu_1, \ldots, \mu_K, \pi_1, \ldots, \pi_K, y_1, \ldots, y_n) \propto \left(\prod_{k=1}^{K} \pi_k^{\alpha_k - 1} \right) \cdot$$

$$\left(\prod_{k=1}^{K} \exp\left(-\tau_0(\mu_k - \mu_0)^2/2\right) \right) \cdot \left(\prod_{i=1}^{n} \sum_{k=1}^{K} \pi_k \exp\left(-\tau(y_i - \mu_k)^2/2\right) \right)$$

The full conditionals do not seem to come from "nice" distributions.

Use data augmentation: include auxiliary variables $Z_1, \ldots Z_n$ which indicate which population the i-th individual is from, i.e.

$$\mathbb{P}(Z_i = k) = \pi_k \qquad \text{and} \qquad Y_i | Z_i = k \sim N(\mu_k, 1/\tau).$$

The marginal distribution of Y is as before, so $Z_1, \ldots Z_n$ are indeed a completion.

Example: Mixture of Gaussians — Joint distribution (ctd.)

The joint distribution of the augmented system is

$$\begin{aligned} & f(y_1, \ldots, y_n, z_1, \ldots, z_n, \mu_1, \ldots, \mu_K, \pi_1, \ldots, \pi_K) \\ \propto & \left(\prod_{k=1}^{K} \pi_k^{\alpha_k - 1} \right) \cdot \left(\prod_{k=1}^{K} \exp\left(-\tau_0 (\mu_k - \mu_0)^2 / 2\right) \right) \\ & \cdot \left(\prod_{i=1}^{n} \pi_{z_i} \exp\left(-\tau (y_i - \mu_{z_i})^2 / 2\right) \right) \end{aligned}$$

The full conditionals now come from "nice" distributions.

Example: Mixture of Gaussians — Full conditionals

$$\begin{aligned}
&\mathbb{P}(Z_i = k | Y_1, \ldots, Y_n, \mu_1, \ldots, \mu_K, \pi_1, \ldots, \pi_K) \\
&\quad = \frac{\pi_k \phi_{(\mu_k, 1/\tau)}(y_i)}{\sum_{\iota=1}^{K} \pi_\iota \phi_{(\mu_\iota, 1/\tau)}(y_i)}
\end{aligned}$$

$$\begin{aligned}
&\mu_k | Y_1, \ldots, Y_n, Z_1, \ldots, Z_n, \pi_1, \ldots, \pi_K \\
&\quad \sim \mathsf{N}\left(\frac{\tau \left(\sum_{i:\ Z_i = k} Y_i \right) + \tau_o \mu_0}{|\{:\ Z_i = k\}| \tau + \tau_0}, \frac{1}{|\{i:\ Z_i = k\}| \tau + \tau_0} \right)
\end{aligned}$$

$$\begin{aligned}
&\pi_1, \ldots, \pi_K | Y_1, \ldots, Y_n, Z_1, \ldots, Z_n, \mu_1, \ldots, \mu_K \\
&\quad \sim \mathsf{Dirichlet}\left(\alpha_1 + |\{i:\ Z_i = 1\}|, \ldots, \alpha_K + |\{I:\ Z_i = K\}| \right).
\end{aligned}$$

Example: Mixture of Gaussians — Gibbs sampler

Starting with initial values $\mu_1^{(0)}, \ldots, \mu_K^{(0)}, \pi_1^{(0)}, \ldots, \pi_K^{(0)}$ iterate the following steps for $t = 1, 2, \ldots$

1. For $i = 1, \ldots, n$:

   Draw $Z_i^{(t)}$ from the discrete distribution on $\{1, \ldots, K\}$ specified by

$$p(Z_i^{(t)}) = \left(\frac{\pi_k \phi_{(\mu_k^{(t-1)}, 1/\tau)}(y_i)}{\sum_{\iota=1}^{K} \pi_\iota^{(t-1)} \phi_{(\mu_\iota^{(t-1)}, 1/\tau)}(y_i)} \right).$$

2. For $k = 1, \ldots, K$:

   Draw

$$\mu_k^{(t)} \sim \mathsf{N}\left(\frac{\tau \left(\sum_{i:\ Z_i^{(t)} = k} Y_i \right) + \tau_o \mu_0}{|\{i:\ Z_i^{(t)} = k\}|\tau + \tau_0}, \frac{1}{|\{i:\ Z_i^{(t)} = k\}|\tau + \tau_0} \right).$$

3. Draw

$$(\pi_1^{(t)}, \ldots, \pi_K^{(t)}) \sim \text{Dirichlet}\left(\alpha_1 + |\{i:\ Z_i^{(t)} = 1\}|, \ldots, \alpha_K + |\{i:\ Z_i^{(t)} = K\}| \right).$$

Two More Difficult Statistical Optimisation Problems

Marginal Maximum Likelihood Estimation :

Given $l(\theta; \mathbf{x}) = \int f_{\mathbf{X},\mathbf{Z}}(\mathbf{x}, \mathbf{z}; \theta) d\mathbf{z}$ compute

$$\hat{\theta}_{\mathrm{ML}} = \arg\max_{\theta \in \Theta} l(\theta; \mathbf{x}).$$

Marginal Maximum a Posteriori Estimation :

Given $l(\theta; \mathbf{x}) = \int f_{\mathbf{X},\mathbf{Z}}(\mathbf{x}, \mathbf{z}; \theta) d\mathbf{z}$ and prior $f^{\mathrm{prior}}(\theta)$ compute

$$\hat{\theta}_{\mathrm{MMAP}} = \arg\max_{\theta \in \Theta} f^{\mathrm{prior}}(\theta) l(\theta; \mathbf{x}).$$

We can't typically evaluate the marginal likelihoods.

Data augmentation

- Recall the *demarginalisation* technique for sampling from $f(\mathbf{x})$ when $f(\mathbf{x}, \mathbf{z})$ is known:
  Introduce a set of auxiliary random variables $Z_1, \ldots, Z_r$ such that f is the marginal density of $(X_1, \ldots, X_p, Z_1, \ldots, Z_r)$, i.e.

$$f(x_1, \ldots, x_p) = \int f(x_1, \ldots, x_n, z_1, \ldots, z_r)\, d(z_1, \ldots, z_r).$$

- We could do something similar making some $f_{(\beta)}(\mathbf{x})(\theta)$ the marginal...

Combining Data Augmentation and Simulated Annealing

- Consider

$$l(\theta; \mathbf{x}, \mathbf{z}) = f_{X,Z}(\mathbf{x}, \mathbf{z}|\theta) = f_Z(\mathbf{z}|\theta) f_X(\mathbf{x}|\mathbf{z}, \theta).$$

- Multiple augmentation for MMAP estimation, set:

$$f_\beta^{MMAP}(\theta, \mathbf{z}_1, \ldots, \mathbf{z}_\beta|\mathbf{x}) \propto \prod_{i=1}^{\beta} [\pi(\theta) f_Z(\mathbf{z}_i) f_X(\mathbf{x}|\mathbf{z}_i, \theta)]$$

- Then:

$$\begin{aligned} f_\beta^{MMAP}(\theta|\mathbf{x}) \propto & \int f_\beta^{MMAP}(\theta, \mathbf{z}_1, \ldots, \mathbf{z}_\beta|\mathbf{x}) d\mathbf{z}_1, \ldots d\mathbf{z}_\beta \\ & \propto \pi(\theta)^\beta f_X(\mathbf{x}|\theta)^\beta = f^{\text{post}}(\theta|\mathbf{x})^\beta \end{aligned}$$

Combining Data Augmentation and Simulated Annealing

- Consider

$$l(\theta; \mathbf{x}, \mathbf{z}) = f_{X,Z}(\mathbf{x}, \mathbf{z}|\theta) = f_Z(\mathbf{z}|\theta) f_X(\mathbf{x}|\mathbf{z}, \theta).$$

- Multiple augmentation for MMLE estimation, set:

$$f_\beta^{MMLE}(\theta, \mathbf{z}_1, \ldots, \mathbf{z}_\beta|\mathbf{x}) \propto \pi(\theta) \prod_{i=1}^{\beta} [f_Z(\mathbf{z}_i) f_X(\mathbf{x}|\mathbf{z}_i, \theta)]$$

- Then:

$$\begin{aligned} f_\beta^{MMLE}(\theta|\mathbf{x}) &\propto \int f_\beta^{MMLE}(\theta, \mathbf{z}_1, \ldots, \mathbf{z}_\beta|\mathbf{x}) d\mathbf{z}_1, \ldots d\mathbf{z}_\beta \\ &\propto \left[\pi(\theta)^{(1/\beta)} f_X(\mathbf{x}|\theta)\right]^\beta \approx l(\theta; \mathbf{x})^\beta \end{aligned}$$

under conditions on $\pi(\cdot)$ an *instrumental* prior.

State Augmentation for Maximisation of Expectations

Algorithm: SAME Gibbs Sampler

- Iteration 1: initialise $\theta^{(1)}$.
- For $t = 2, \ldots, T$:
  - For $k = 1, \ldots, \beta_t$, sample:

$$\mathbf{z}_k^{(t)} \sim f_Z(\mathbf{z}_k^{(t)} | x, \theta^{(t-1)})$$

  - Sample:

$$\theta^{(t)} \sim f_{(\beta_t)}^{\cdots}(\theta | \mathbf{x}, \mathbf{z}_1^{(t)}, \ldots, \mathbf{z}_{\beta_t}^{(t)})$$

A Toy Example — ML Estimation (1)

- Student t-distribution of unknown location parameter θ with 0.05 degrees of freedom. Four observations are available, $y = (-20, 1, 2, 3)$.
- Known marginal likelihood:

$$\log p(\mathbf{x}|\theta) = -0.525 \sum_{i=1}^{4} \log\left(0.05 + (x_i - \theta)^2\right)$$

- Augmented complete likelihood (student t is a scale mixture of normals):

$$\log p(\mathbf{x}, \mathbf{z}|\theta) = -\sum_{i=1}^{4} \left[0.475 \log z_i + 0.025 z_i + 0.5 z_i (x_i - \theta)^2\right]$$

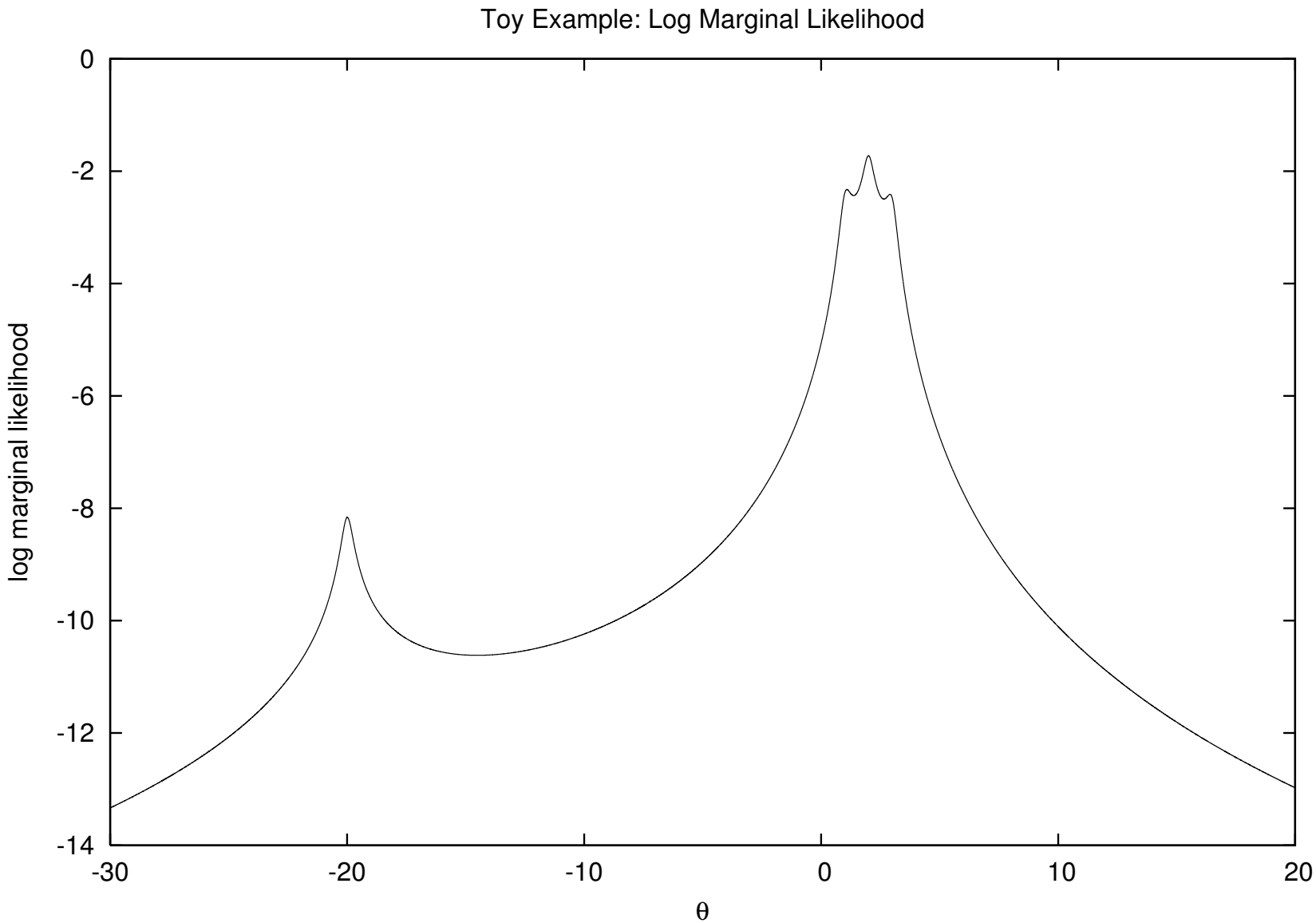
A Toy Example — ML Estimation (2)

$$p_{(\beta_t)}(\mathbf{z}_{1:\beta_t}|\theta,\mathbf{x}) = \prod_{i=1}^{\beta_t}\prod_{j=1}^{4} \text{Gamma}\left(z_{i,j}\left|0.525, 0.025+\frac{(x_j-\theta)^2}{2}\right.\right),$$

$$p_{(\beta_t)}(\theta|\mathbf{z}_{1:\beta_t}) \propto \mathcal{N}\left(\theta\left|\mu_t^{(\theta)}, \Sigma_t^{(\theta)}\right.\right),$$

where the parameters,

$$\Sigma_t^{(\theta)} = \left[\sum_{i=1}^{\beta_t}\sum_{j=1}^{4} z_{i,j}\right]^{-1} \qquad \mu_t^{(\theta)} = \Sigma_t^{(\theta)} \sum_{i=1}^{\beta_t} y^T z_i$$


Toy Example: Log Marginal Likelihood
log marginal likelihood
θ
0
-2
-4
-6
-8
-10
-12
-14
-30
-20
-10
0
10
20

Example: Gaussian Mixture Model — MAP Estimation (1)

- n iid observations, $x_1, \ldots, x_n$.
- Likelihood $f_{X,Z}(x_i, z_i|\omega, \mu, \sigma) = \omega_{z_i} \mathsf{N}(x_i|\mu_{z_i}, \sigma^2_{z_i})$.
- Marginal likelihood $f_X(x_i|\omega, \mu, \sigma) = \sum_{j=1}^{K} \omega_j \mathsf{N}(x_i|\mu_j, \sigma^2_j)$.
- Diffuse conjugate priors were employed:

$$\begin{aligned} \omega &\sim \mathsf{Dirichlet}(\chi, \ldots, \chi) \\ \sigma_i^2 &\sim \mathsf{IG}\left(\frac{\lambda_i + 3}{2}, \frac{b_i}{2}\right) \\ \mu_i|\sigma_i^2 &\sim \mathsf{N}(a_i, \sigma_i^2/\lambda_i) \end{aligned}$$

- All full conditional distributions of interest are available.
- Marginal posterior can be calculated...

