Bayesian modelling

Introduction to Monte Carlo methods and the Metropolis–Hastings algorithm

Léo Belzile

2025

HEC MONTRÉAL

Bayesian inference beyond conjugate models

How to circumvent the problem of intractable posteriors?

- simulation-based methods: accept-reject, Markov chain Monte Carlo, particle filters, etc.
- deterministic methods: (integrated nested) Laplace approximations, variational Bayes, expectation propagation, etc.

We focus on Monte Carlo methods.

Simulation algorithms: inversion method

If F is an absolutely continuous distribution function, then

$$F(X) \sim \mathsf{U}(0,1).$$

The inversion method consists in applying the quantile function F^{-1} to $U \sim \mathsf{U}(0,1)$, viz.

$$F^{-1}(U) \sim X.$$

Inversion method for truncated distributions

Consider a random variable Y with distribution function F.

If X follows the same distribution as Y, but restricted over the interval $[a, b]$, then

$$\Pr(X \leq x) = \frac{F(x) - F(a)}{F(b) - F(a)}, \qquad a \leq x \leq b,$$

Therefore,

$$F^{-1}[F(a) + \{F(b) - F(a)\}U] \sim X$$

Simulation algorithms: accept-reject

- **Target**: sample from density $p(x)$ (hard to sample from)
- **Proposal**: find a density $q(x)$ with nested support, $\text{supp}(p) \subseteq \text{supp}(q)$, such that

$$\frac{p(x)}{q(x)} \leq C, \quad C \geq 1.$$

Rejection sampling algorithm

1. Generate X from proposal with density $q(x)$.
2. Compute the ratio $R \leftarrow p(X)/q(X)$.
3. If $CU \leq R$ for $U \sim \mathsf{U}(0,1)$, return X, else go back to step 1.

Remarks on rejection sampling

- Acceptance rate is $1/C$
  - we need on average C draws from q to get one from p
- q must be more heavy-tailed than p
  - e.g., $q(x)$ Student-t for $p(x)$ Gaussian
- q should be cheap and easy to sample from!

Designing a good proposal density

Good choices must satisfy the following constraints:

- pick a family $q(x)$ so that

$$C = \sup_x \frac{p(x)}{q(x)}$$

  is as close to 1 as possible.

- you can use numerical optimization with $f(x) = \log p(x) - \log q(x)$ to find the mode $x^\star$ and the upper bound $C = \exp f(x^\star)$.