Example: Gaussian Mixture Model — MAP Estimation (2)

SAME Iteration at step t:

- Sample:

$$\omega \leftarrow \text{Dirichlet}\left(\beta_t(\chi-1)+1+n_1(\beta_t), \ldots, \beta_t(\chi-1)+1+n_K(\beta_t)\right)$$

$$\sigma_i^2 \leftarrow \text{IG}(A_i, B_i)$$

$$\mu_i|\sigma_i^2 \leftarrow \text{Normal}\left(\frac{\beta_t\lambda_i a_i + \bar{\mathbf{x}}_i^{\beta_t}}{\beta_t\lambda_i + n_i^{\beta_t}}, \frac{\sigma_i^2}{\beta_t\lambda_i + n_i^{\beta_t}}\right)$$

where

$$n_i^{\beta_t} = \sum_{l=1}^{\beta_t}\sum_{p=1}^{n}\mathbb{I}_i(Z_{l,p}^{(t-1)}) \qquad \bar{\mathbf{x}}_i^{\beta_t} = \sum_{l=1}^{\beta_t}\sum_{p=1}^{n}\mathbb{I}_i(Z_{l,p}^{(t-1)})x_j$$

$$\overline{\mathbf{x}^2}_i^{\beta_t} = \sum_{l=1}^{\beta_t}\sum_{p=1}^{n}\mathbb{I}_i(Z_{l,p})x_j^2$$

- and

$$A_i = \frac{\beta_t(\lambda_i + 1) + n_i^{\beta_t}}{2} + 1$$

$$B_i = \frac{1}{2}\left(\beta_t(b_i + \lambda_i a_i^2) + \bar{\mathbf{x}^2}_i^{\beta_t} - \sum_{g=1}^{\beta_t} \frac{(\bar{\mathbf{x}}_i^g - \bar{\mathbf{x}}_i^{g-1} + \lambda_i a_i)^2}{\lambda_i + n_i^g - n_i^{g-1}}\right)$$

- Sample, for $j = 1, \ldots, \beta_t$:

$$\mathbf{z}_j^{(t)} \sim f^{\text{posterior}}(\mathbf{z}|\mathbf{x}, \pi^{(t)}, \sigma^{(t)}, \mu^{(t)})$$

Some Results at Last: Simulated Data

Algorithm	T	Cost	Mean	Std. Dev.	Min	Max
EM	500	500	-158.06	3.23	-166.39	-153.85
EM	5000	5000	-157.73	3.83	-165.81	-153.83
SAME(6)	4250	8755	-155.32	0.87	-157.35	-154.03
SAME(50)	4250	112522	-155.05	0.82	-156.11	-153.98

SAME(6) set $\beta_t = 1$ for the first half of the iterations and then increasing linearly to a final maximum value of 6.

SAME(50) set $\beta_t = 1$ for the first 250 iterations, and then increasing linearly to 50

True parameters The log posterior density of the generating parameters was -155.87.

$$\pi = [0.2, 0.3, 0.5] \quad \mu = [0, 2, 3] \quad \text{and } \sigma = \left[1, \frac{1}{4}, \frac{1}{16}\right].$$

Some Results at Last: Galaxy Data

Algorithm	T	**Cost**	**Mean**	**Std. Dev.**	**Min**	**Max**
EM	500	500	-46.54	2.92	-54.12	-44.32
EM	5000	5000	-46.91	3.00	-56.68	-44.34
SAME(6)	4250	8755	-45.18	0.54	-46.61	-44.17
SAME(50)	4250	112522	-44.93	0.21	-45.52	-44.47

SAME(6) set $\beta_t = 1$ for the first half of the iterations and then increasing linearly to a final maximum value of 6.

SAME(50) set $\beta_t = 1$ for the first 250 iterations, and then increasing linearly to 50

Variant a more sophisticated algorithm suggests that -43.96 ± 0.03 is about optimal.

Part 4— Section 14

Recent Innovations

Bayesian Computation (Towards ABC)

- Consider a target distribution $f_{\mathbf{X}|\mathbf{Y}}(\mathbf{x}|\mathbf{y})$ written as:

$$f_{\mathbf{X}|\mathbf{Y}}(\mathbf{x}|\mathbf{y}) = \frac{f_{\mathbf{Y}|\mathbf{X}}(\mathbf{y}|\mathbf{x})f_{\mathbf{X}}(\mathbf{x})}{f_{\mathbf{Y}}(\mathbf{y})}.$$

- If both $f_{\mathbf{X}}(\mathbf{x})$ and $f_{\mathbf{Y}|\mathbf{X}}(\mathbf{y}|\mathbf{x})$ can be evaluated we're done.
- If we *cannot* evaluate $f_{\mathbf{Y}|\mathbf{X}}$ even pointwise, then we *can't* directly use the techniques which we've described previously.
- Consider the case in which $\mathbf{Y}$ is *discrete*.
- We can invoke a clever data augmentation trick which requires only that we can *sample* from $f_{\mathbf{Y}|\mathbf{X}}$.

- We can define an extended distribution:

$$f_{\mathbf{X},\mathbf{Z}|\mathbf{Y}}(\mathbf{x},\mathbf{z}|\mathbf{y}) \propto f_{\mathbf{Y}|\mathbf{X}}(\mathbf{z}|\mathbf{x}) f_{\mathbf{X}}(\mathbf{x}) \delta_{\mathbf{y},\mathbf{z}}$$

  and note that it has, as a marginal distribution, our target:

$$\sum_{\mathbf{z}} f_{\mathbf{X},\mathbf{Z}|\mathbf{Y}}(\mathbf{x},\mathbf{z}|\mathbf{y}) \propto \sum_{\mathbf{z}} f_{\mathbf{Y}|\mathbf{X}}(\mathbf{z}|\mathbf{x}) f_{\mathbf{X}}(\mathbf{x}) \delta_{\mathbf{y},\mathbf{z}} = f_{\mathbf{Y}|\mathbf{X}}(\mathbf{y}|\mathbf{x}) f_{\mathbf{X}}(\mathbf{x}).$$

- We can sample $(\mathbf{X},\mathbf{Z}) \sim f_{\mathbf{Y}|\mathbf{X}}(\mathbf{z}|\mathbf{x}) f_{\mathbf{X}}(\mathbf{x})$ and use this as a rejection sampling proposal for our target distribution, keeping samples with probability proportional to

$$f_{\mathbf{X},\mathbf{Z}|\mathbf{Y}}(\mathbf{x},\mathbf{z}|\mathbf{y}) / f_{\mathbf{Y}|\mathbf{X}}(\mathbf{z}|\mathbf{x}) f_{\mathbf{X}}(\mathbf{x}) \propto \delta_{\mathbf{y},\mathbf{z}}$$

Approximate Bayesian Computation

- When data is not discrete / takes many values, exact matches have no or negligible probability.
- Instead, we keep samples for which $||\mathbf{z} - \mathbf{y}|| \leq \epsilon$.
- This leads to a *different* target distribution:

$$f^{\text{ABC}}_{\mathbf{X},\mathbf{Z}|\mathbf{Y}} \propto f_{\mathbf{Y}|\mathbf{X}}(\mathbf{z}|\mathbf{x}) f_{\mathbf{X}}(\mathbf{x}) \mathbb{I}_{B(\mathbf{y},\epsilon)}(\mathbf{z})$$

where $B(\mathbf{y}, \epsilon) := \{\mathbf{x} : |\mathbf{x} - \mathbf{y}| \leq \epsilon\}$, so

$$\begin{aligned} f^{\text{ABC}}_{\mathbf{x}|\mathbf{Y}} &\propto \int f_{\mathbf{Y}|\mathbf{X}}(\mathbf{z}|\mathbf{x}) f_{\mathbf{X}}(\mathbf{x}) \mathbb{I}_{B(\mathbf{y},\epsilon)}(\mathbf{z}) d\mathbf{z} \\ &\propto \int f_{\mathbf{Y}|\mathbf{X}}(\mathbf{z}|\mathbf{x}) \mathbb{I}_{B(\mathbf{y},\epsilon)}(\mathbf{z}) d\mathbf{z} f_{\mathbf{X}}(\mathbf{x}) \\ &\propto \int_{\mathbf{z} \in B(\mathbf{y},\epsilon)} f_{\mathbf{Y}|\mathbf{X}}(\mathbf{z}|\mathbf{x}) d\mathbf{z} f_{\mathbf{X}}(\mathbf{x}) \end{aligned}$$

this approximation amounts to a *smoothing* of the likelihood function.

Even More Approximate Bayesian Computation

- Often a further approximation is introduced by considering not the data itself but some low dimensional summary of the data: This leads to a *different* target distribution:

$$f^{\text{ABC}}_{\mathbf{X},\mathbf{Z}|\mathbf{Y}} \propto f_{\mathbf{Y}|\mathbf{X}}(\mathbf{z}|\mathbf{x}) f_{\mathbf{X}}(\mathbf{x}) \mathbb{I}_{B(s(\mathbf{y}),\epsilon)}(s(\mathbf{z}))$$

- Unless the summary is a sufficient statistic (which it probably isn't) this introduces a difficult to understand approximation.
- Be very careful.

Pseudomarginal methods can also be considered as augmentation techniques, but we don't have enough time to do that here.

Part 5

Theory and Practice

Part 5— Section 15

Theoretical Considerations and Convergence Results

Some reassurance about Gibbs Samplers

Definition (Positivity condition)

A distribution with density $f(x_1, \ldots, x_p)$ *and marginal densities* $f_{X_i}(x_i)$ *is said to satisfy the positivity condition if* $f(x_1, \ldots, x_p) > 0$ *for all* $x_1, \ldots, x_p$ *with* $f_{X_i}(x_i) > 0$.

Theorem (Hammersley-Clifford)

Let $(X_1, \ldots, X_p)$ *satisfy the positivity condition and have joint density* $f(x_1, \ldots, x_p)$. *Then for all* $(\xi_1, \ldots, \xi_p) \in supp(f)$

$$f(x_1, \ldots, x_p) \propto \prod_{j=1}^{p} \frac{f_{X_j|X_{-j}}(x_j|x_1, \ldots, x_{j-1}, \xi_{j+1}, \ldots, \xi_p)}{f_{X_j|X_{-j}}(\xi_j|x_1, \ldots, x_{j-1}, \xi_{j+1}, \ldots, \xi_p)}$$

A Cautionary Example

Note the theorem does *not* guarantee the existence of a joint distribution for every set of "full conditionals"!

- Consider the following "model"

$$\begin{aligned} X_1|X_2 &\sim \text{Expo}(\lambda X_2) \\ X_2|X_1 &\sim \text{Expo}(\lambda X_1), \end{aligned}$$

- Trying to apply the Hammersley-Clifford theorem, we obtain

$$\begin{aligned} f(x_1, x_2) &\propto \frac{f_{X_1|X_2}(x_1|\xi_2) \cdot f_{X_2|X_1}(x_2|x_1)}{f_{X_1|X_2}(\xi_1|\xi_2) \cdot f_{X_2|X_1}(\xi_2|x_1)} \\ &\propto \exp(-\lambda x_1 x_2) \end{aligned}$$

- $\int \int \exp(-\lambda x_1 x_2)\, dx_1\, dx_2 = +\infty$
  $\rightsquigarrow$ joint density cannot be normalised.
- There is no joint density with the above full conditionals.

Irreducibility and recurrence of Gibbs Samplers

Proposition

If the joint distribution $f(x_1, \ldots, x_p)$ satisfies the positivity condition, the Gibbs sampler yields an f-irreducible, recurrent Markov chain.

Outline Proof

Given an $\mathcal{X}$ such that $\int_{\mathcal{X}} f(x_1^{(t)}, \ldots, x_p^{(t)}) d(x_1^{(t)}, \ldots, x_p^{(t)}) > 0$.

$$\int_{\mathcal{X}} K(\mathbf{x}^{(t-1)}, \mathbf{x}^{(t)}) d\mathbf{x}^{(t)} = \int_{\mathcal{X}} \underbrace{f_{X_1|X_{-1}}(x_1^{(t)}|x_2^{(t-1)}, \ldots, x_p^{(t-1)})}_{>0} \cdots$$

$$\underbrace{f_{X_p|X_{-p}}(x_p^{(t)}|x_1^{(t)}, \ldots, x_{p-1}^{(t)})}_{>0} d\mathbf{x}^{(t)}$$

Ergodic theorem

Theorem (Ergodicity of the Gibbs Sampler)

If the Markov chain generated by the Gibbs sampler is irreducible and recurrent (which is e.g. the case when the positivity condition holds), then for any integrable function $\varphi : E \to \mathbb{R}$

$$\lim_{n\to\infty} \frac{1}{n} \sum_{t=1}^{n} \varphi(\mathbf{X}^{(t)}) \to \mathbb{E}_f\left(\varphi(\mathbf{X})\right)$$

for almost every starting value $\mathbf{X}^{(0)}$.

Thus we can approximate expectations $\mathbb{E}_f\left(\varphi(\mathbf{X})\right)$ by their empirical counterparts using *a single* Markov chain.

A Simple Example

- Consider

$$\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \sim \mathsf{N}_2 \left(\begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \begin{pmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{pmatrix} \right)$$

- Associated marginal distributions

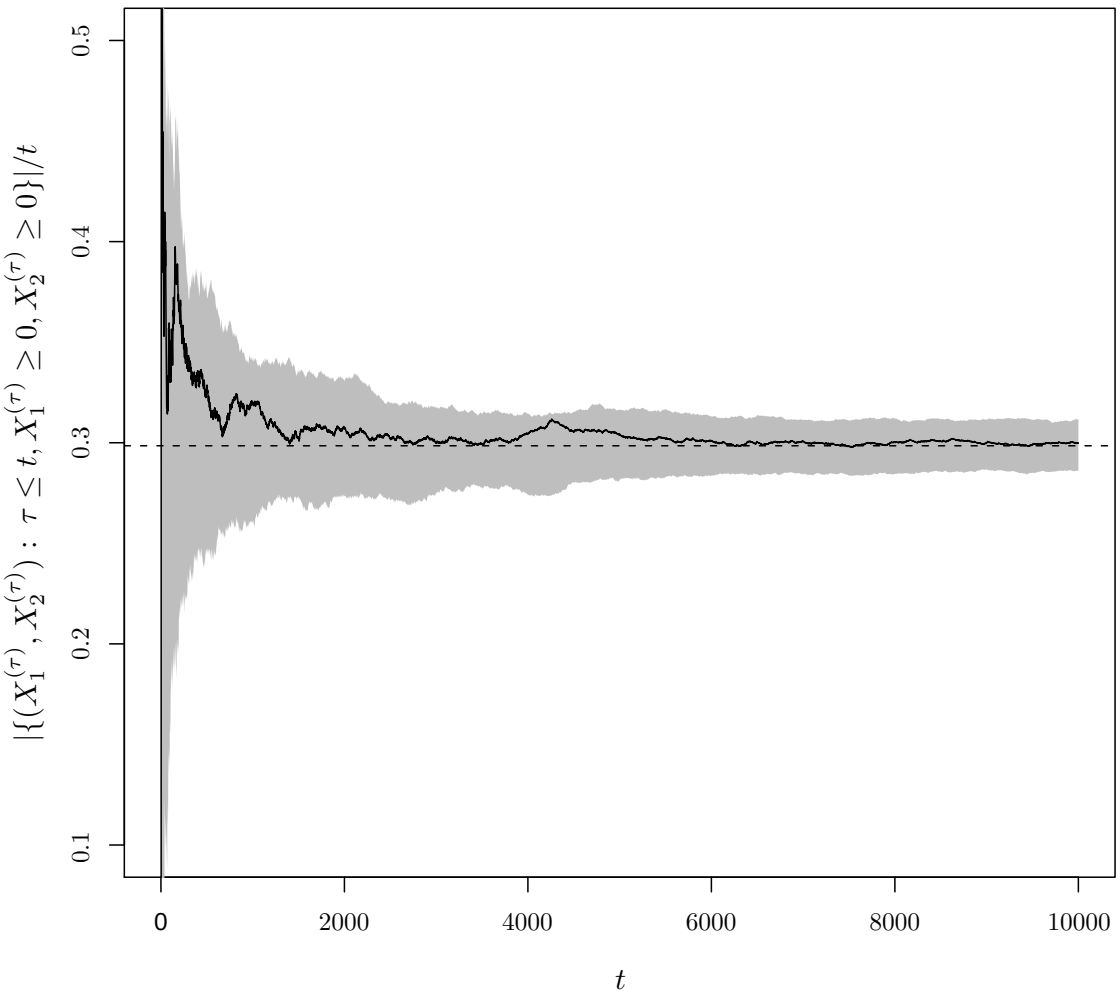
$$\begin{aligned} X_1 &\sim \mathsf{N}(\mu_1, \sigma_1^2) \\ X_2 &\sim \mathsf{N}(\mu_2, \sigma_2^2) \end{aligned}$$

- Associated full conditionals

$$\begin{aligned} X_1 | X_2 = x_2 &\sim \mathsf{N}(\mu_1 + \sigma_{12}/\sigma_2^2(x_2 - \mu_2), \sigma_1^2 - (\sigma_{12})^2\sigma_2^2) \\ X_2 | X_1 = x_1 &\sim \mathsf{N}(\mu_2 + \sigma_{12}/\sigma_1^2(x_1 - \mu_1), \sigma_2^2 - (\sigma_{12})^2\sigma_1^2) \end{aligned}$$

- Gibbs sampler consists of iterating for $t = 1, 2, \ldots$
  1. Draw $X_1^{(t)} \sim \mathsf{N}(\mu_1 + \sigma_{12}/\sigma_2^2(X_2^{(t-1)} - \mu_2), \sigma_1^2 - (\sigma_{12})^2\sigma_2^2)$
  2. Draw $X_2^{(t)} \sim \mathsf{N}(\mu_2 + \sigma_{12}/\sigma_1^2(X_1^{(t)} - \mu_1), \sigma_2^2 - (\sigma_{12})^2\sigma_1^2)$.

Using the ergodic theorem we can estimate $\mathbb{P}(X_1 \geq 0, X_2 \geq 0)$ by the proportion of samples $(X_1^{(t)}, X_2^{(t)})$ with $X_1^{(t)} \geq 0$ and $X_2^{(t)} \geq 0$:



Theoretical properties of Metropolis-Hastings

- The Markov chain $(\mathbf{X}^{(0)}, \mathbf{X}^{(1)}, \ldots)$ is (strongly) irreducible if $q(\mathbf{x}|\mathbf{x}^{(t-1)}) > 0$ for all $\mathbf{x}, \mathbf{x}^{(t-1)} \in \text{supp}(f)$.
  (see, e.g.,(see Roberts & Tweedie, 1996) for weaker conditions)
- Such a chain is recurrent if it is irreducible.
  (see e.g. Tierney, 1994)
- The chain is aperiodic if there is positive probability that the chain remains in the current state, i.e. $\mathbb{P}(\mathbf{X}^{(t)} = \mathbf{X}^{(t-1)}) > 0$
  (for a suitable group of "current states").

Theorem (A Simple Ergodic Theorem)

If $(X_i)_{i\in\mathbb{N}}$ is an f-irreducible, f-invariant, recurrent $\mathbb{R}^d$-valued Markov chain then the following strong law of large numbers holds for any integrable function $\varphi : \mathbb{R}^d \to \mathbb{R}$:

$$\lim_{t\to\infty} \frac{1}{t} \sum_{i=1}^{t} \varphi(\xi_i) \overset{a.s.}{=} \int \varphi(x) f(x) dx.$$

for almost every starting value x.

Theorem (A Central Limit Theorem)

Under technical regularity conditions the following CLT holds for a recurrent, f-invariant Markov chain, and a function $\varphi : E \to \mathbb{R}$ which has at least two finite moments:

$$\lim_{t\to\infty} \sqrt{t}\left[\frac{1}{t}\sum_{i=1}^{t}\varphi(\xi_i) - \int \varphi(x)\mu(x)dx\right] \stackrel{\mathcal{D}}{=} N\left(0, \sigma^2(\varphi)\right),$$

$$\sigma^2(\varphi) = \mathbb{E}\left[(f(\xi_1) - \bar{\varphi})^2\right] + 2\sum_{k=2}^{\infty}\mathbb{E}\left[(\varphi(\xi_1) - \bar{\varphi})(\varphi(\xi_k) - \bar{\varphi})\right],$$

where $\bar{\varphi} = \int \varphi(x)f(x)dx$.

Optimal Scaling

Much effort has gone into determining optimal scaling rules:

Diffusion Limits Under strong assumptions:

$$\lim_{p\to\infty} \frac{X_1^{(\lfloor tp \rfloor)}}{\sqrt{p}} \xrightarrow{d} \text{Diffusion}$$

where p is *dimension* and the *speed* of the diffusion depends upon proposal scale.

ESJD Seek to maximise:

$$\int f(x)K(x,y;\theta)(y-x)^2 dxdy$$

Rule of Thumb Optimal RWM Scaling depends upon dimension:

- $p = 1$ Acceptance rate of around 0.44.
- $p \geq 5$ Acceptance rate of around 0.234.

The Metropolis-Adjusted Langevin Algorithm

- Based on the Langevin diffusion:

$$d\mathbf{X}_t = \frac{1}{2}\nabla \log(f(\mathbf{X}_t))dt + d\mathbf{B}_t$$

  which is f-invariant *in continuous time*.
- Given target f the MALA proposal proposes:

$$\mathbf{X} \leftarrow \mathbf{X}^{(t-1)} + \epsilon$$
$$\epsilon \sim \mathsf{N}\left(\frac{\sigma^2}{2}\nabla \log f(\mathbf{X}^{(t-1)}), \sigma^2 I_p\right)$$

  at time t.
- Accepts X with the usual MH acceptance probability.
- Optimal acceptance rate (under similar strong conditions) now 0.574.

MALA Example: Normal (1)

Target $f(x) = \mathsf{N}(0, 1)$

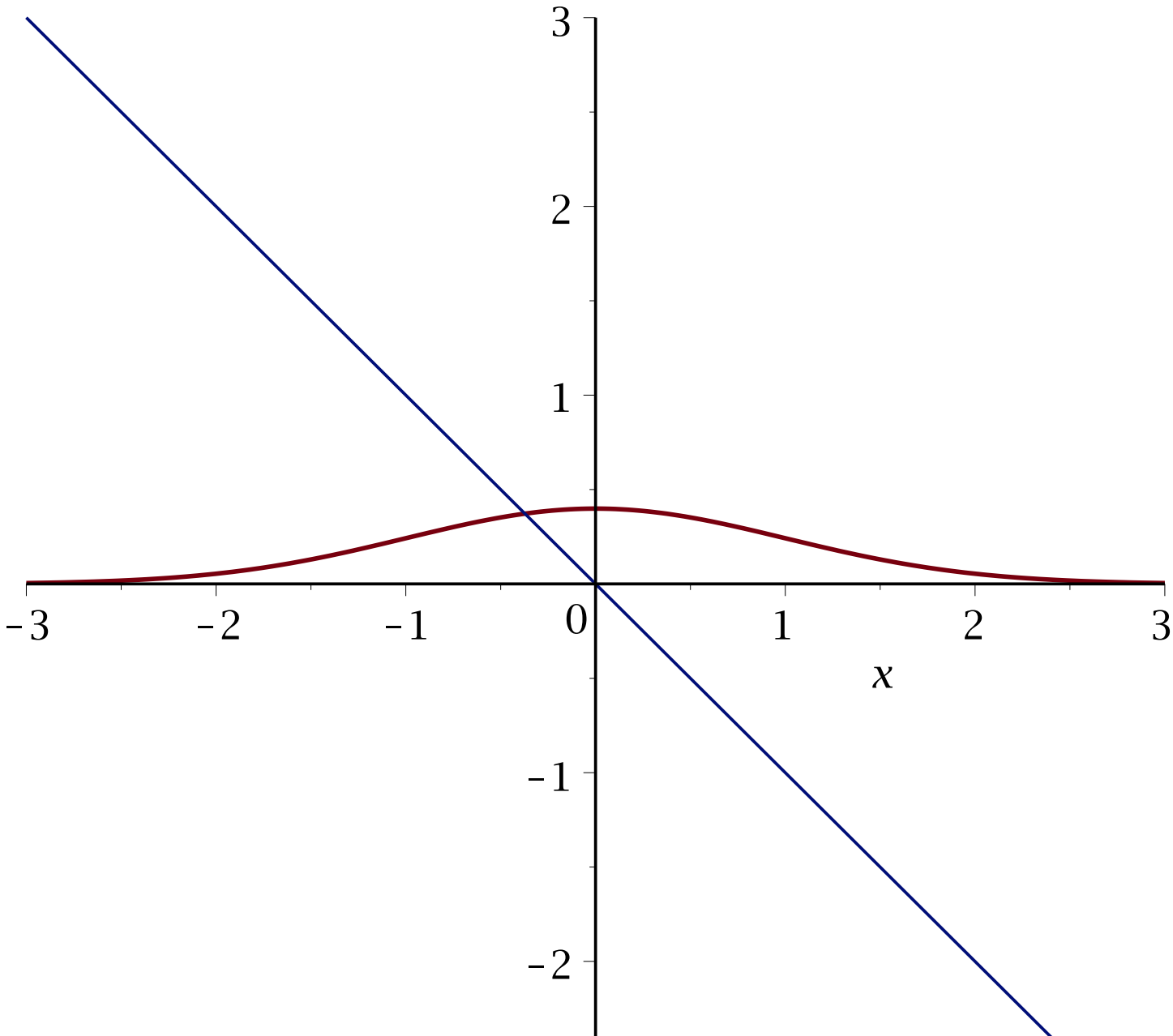
Proposal

$$q(X^{(t-1)}, X) = \mathsf{N}\left(X^{(t-1)} - \frac{\sigma^2 X^{(t-1)}}{2}, \sigma^2\right)$$