Accept-reject illustration

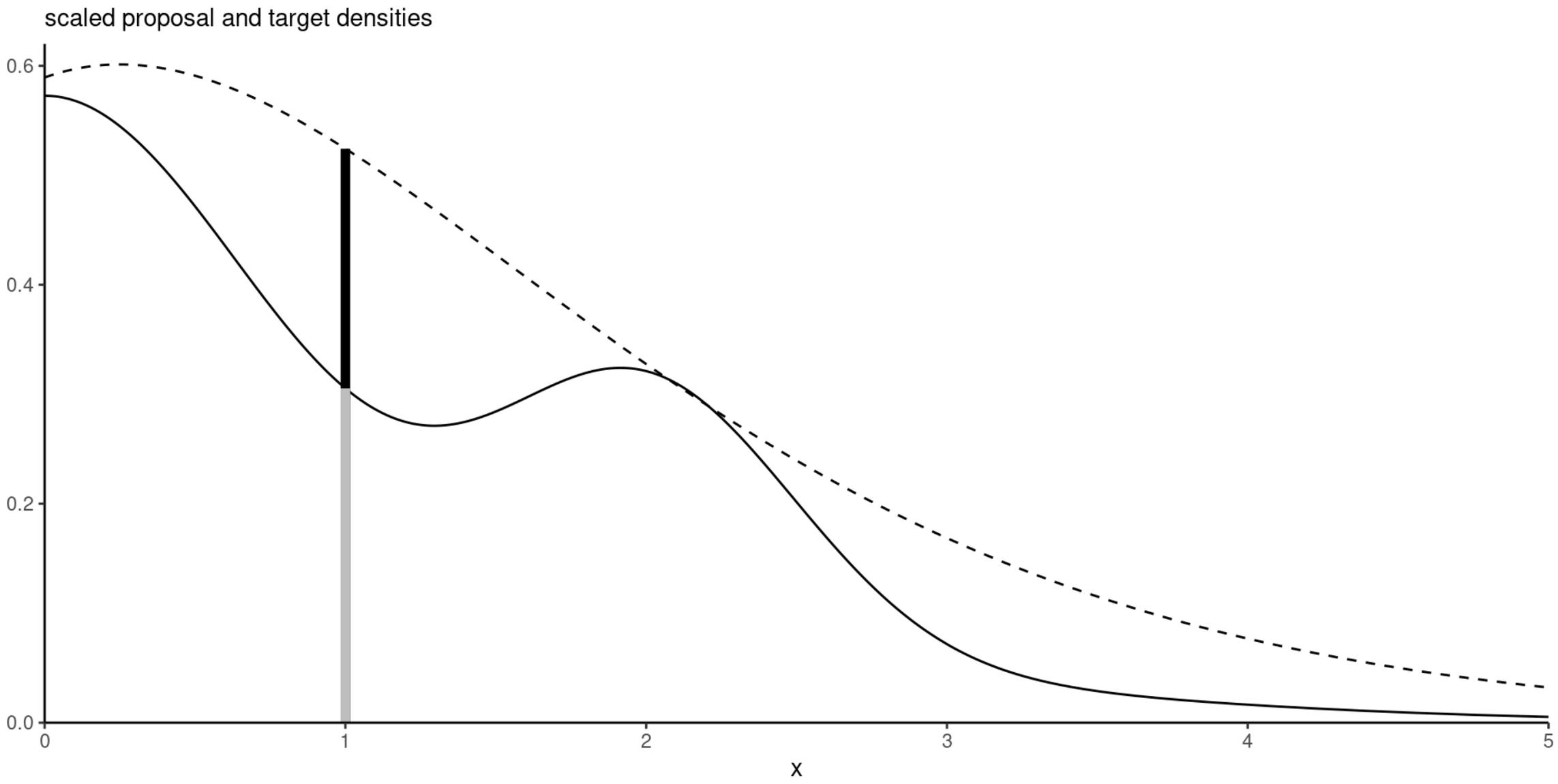


Figure 1: Target density (full) and scaled proposal density (dashed): the vertical segment at $x = 1$ shows the percentage of acceptance for a uniform slice under the scaled proposal, giving an acceptance ratio of 0.58.

Truncated Gaussian via accept-reject

Consider sampling $Y \sim \mathsf{No}(\mu, \sigma^2)$, but truncated in the interval (a, b). The target density is

$$p(x; \mu, \sigma, a, b) = \frac{1}{\sigma} \frac{\phi\left(\frac{x-\mu}{\sigma}\right)}{\Phi(\beta) - \Phi(\alpha)}.$$

for $\alpha = (a - \mu)/\sigma$ and $\beta = (b - \mu)/\sigma$. where $\phi(\cdot)$, $\Phi(\cdot)$ are respectively the density and distribution function of the standard Gaussian distribution.

Accept-reject (crude version)

1. Simulate $X \sim \text{No}(\mu, \sigma^2)$
2. reject any draw if $X < a$ or $X > b$.

The acceptance rate is $C^{-1} = \{\Phi(\beta) - \Phi(\alpha)\}$

```r
# Standard Gaussian truncated on [0,1]
candidate <- rnorm(1e5)
trunc_samp <- candidate[candidate >= 0 & candidate <= 1]
# Acceptance rate
length(trunc_samp)/1e5
```

```
[1] 0.34289
```

```r
# Theoretical acceptance rate
pnorm(1)-pnorm(0)
```

```
[1] 0.3413447
```

Accept-reject for truncated Gaussian

Since the Gaussian is a location scale family, the inversion method gives

$$X \sim \mu + \sigma\Phi^{-1}\left[\Phi(\alpha) + \{\Phi(\beta) - \Phi(\alpha)\}U\right]$$

We however need to evaluate Φ numerically (no closed-form expression).