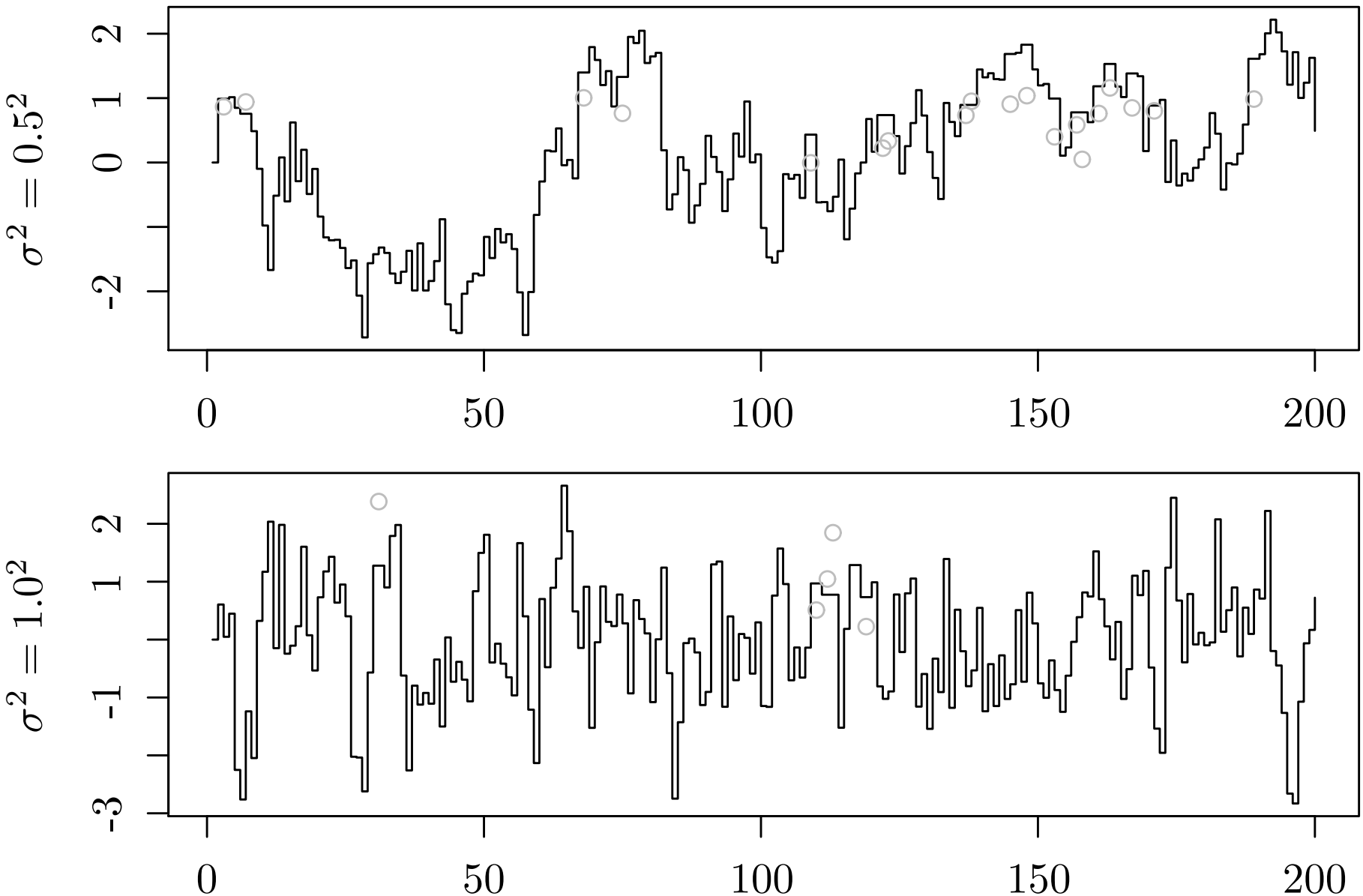
Acceptance Probability

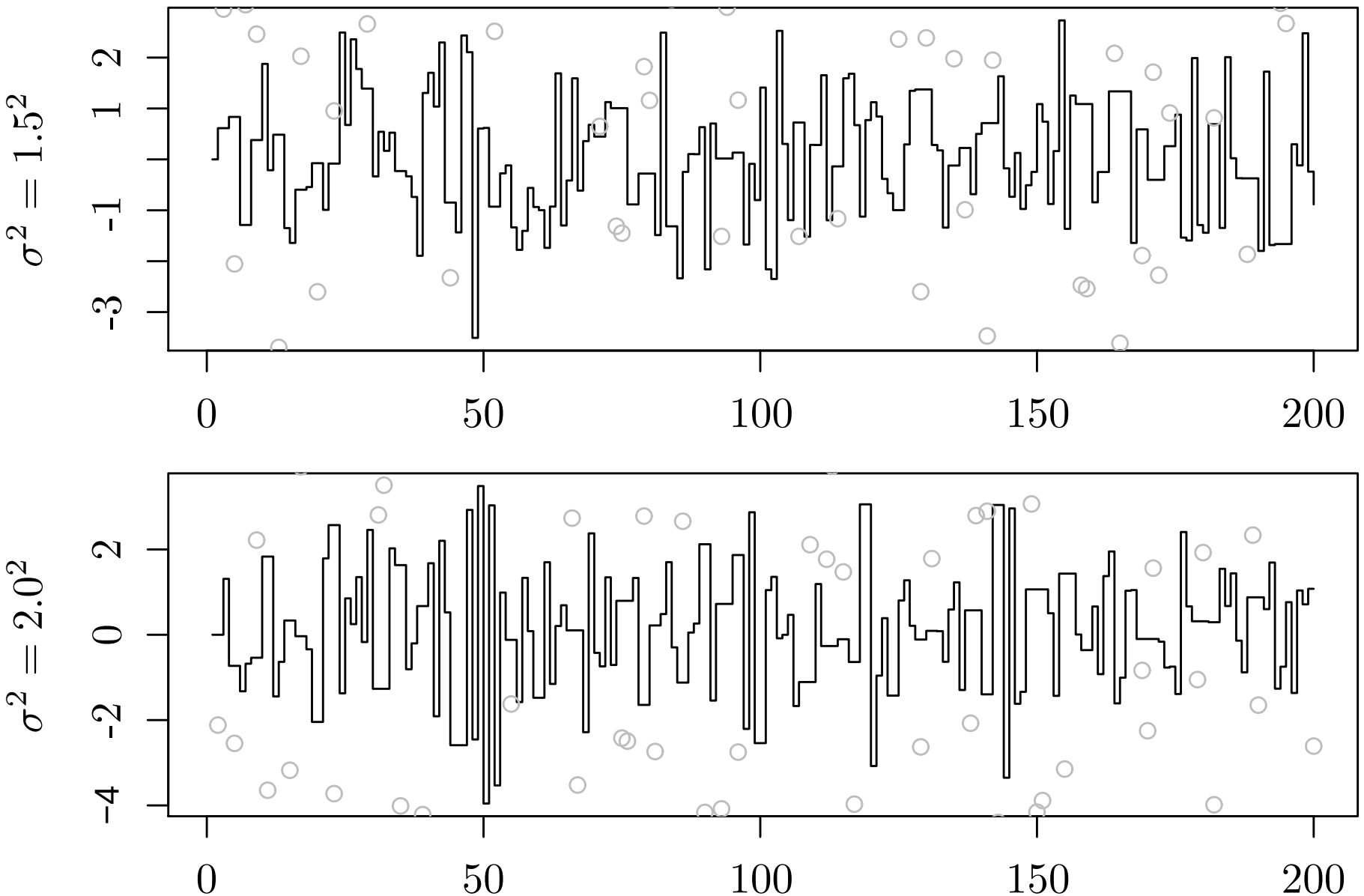
$$\begin{aligned}\alpha(X^{(t-1)}, X) =& 1 \wedge \frac{f(X)}{f(X^{(t-1)})} \frac{q(X, X^{(t-1)})}{q(X^{(t-1)}, X)} \\ =& 1 \wedge \exp\left(\frac{1}{2}\left[(X^{(t-1)})^2 - X^2\right]\right) \times \\ & \exp\left(\frac{1}{2\sigma^2}\left[\left\{X - \mu(X^{(t-1)})\right\}^2 - \left\{X^{(t-1)} - \mu(X)\right\}^2\right]\right)\end{aligned}$$

where $\mu(x) := x - \frac{x\sigma^2}{2}$.


3
2
1
-1
-2
-3
-2
-1
0
1
2
3
x

Scaling of Proposal Distributions




$\sigma^2 = 1.5^2$
-3
-1
1
2
0
50
100
150
200
$\sigma^2 = 2.0^2$
-4
-2
0
2
0
50
100
150
200

MALA Example: Normal (2)

RWM	Autocorrelation $\rho(X^{(t-1)}, X^{(t)})$	Probability of acceptance $\alpha(X, X^{(t-1)})$	ESJD
$\sigma^2 = 0.1^2$	0.9901	0.9694	0.010
$\sigma^2 = 1$	0.7733	0.7038	0.448
$\sigma^2 = 2.38^2$	0.6225	0.4426	0.742
$\sigma^2 = 10^2$	0.8360	0.1255	0.337

MALA	Autocorrelation $\rho(X^{(t-1)}, X^{(t)})$	Probability of acceptance $\alpha(X, X^{(t-1)})$	ESJD
$\sigma^2 = 0.5^2$	0.898	0.877	0.246
$\sigma^2 = 1$	0.492	0.961	1.293
$\sigma^2 = 1.5^2$	0.047	0.774	2.137
$\sigma^2 = 2.0^2$	0.011	0.631	4.119

Part 5— Section 16

Convergence Diagnostics

The need for convergence diagnostics

- Theory guarantees (under certain conditions) the convergence of the Markov chain $\mathbf{X}^{(t)}$ to the desired distribution.
- This does not imply that a *finite* sample from such a chain yields a good approximation to the target distribution.
- Validity of the approximation must be confirmed in practice.
- Convergence diagnostics help answering this question.
- Convergence diagnostics are *not* perfect and should be treated with a good amount of scepticism.

Different diagnostic tasks

Convergence to the target distribution Does $\mathbf{X}^{(t)}$ yield a sample from the target distribution?

- Has reached $(\mathbf{X}^{(t)})_t$ a stationary regime?
- Does $(\mathbf{X}^{(t)})_t$ cover the support of the target distribution?

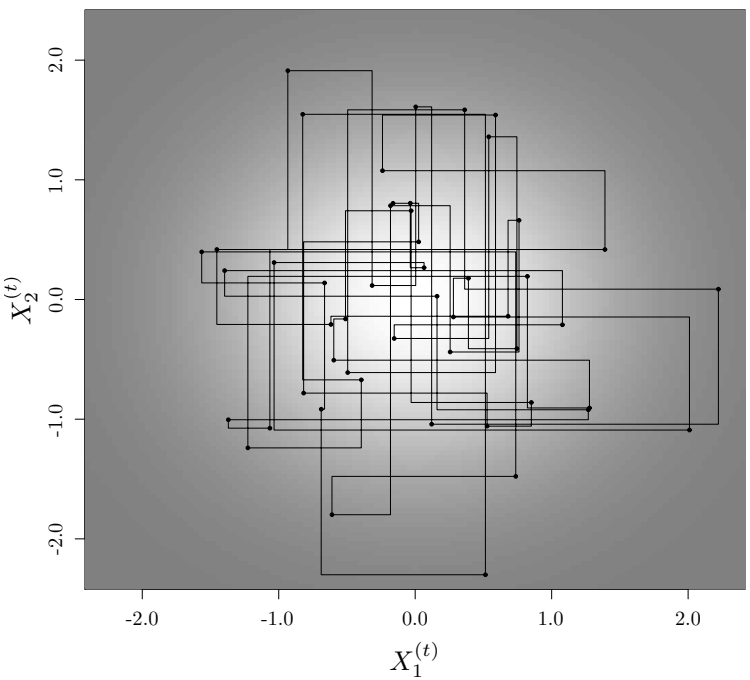
Convergence of averages Is $\sum_{t=1}^{T} \varphi(\mathbf{X}^{(t)})/T \approx \mathbb{E}_f(\varphi(\mathbf{X}))$?

Comparison to i.i.d. sampling How much information is contained in the sample from the Markov chain compared to an i.i.d. sample?

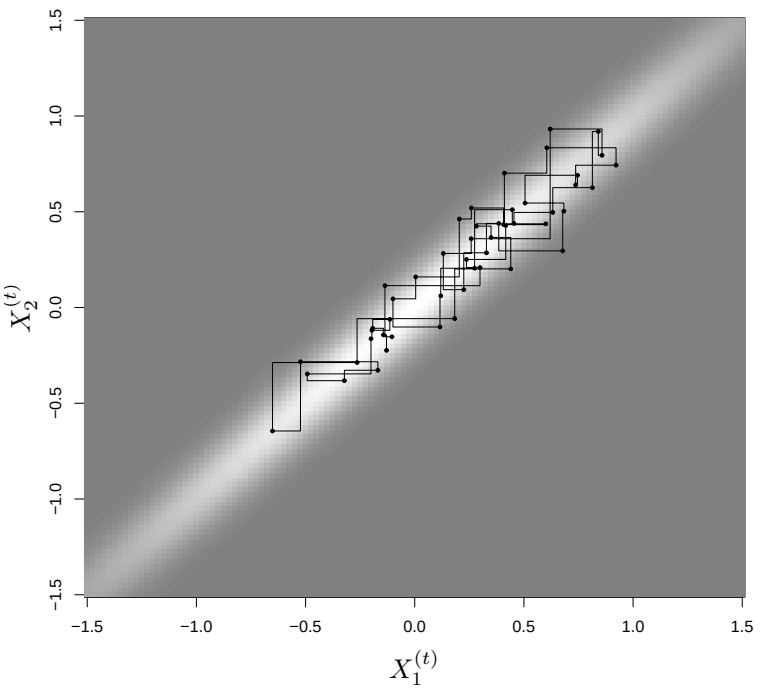
Pathological example 1: potentially slowly mixing

Gibbs sampler from a bivariate Gaussian with correlation $\rho(X_1, X_2)$

$\rho(X_1, X_2) = 0.3$



$\rho(X_1, X_2) = 0.99$



For correlations $\rho(X_1, X_2)$ close to ± 1 the chain can be poorly mixing.

Pathological example 2: no central limit theorem

The following MCMC algorithm has the Beta$(\alpha, 1)$ distribution as stationary distribution:

Starting with any $X^{(0)}$ iterate for $t = 1, 2, \ldots$

1. With probability $1 - X^{(t-1)}$, set $X^{(t)} = X^{(t-1)}$.
2. Otherwise draw $X^{(t)} \sim \text{Beta}(\alpha + 1, 1)$.

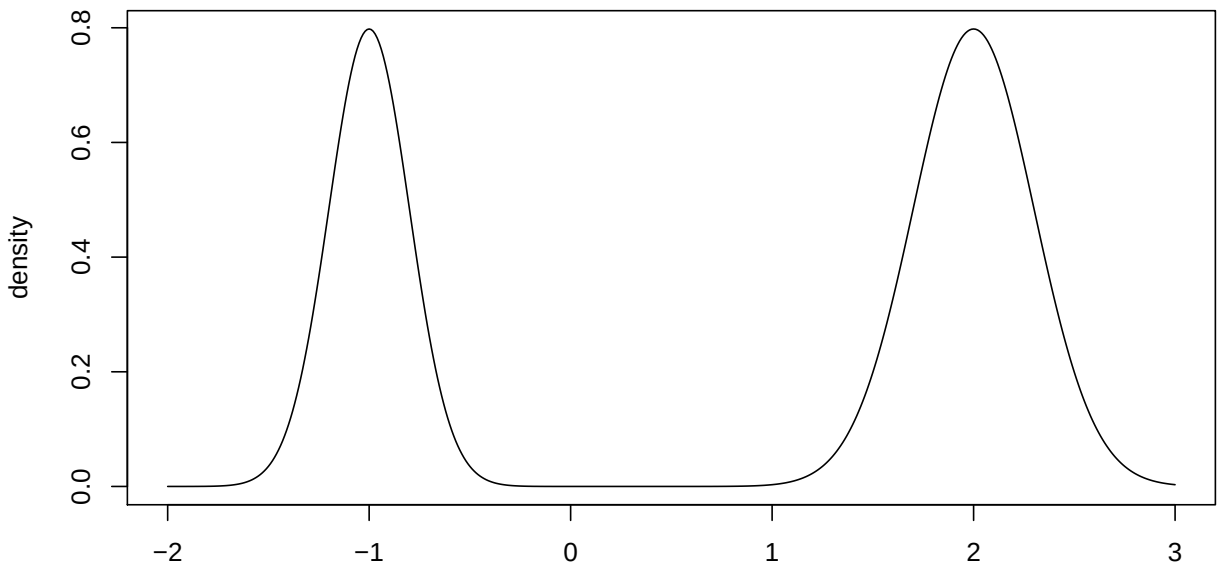
Markov chain converges very slowly (no central limit theorem applies).

Pathological example 3: nearly reducible chain

Metropolis-Hastings sample from a mixture of two well-separated Gaussians, i.e. the target is

$$f(x) = 0.4 \cdot \phi_{(-1,0.2^2)}(x) + 0.6 \cdot \phi_{(2,0.3^2)}(x)$$

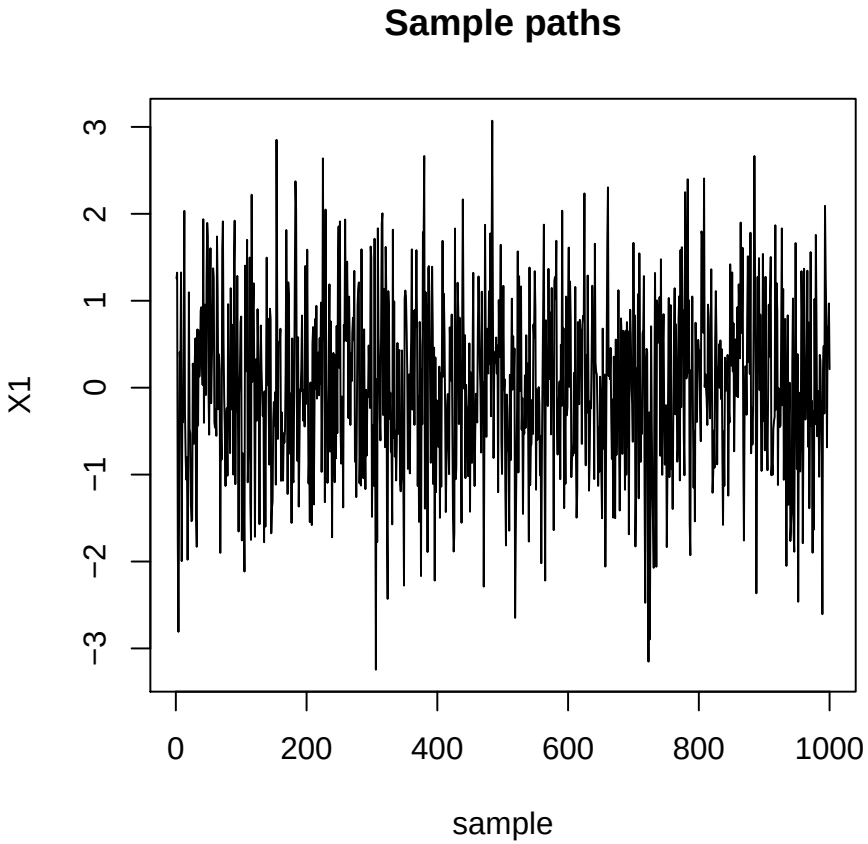
If the variance of the proposal is too small, the chain cannot move from one population to the other.

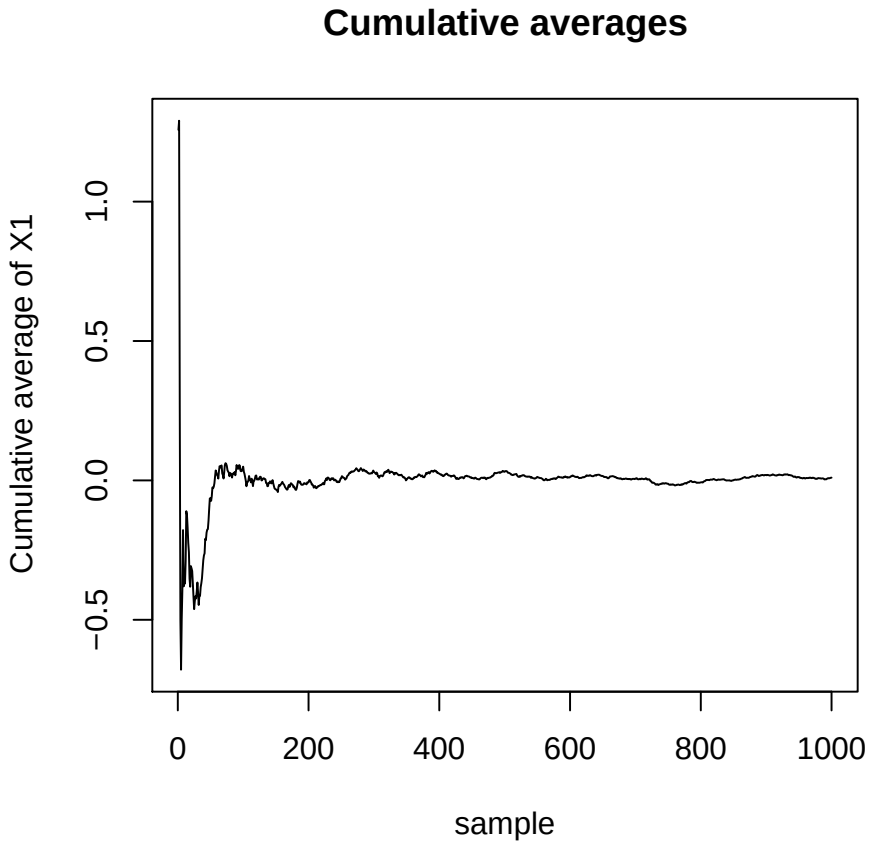


Basic plots

- Plot the sample paths $(X_j^{(t)})_t$.
  should be oscillating very fast and show very little structure.
- Plot the cumulative averages $(\sum_{\tau=1}^{t} X_j^{(\tau)}/t)_t$.
  should be converging to a value.
- Alternatively plot CUSUM $(\bar{X}_j - \sum_{\tau=1}^{t} X_j^{(\tau)}/t)_t$ with $\bar{X}_j = \sum_{\tau=1}^{T} X_j^{(\tau)}/T$.
  should be converging to 0.
- Only very obvious problems visible in these plots.
- Difficult to assess multivariate distributions from univariate projections.

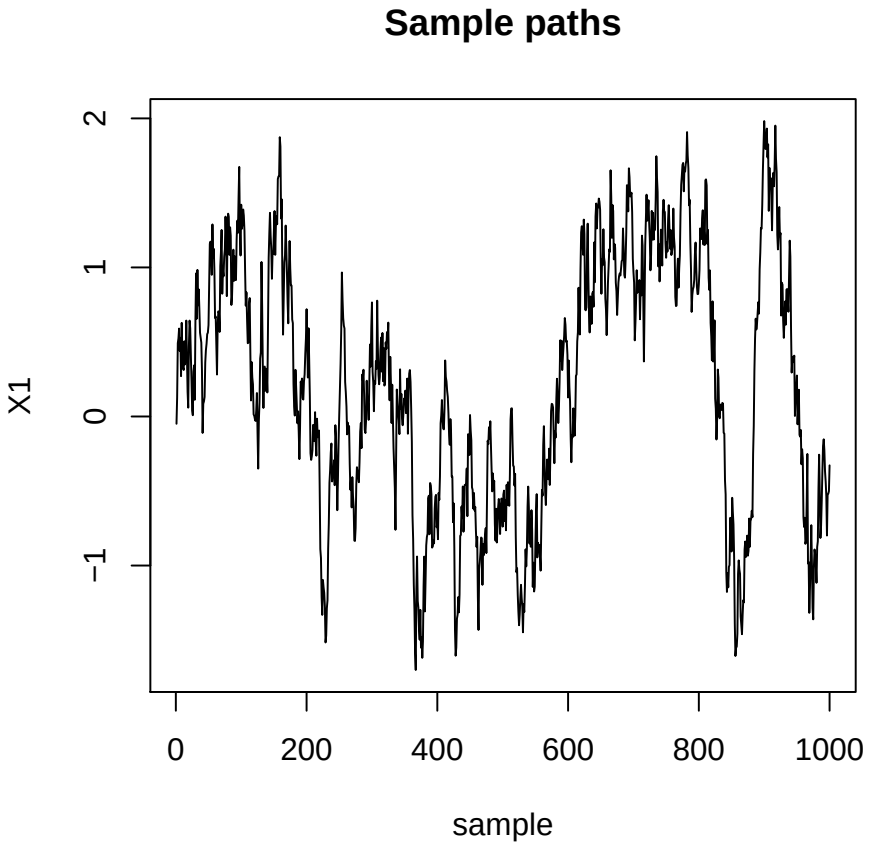
Basic plots for pathological example 1 ($\rho(X_1, X_2) = 0.3$)

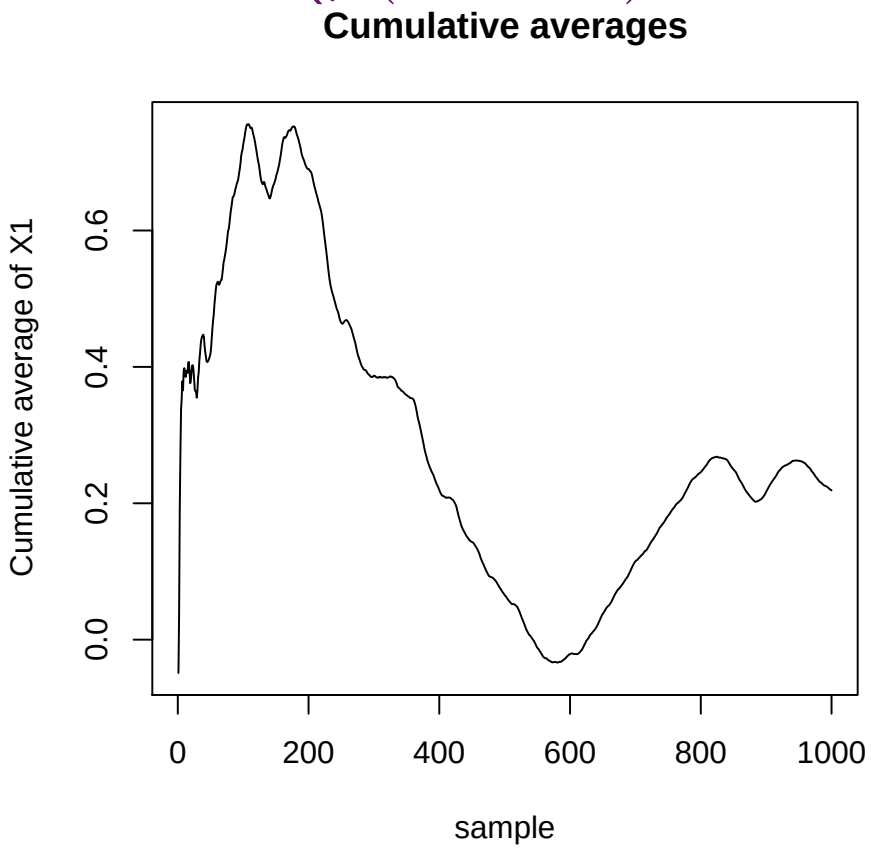




Looks OK.

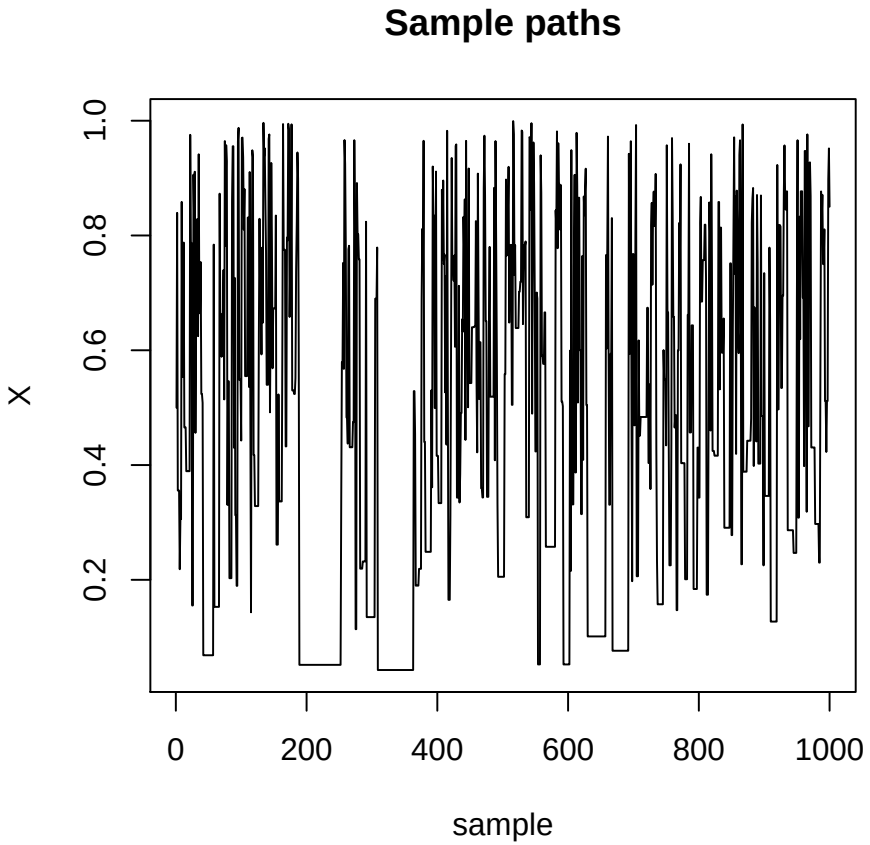
Basic plots for pathological example 1 ($\rho(X_1, X_2) = 0.99$)

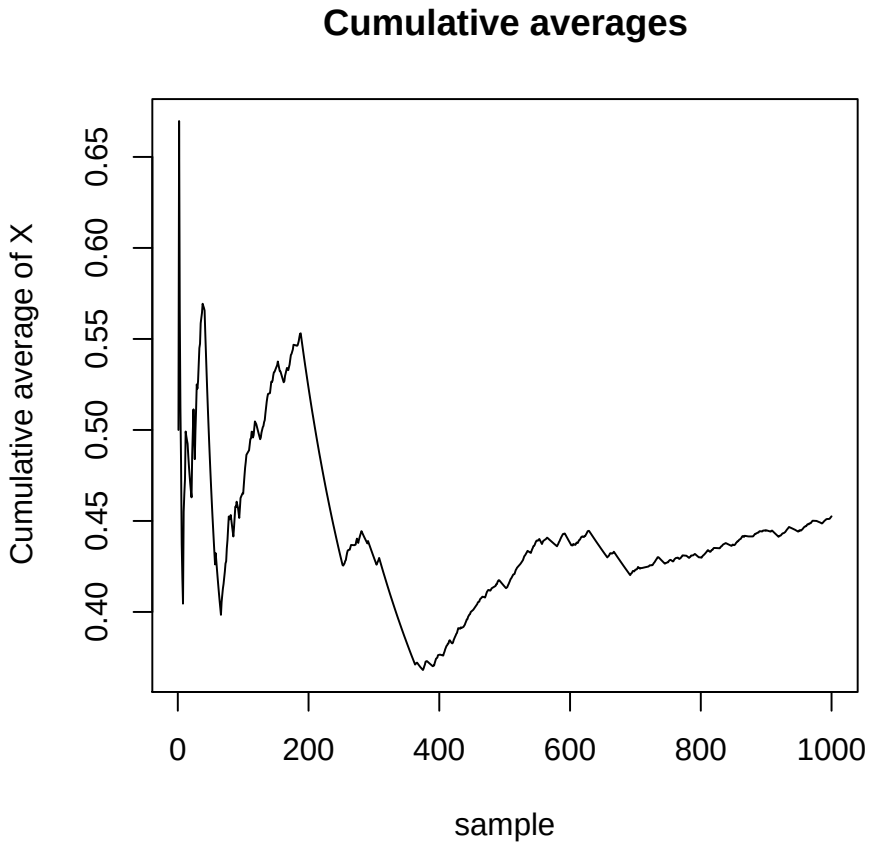




Slow mixing speed can be detected.

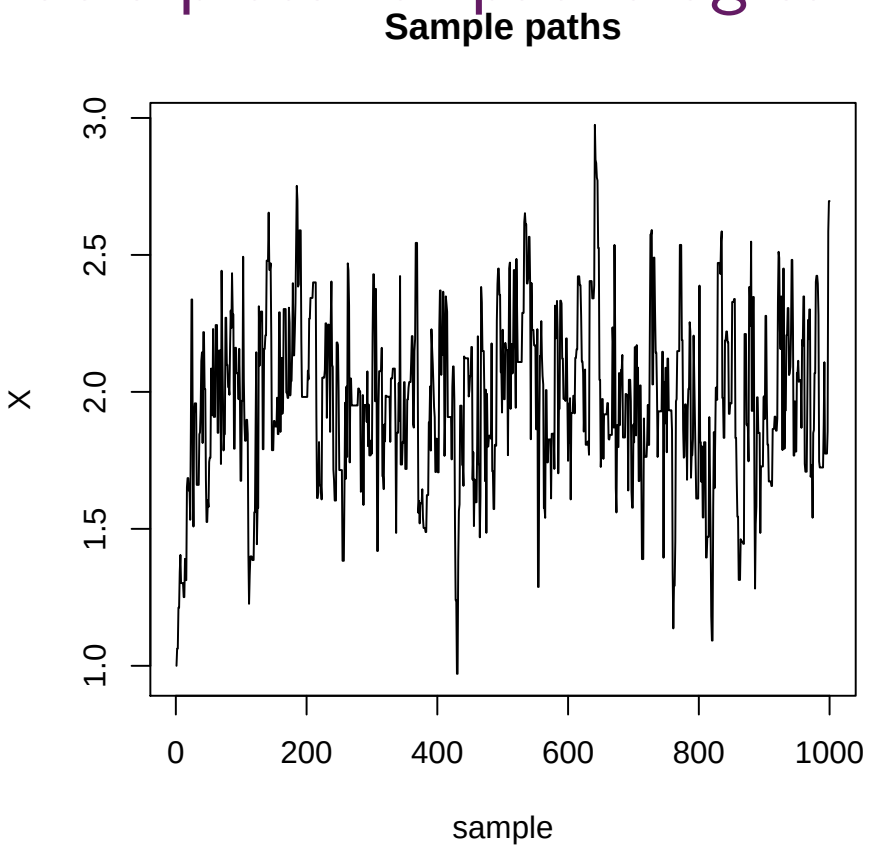
Basic plots for pathological example 2

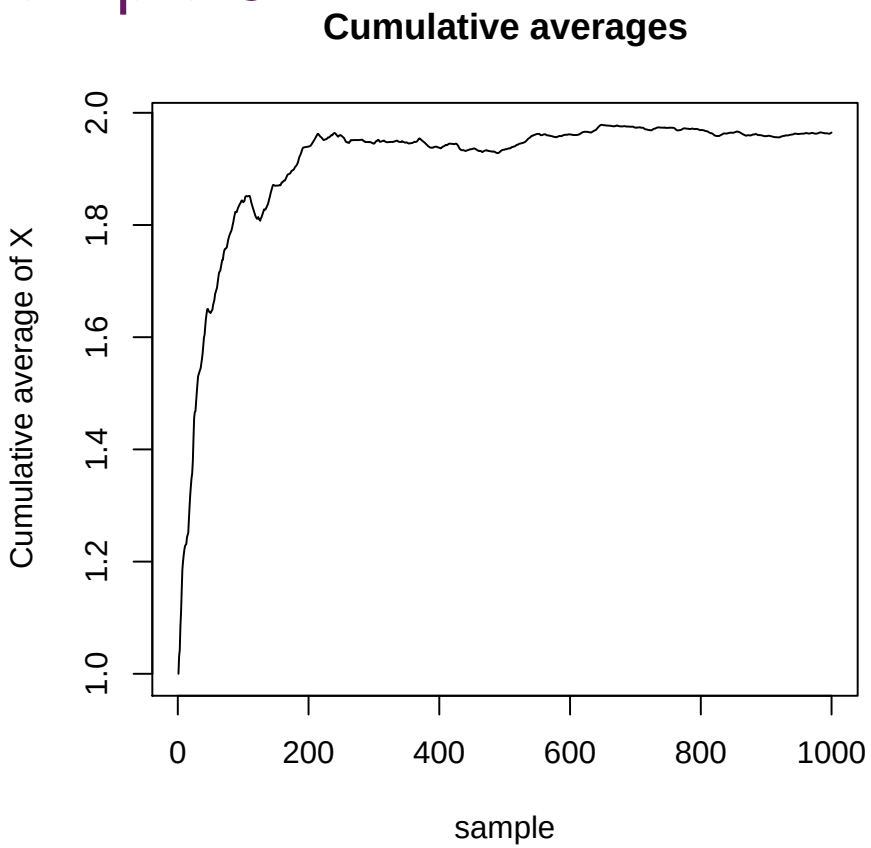




Slow convergence of the mean can be detected.

Basic plots for pathological example 3





We *cannot* detect that the sample only covers one part of the distribution.
("you've only seen where you've been")

Non-parametric tests of convergence

- Partition chain in 3 blocks:

  burn-in $(\mathbf{X}^{(t)})_{t=1,\ldots,\lfloor T/3 \rfloor}$

  first block $(\mathbf{X}^{(t)})_{t=\lfloor T/3 \rfloor+1,\ldots,2\lfloor T/3 \rfloor}$

  second block $(\mathbf{X}^{(t)})_{t=2\lfloor T/3 \rfloor+1,\ldots,T}$

- Distribution of $\mathbf{X}^{(t)}$ in both blocks should be identical.
- Idea: Use of a non-parametric test to test whether the two distributions are identical.
- Problem: Tests designed for i.i.d. samples.
  $\rightsquigarrow$ Resort to a (less correlated) thinned chain $\mathbf{Y}^{(t)} = \mathbf{X}^{(m \cdot t)}$.

Kolmogorov-Smirnov test

- Two i.i.d. populations: $Z_{1,1}, \ldots, Z_{1,n}$ and $Z_{2,1}, \ldots, Z_{2,n}$
- Estimate empirical CDF in each population:

$$\hat{F}_k(z) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}_{(-\infty, z]}(Z_{k,i})$$

- Test statistic is the maximum difference between the two empirical CDFs: $K = \sup_{x \in \mathbb{R}} |\hat{F}_1(x) - \hat{F}_2(x)|$
- For $n \to \infty$ the CDF of $\sqrt{n} \cdot K$ converges to the CDF

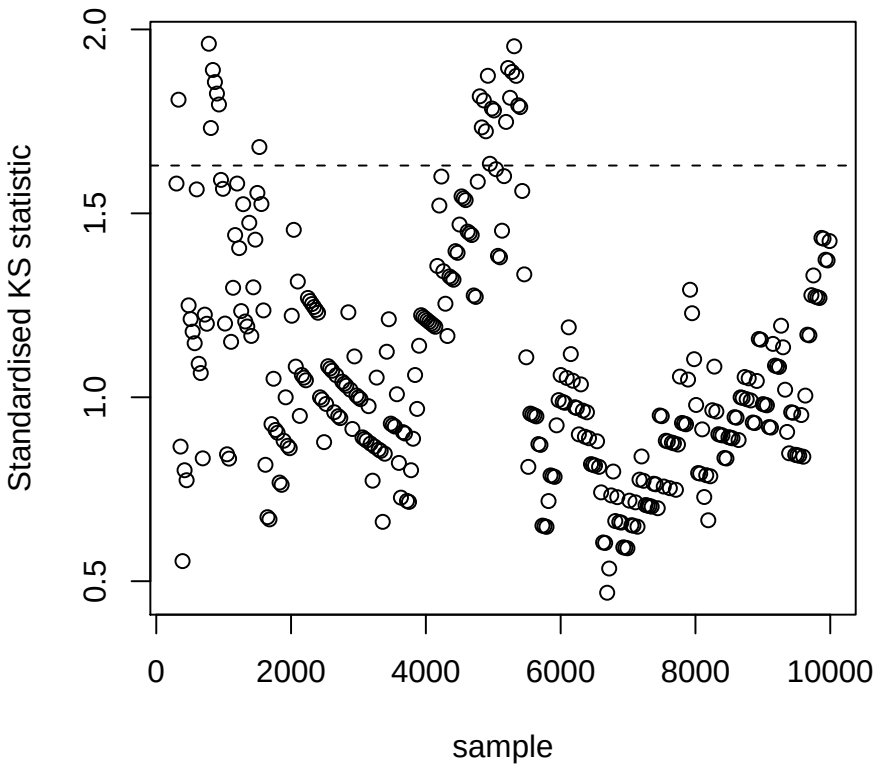
$$R(k) = 1 - \sum_{i=1}^{+\infty} (-1)^{i-1} \exp(-2i^2 k^2)$$

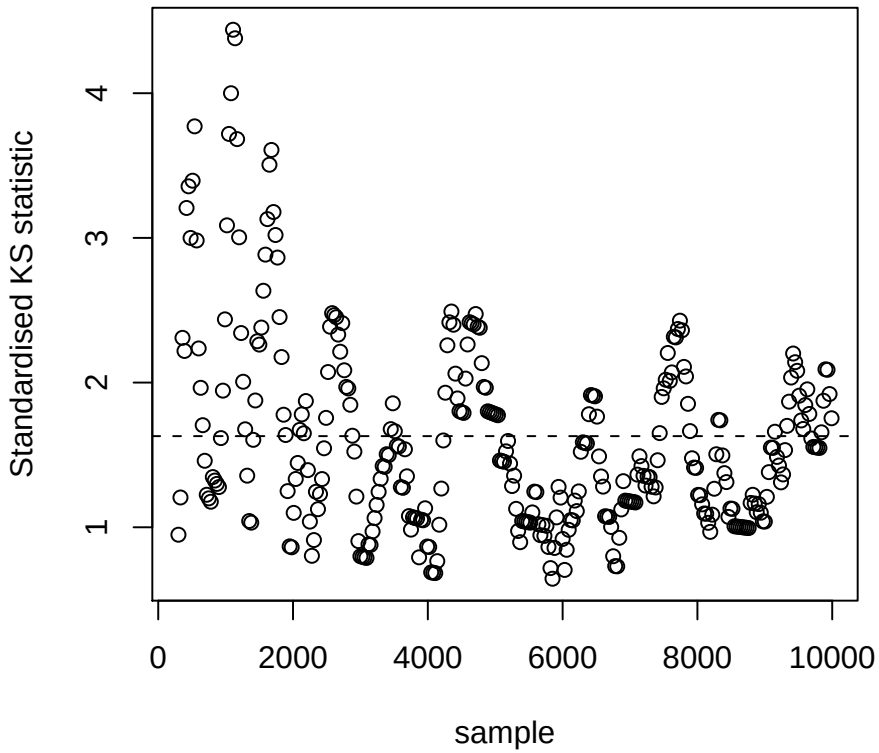
Kolmogorov-Smirnov test

- In our case the two populations are
  thinned first block $(\mathbf{Y}^{(t)})_{t=\lfloor T/(3\cdot m)\rfloor+1,\ldots,2\lfloor T/(3\cdot m)\rfloor}$
  thinned second block $(\mathbf{X}^{(t)})_{t=2\lfloor T/(3\cdot m)\rfloor+1,\ldots,\lfloor T/m\rfloor}$
- Even the thinned chain $(\mathbf{Y}^{(t)})_t$ is autocorrelated
  $\rightsquigarrow$ test invalid from a formal point of view.
- Standardised test statistic $\sqrt{\lfloor T/(3\cdot m)\rfloor}\cdot K$ can still be used a heuristic tool.

KS test for pathological example 1

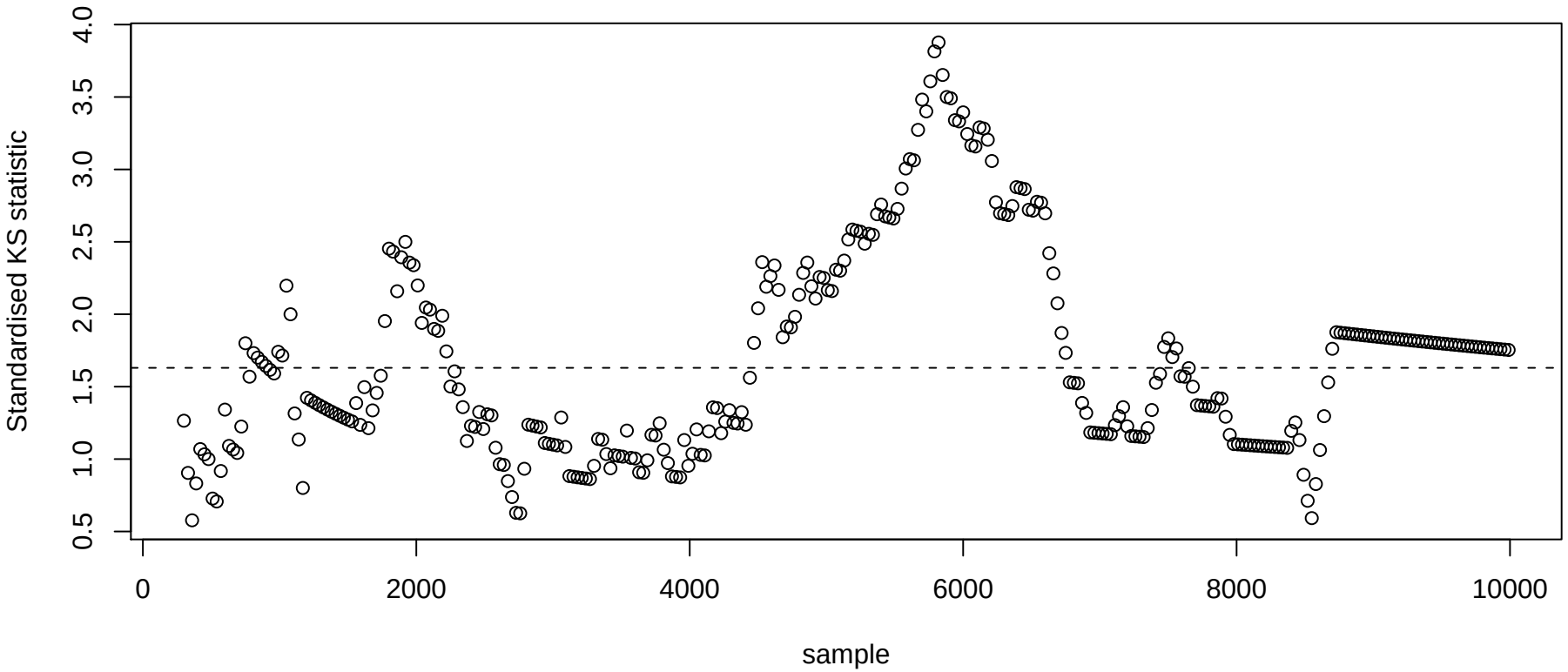
$\rho(X_1, X_2) = 0.3$ $\rho(X_1, X_2) = 0.99$





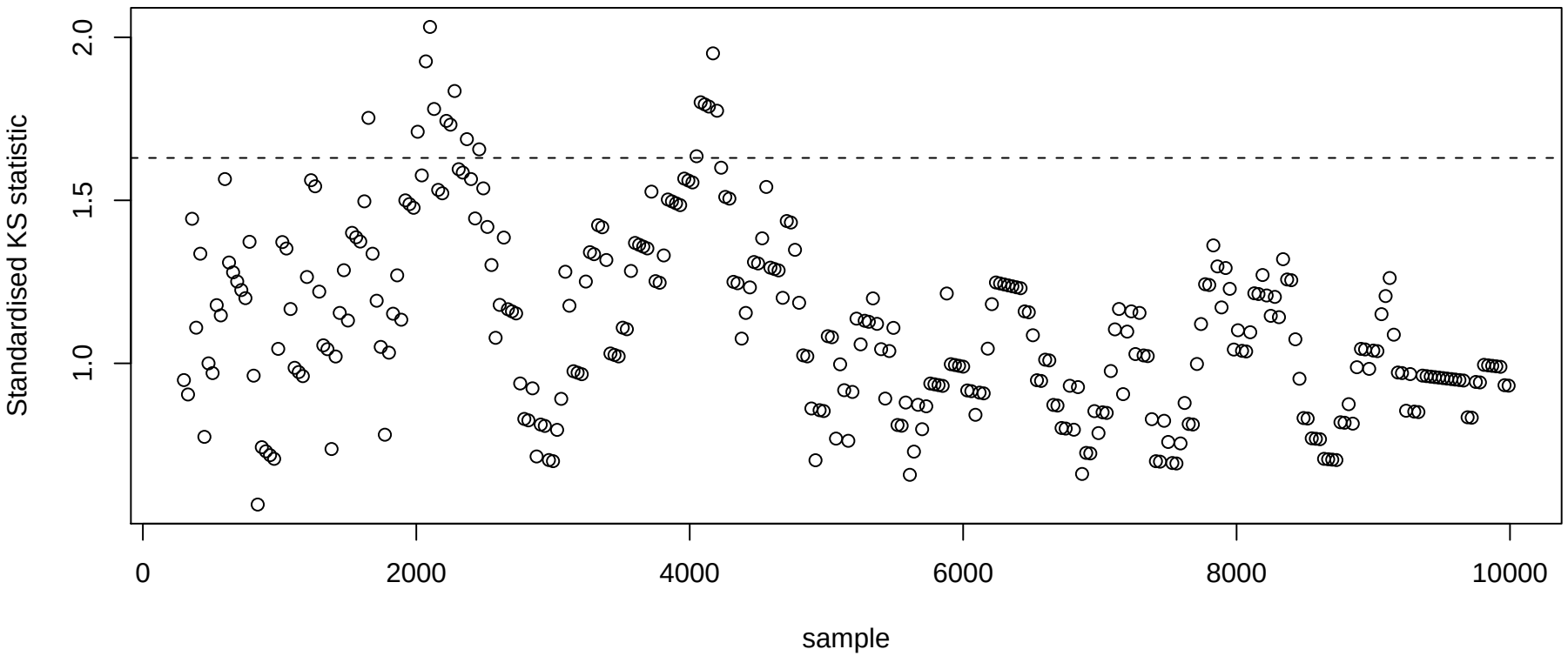
Slow mixing speed can be detected for the highly correlated chain.

KS test for pathological example 2



Problems can be detected.

KS test for pathological example 3

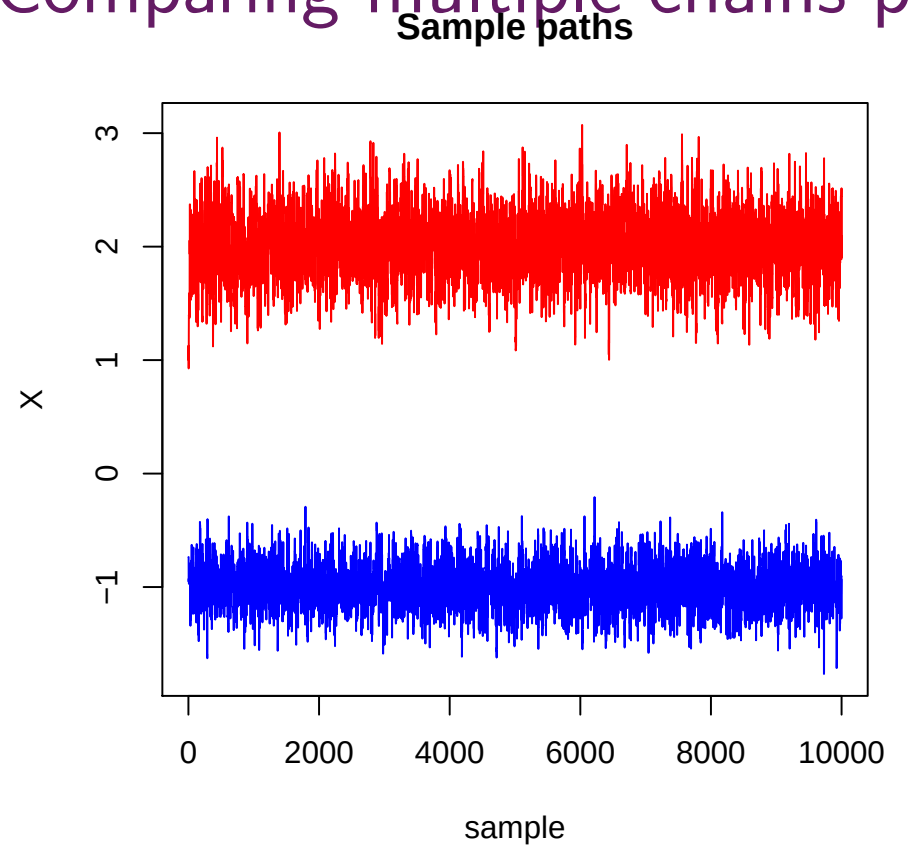


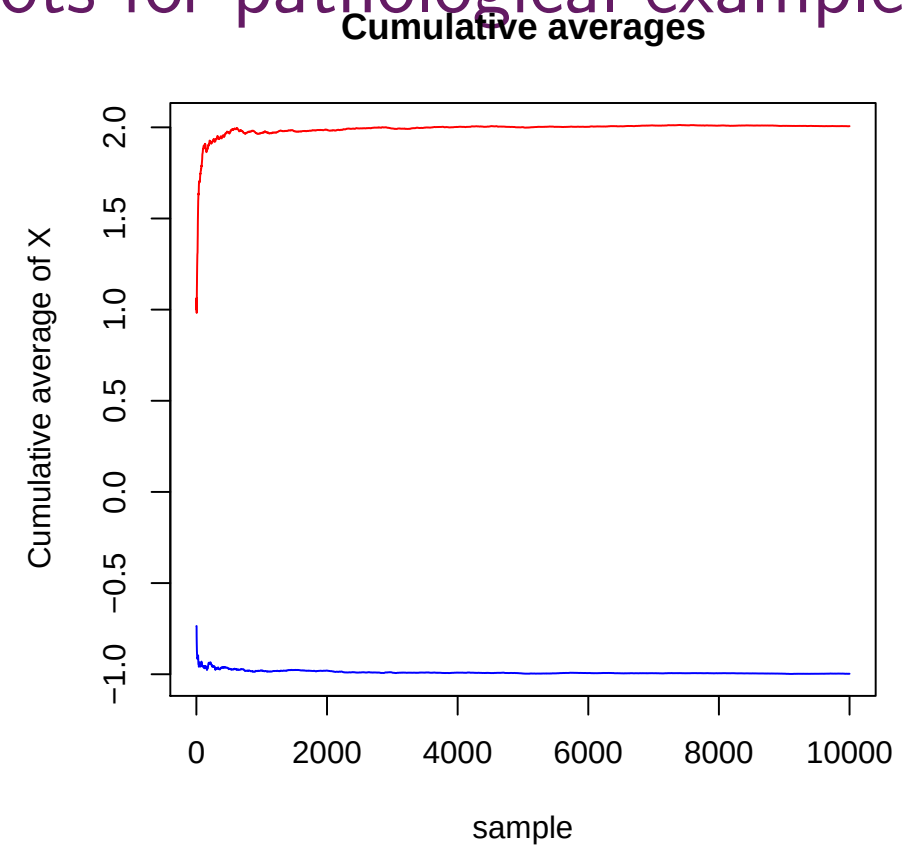
We *cannot* detect that the sample only covers one part of the distribution.
("you've only seen where you've been")

Comparing multiple chains

- Compare $L > 1$ chains $(\mathbf{X}^{(1,t)})_t, \ldots, (\mathbf{X}^{(L,t)})_t$.
- Initialised using overdispersed starting values $\mathbf{X}^{(1,0)}, \ldots, \mathbf{X}^{(L,0)}$.
- Idea: Variance and range of each chain $(\mathbf{X}^{(l,t)})_t$ should equal the range and variance of all chains pooled together.
- Compare basic plots for the different chains.
- Quantitative measure:
  - Compute distance $\delta_\alpha^{(l)}$ between α and $(1-\alpha)$ quantile of $(X_k^{(l,t)})_t$.
  - Compute distance $\delta_\alpha^{(\cdot)}$ between α and $(1-\alpha)$ quantile of the pooled data.
  - The ratio $\hat{S}_\alpha^{\text{interval}} = \dfrac{\sum_{l=1}^{L} \delta_\alpha^{(l)}/L}{\delta_\alpha^{(\cdot)}}$ should be around 1.
- Alternative: compare variance within each chain with the pooled variance estimate.
- Choosing suitable initial values $\mathbf{X}^{(1,0)}, \ldots, \mathbf{X}^{(L,0)}$ difficult.

Comparing multiple chains plots for pathological example 3





$$\hat{S}_{\alpha}^{\text{interval}} = 0.2703 \ll 1$$

We can detect that the sample only covers one part of the distribution (provided the chains are initialised appropriately).

Riemann sums and control variates

- Consider order statistic $X^{[1]} \leq \ldots \leq X^{[T]}$.
- Provided $(X^{[t]})_t = 1 \ldots, T$ covers the support of the target, the Riemann sum

$$\sum_{t=2}^{T} (X^{[t]} - X^{[t-1]}) f(X^{[t]})$$

converges to

$$\int f(x) dx = 1.$$

- Thus if $\sum_{t=2}^{T} (X^{[t]} - X^{[t-1]}) f(X^{[t]}) \ll 1$, the Markov chain has failed to explore all the support of the target.
- Requires that target density f is available inclusive of normalisation constants.
- Only effective in 1D.

Riemann sums for pathological example 3

For the chain stuck in the population with mean 2 we obtain

$$\sum_{t=2}^{T}(X^{[t]} - X^{[t-1]})f(X^{[t]}) = 0.598 \ll 1,$$

so we can detect that we have not explored the whole distribution.

Effective sample size

- MCMC algorithms yield a positively correlated sample $(\mathbf{X}^{(t)})_{t=1,\ldots,T}$.
- How much less useful is an MCMC sample of size T than an i.i.d. sample of size T?
- Approximate $(\varphi(\mathbf{X}^{(t)}))_{t=1,\ldots,T}$ by an $AR(1)$ process, i.e.:

$$\rho(\varphi(\mathbf{X}^{(t)}), \varphi(\mathbf{X}^{(t+\tau)})) = \rho^{|\tau|}.$$

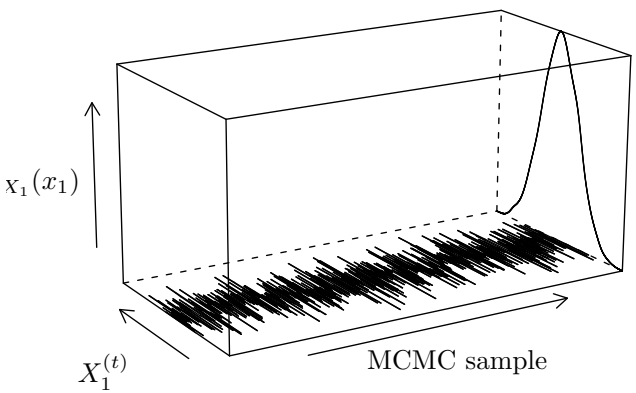
- Variance of the estimator is

$$\mathrm{Var}\left(\frac{1}{T}\sum_{t=1}^{T}\varphi(\mathbf{X}^{(t)})\right) \approx \frac{1+\rho}{1-\rho}\cdot\frac{1}{T}\mathrm{Var}\left(\varphi(\mathbf{X}^{(t)})\right)$$

- Same variance as an i.i.d. sample of the size $T\cdot\dfrac{1-\rho}{1+\rho}$.
- Thus define $T\cdot\dfrac{1-\rho}{1+\rho}$ as *effective sample size*.

Effective sample for pathological example 1

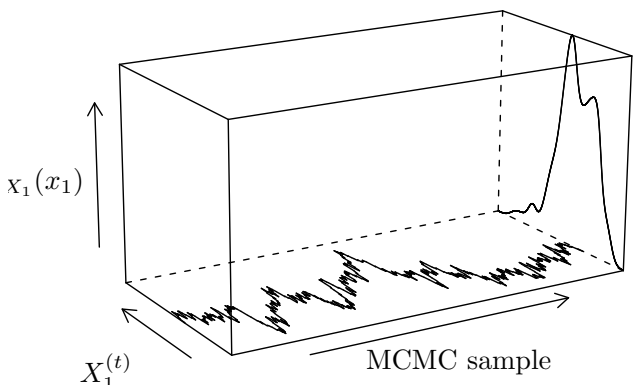
Rapidly mixing chain
$(\rho(X_1, X_2) = 0.3)$
10,000 samples



$\rho(X_1^{(t-1)}, X_1^{(t)}) = 0.078$

ESS for estimating $\mathbb{E}_f(X_1)$ is 8,547.

Slowly mixing chain
$(\rho(X_1, X_2) = 0.99)$
10,000 samples



$\rho(X_1^{(t-1)}, X_1^{(t)}) = 0.979$

ESS for estimating $\mathbb{E}_f(X_1)$ is 105.

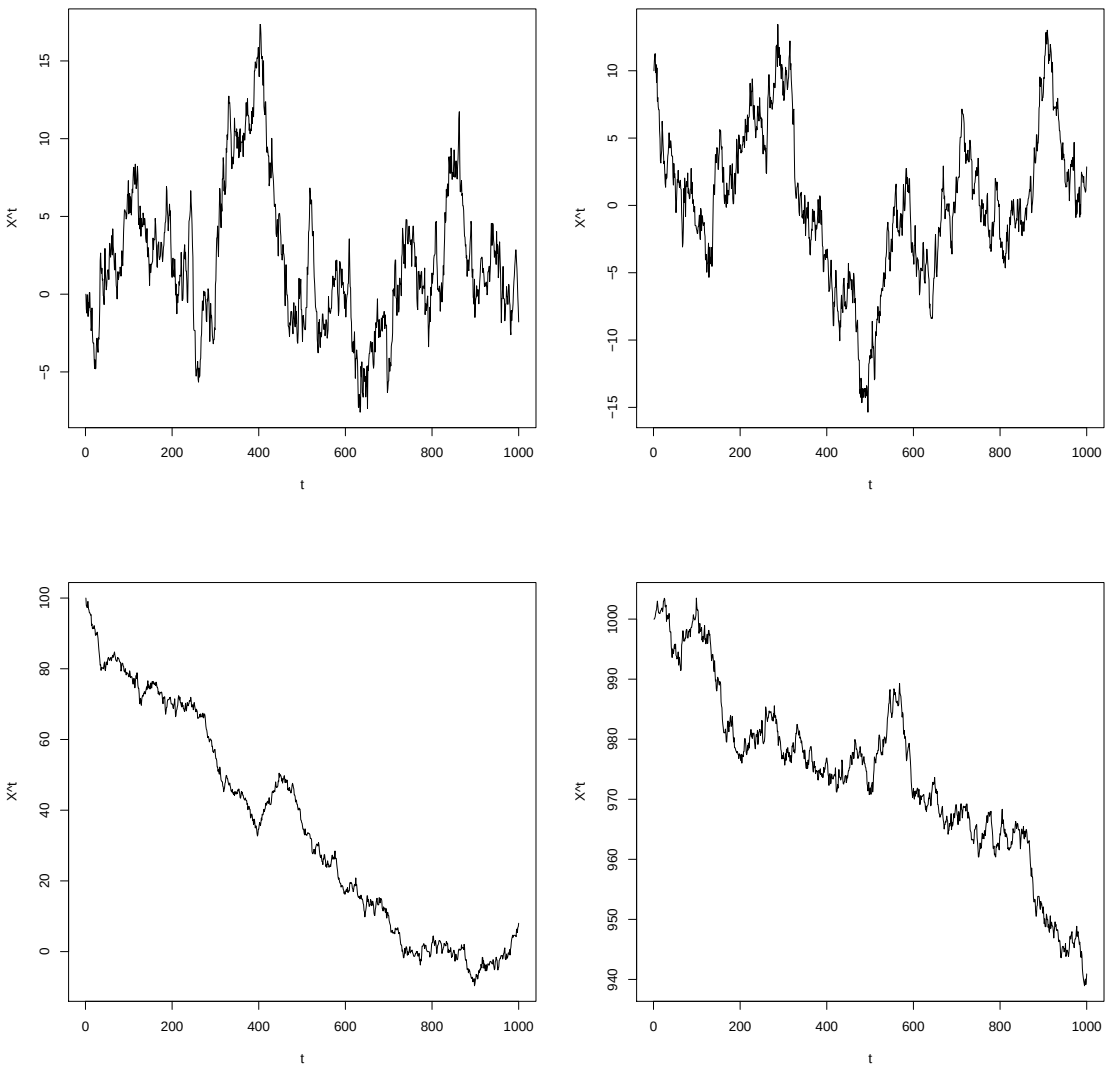
What Else Can We Do?

1. More sophisticated convergence diagnostics:
   - Geweke's method based on spectral analysis
   - Raftery's binary-chain method
   - ⋮
2. Theoretical Computations
   - Convergence rates
   - Mixing times
   - Confidence intervals
3. Perfect Simulation
   - Processes with "ordered transitions".
   - Certain spatial processes.

Part 5— Section 17

Practical Considerations

Where do we start?



RWM Traces.

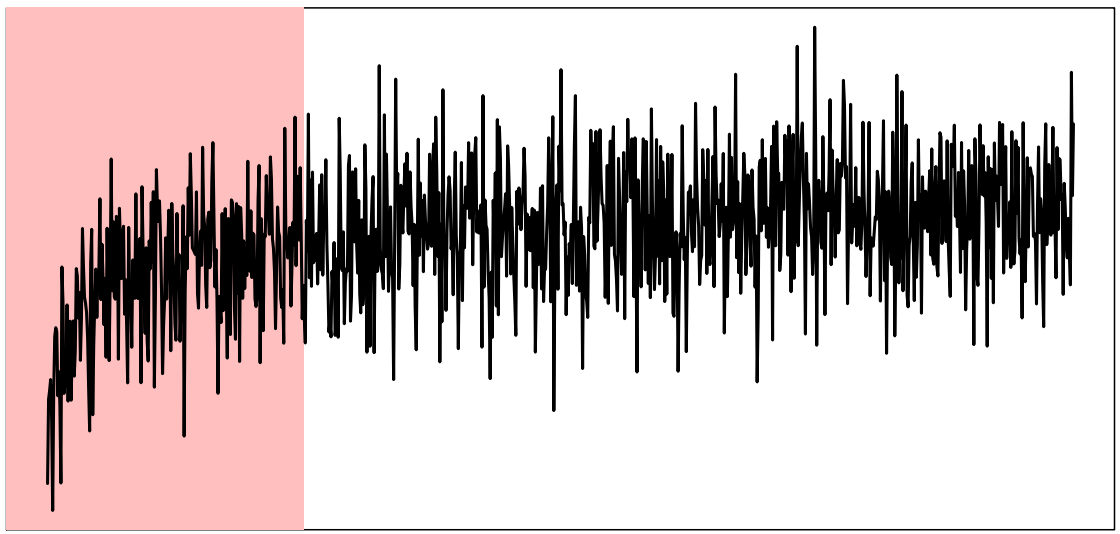
Target:
$f(x) = \mathrm{e}^{-|x|/5}/10$

Starting values:

- $X^{(1)} = 0$
- $X^{(1)} = 10$
- $X^{(1)} = 100$
- $X^{(1)} = 1,000$

Practical considerations: Burn-in period

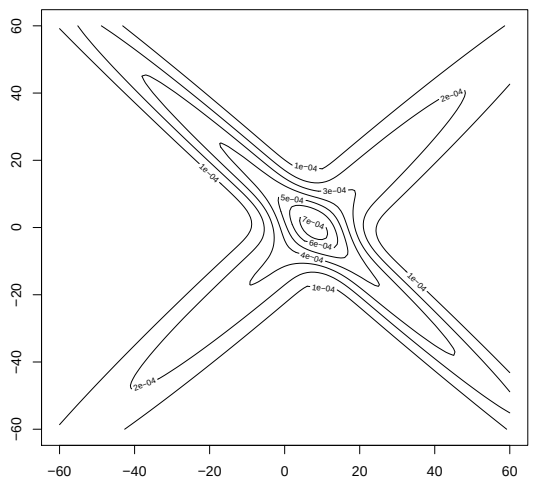
- Theory (ergodic theorems) allows for the use of the entire chain $(\mathbf{X}^{(0)}, \mathbf{X}^{(1)}, \ldots)$.
- However distribution of $(\mathbf{X}^{(t)})$ for small t might still be far from the stationary distribution f.
- Can be beneficial to discard the first iterations $\mathbf{X}^{(t)}$, $t = 1, \ldots, T_0$ (*burn-in period*).
- Optimal T_0 depends on mixing properties of the chain.

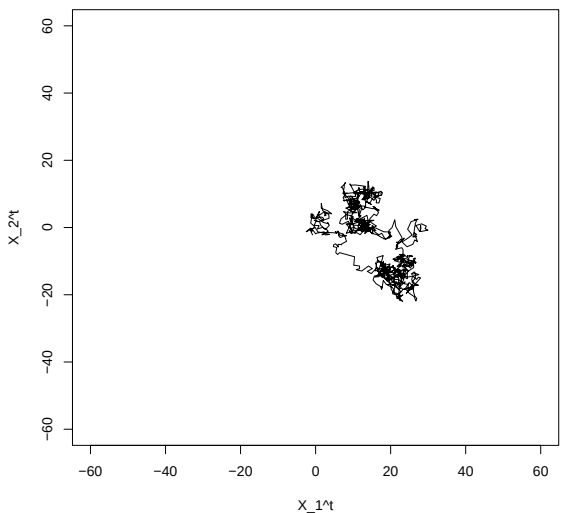


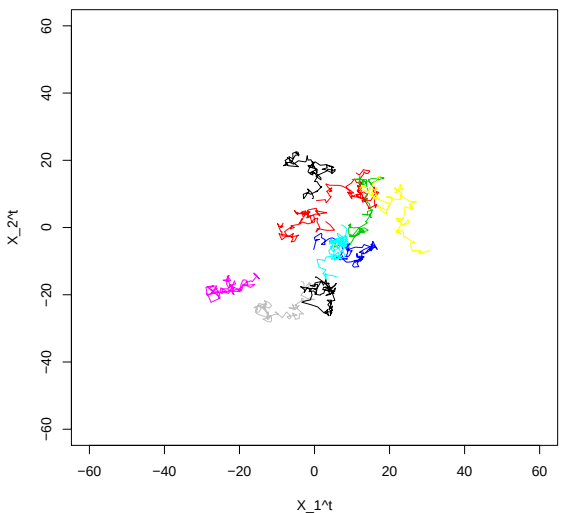
Practical considerations: Multiple Starts?

- Should we use "multiple overdispersed initialisations"?
- Advantages:
  - Exploring different parts of the space.
  - May be useful for assessing convergence.
  - Trivial to parallelize.
- Disadvantages:
  - We need to specify many starting values.
  - What does overdispersed mean, anyway?
  - Every chain needs to reach stationarity.
  - Multiple burn-in periods may be expensive.

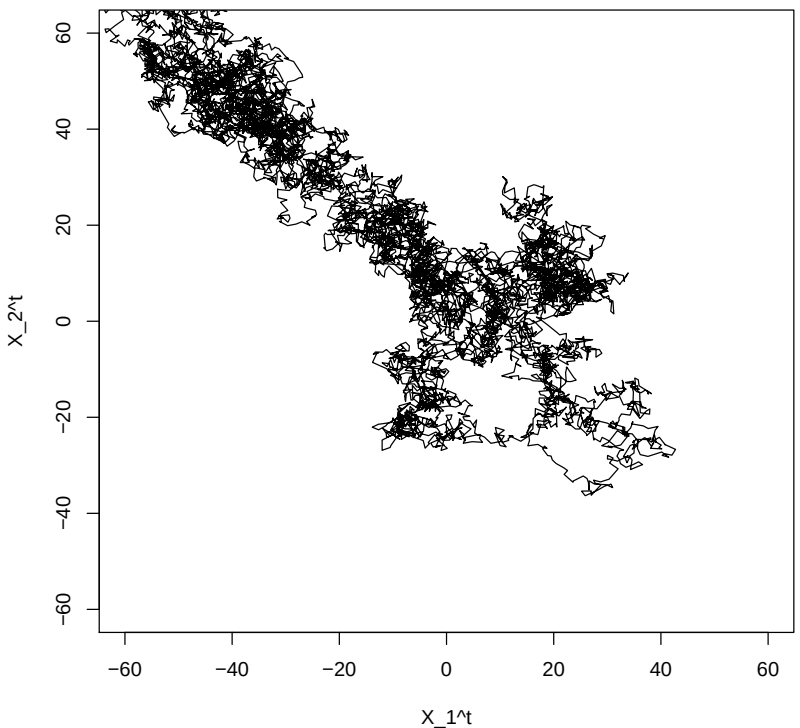
One Chain vs. Many: 1000 or 10×100

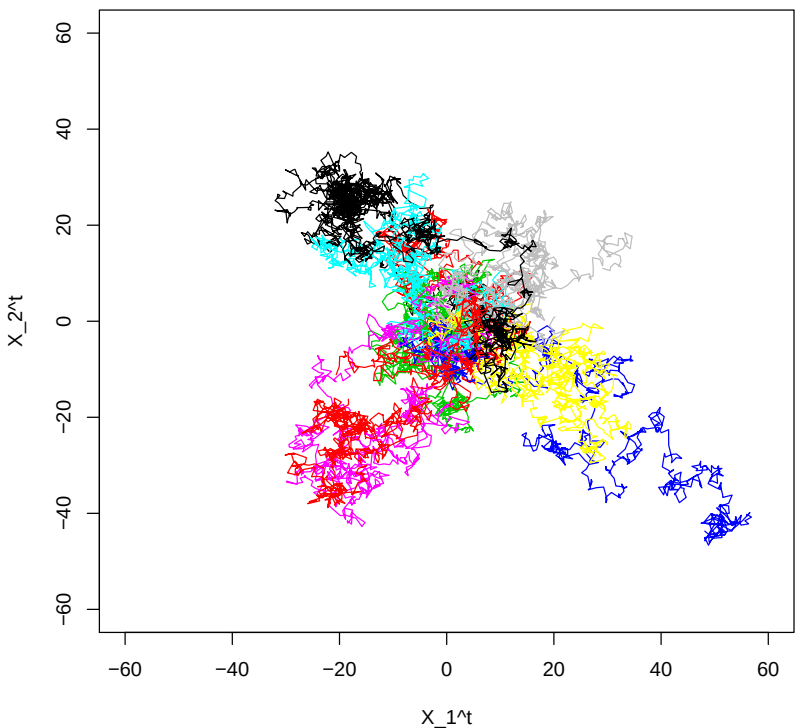




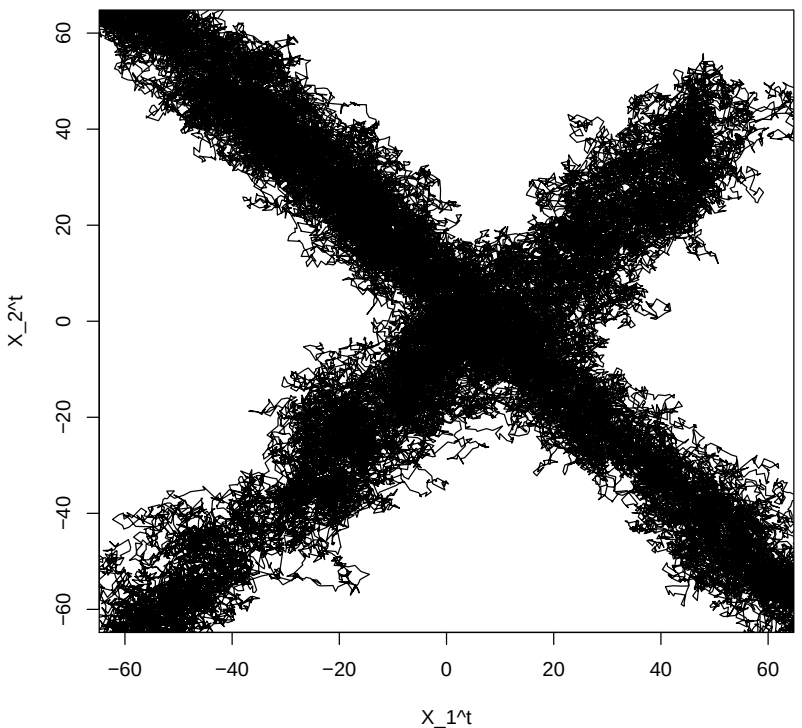


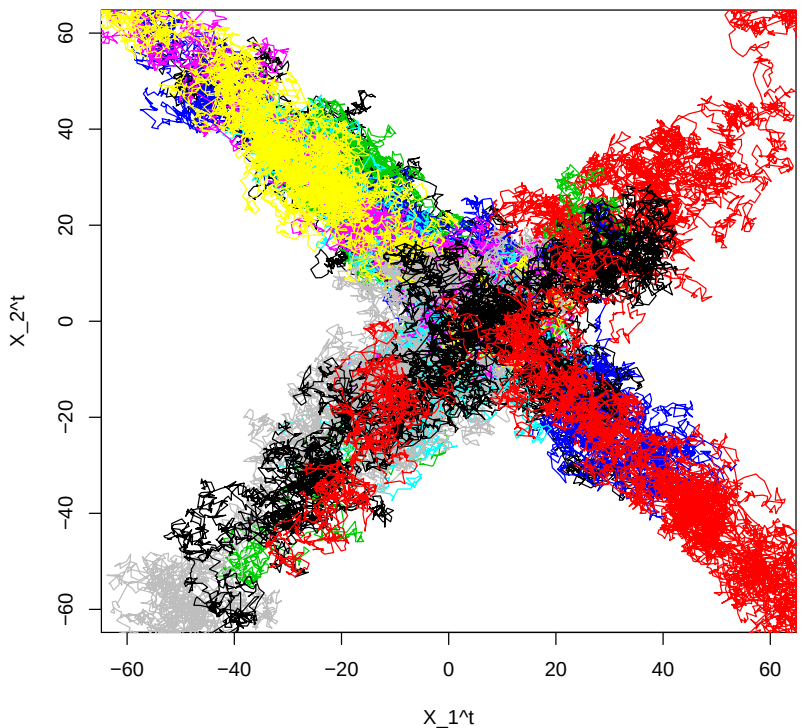
One Chain vs. Many: $10,000$ or 10×1000





One Chain vs. Many: $100,000$ or $10 \times 10,000$





Practical considerations: Thinning (1)

- MCMC methods typically yield positively correlated chain: $\rho(\mathbf{X}^{(t)}, \mathbf{X}^{(t+\tau)})$ large for small τ.
- Idea: keeping only every m-th value: $(\mathbf{Y}^{(t)})_{t=1,\ldots,\lfloor T/m \rfloor}$ with $\mathbf{Y}^{(t)} = \mathbf{X}^{(m \cdot t)}$ instead of $(\mathbf{X}^{(t)})_{t=1,\ldots,T}$ (*thinning*).
- $(\mathbf{Y}^{(t)})_t$ exhibits less autocorrelation than $(\mathbf{X}^{(t)})_t$, i.e.

$$\rho(\mathbf{Y}^{(t)}, \mathbf{Y}^{(t+\tau)}) = \rho(\mathbf{X}^{(t)}, \mathbf{X}^{(t+m \cdot \tau)}) < \rho(\mathbf{X}^{(t)}, \mathbf{X}^{(t+\tau)}),$$

  if the correlation $\rho(\mathbf{X}^{(t)}, \mathbf{X}^{(t+\tau)})$ decreases monotonically in τ.
- Price: length of $(\mathbf{Y}^{(t)})_{t=1,\ldots,\lfloor T/m \rfloor}$ is only $(1/m)$-th of the length of $(\mathbf{X}^{(t)})_{t=1,\ldots,T}$.

Practical considerations: Thinning (2)

- If $\mathbf{X}^{(t)} \sim f$ and corresponding variances exist,

$$\mathrm{Var}\left(\frac{1}{T}\sum_{t=1}^{T}\varphi(\mathbf{X}^{(t)})\right) \leq \mathrm{Var}\left(\frac{1}{\lfloor T/m \rfloor}\sum_{t=1}^{\lfloor T/m \rfloor}\varphi(\mathbf{Y}^{(t)})\right),$$

  i.e. thinning cannot be justified when objective is estimating $\mathbb{E}_f(\varphi(\mathbf{X}))$.
- Thinning can be a useful concept
  - if computer has insufficient memory.
  - for convergence diagnostics: $(\mathbf{Y}^{(t)})_{t=1,\ldots,\lfloor T/m \rfloor}$ is closer to an i.i.d. sample than $(\mathbf{X}^{(t)})_{t=1,\ldots,T}$.

A Closing Thought

It is better to create than to learn! Creating is the essence of life.

Julius Cæsar

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