The method fails for *rare event* simulation because the computer returns

- $\Phi(x) = 0$ for $x \leq -39$
- $\Phi(x) = 1$ for $x \geq 8.3$,

implying that $a \leq 8.3$ for this approach to work (Botev & L'Écuyer, 2017).

Simulating tails of Gaussian variables

We consider simulation from a standard Gaussian truncated above $a > 0$

Write the density of the truncated Gaussian as (Devroye, 1986, p. 381)

$$f(x) = \frac{\exp(-x^2/2)}{\int_a^\infty \exp(-z^2/2)\mathrm{d}z} = \frac{\exp(-x^2/2)}{c_1}.$$

Note that, for $x \geq a$,

$$c_1 f(x) \leq \frac{x}{a}\exp\left(-\frac{x^2}{2}\right) = a^{-1}\exp\left(-\frac{a^2}{2}\right)g(x);$$

where $g(x)$ is the density of a Rayleigh variable shifted by a.[1]

Accept-reject: truncated Gaussian with Rayleigh

The shifted Rayleigh has distribution function

$$G(x) = 1 - \exp\{(a^2 - x^2)/2\}, x \geq a.$$

Marsaglia algorithm

1. Generate a shifted Rayleigh above a, $X \leftarrow \{a^2 - 2\log(U)\}^{1/2}$ for $U \sim \mathsf{U}(0,1)$
2. Accept X if $XV \leq a$, where $V \sim \mathsf{U}(0,1)$.

For sampling on $[a, b]$, propose from a Rayleigh truncated above at b (Botev & L'Écuyer, 2017).

```
a <- 8.3
niter <- 1000L
X <- sqrt(a^2 + 2*rexp(niter))
samp <- X[runif(niter)*X <= a]
```

Markov chains

Plain ordinary Monte Carlo is great, but few algorithms are generic enough to be useful in complex high-dimensional problems.

We will instead typically build Markov chains that target an invariant stationary distribution.

Caveats?

Markov chain Monte Carlo methods generate **correlated** draws.

Questions:

1. can we use them as ordinary independent samples?
2. what is the price to pay?

We need to do a little theoretical detour to answer these questions.

Stationarity and Markov property

A stochastic process is **(weakly) stationary** if

- the distribution of $\{X_1, \ldots, X_t\}$ is the same as that of $\{X_{n+1}, \ldots X_{t+n}\}$ for any value of n and given t.

A stochastic process is **Markov** if

- it satisfies the Markov property: given the current state of the chain, the future only depends on the current state and not on the past.

Autoregressive process of order 1

Consider a first-order autoregressive process, or AR(1),

$$Y_t = \mu + \phi(Y_{t-1} - \mu) + \varepsilon_t,$$

where

- ϕ is the lag-one correlation,
- μ the global mean
- ε_t is an iid innovation with mean zero and variance σ^2

If $|\phi| < 1$, the process is stationary, otherwise variance increases with t

Variance of a stationary distribution

For a correlated sequence, the variance of the stationary distribution is

$$\tau^2 = \mathsf{Va}(Y_t) + 2\sum_{k=1}^{\infty} \mathsf{Co}(Y_t, Y_{t-k}).$$

- for i.i.d. data, $\tau^2 = \mathsf{Va}(Y_t)$
- for stationary $\mathsf{AR}(1)$ process, we get $\sigma^2/(1-\phi^2)$ (geometric series)

Variance of sample average

Intuitively, a sample of correlated observations carries less information than an independent sample of draws.

We want the variance of the sample average, which is

$$\mathsf{Va}\left(\overline{Y}_T\right) = \frac{1}{T}\sum_{t=1}^{T}\mathsf{Va}(Y_t) + \frac{2}{T}\sum_{t=1}^{T-1}\sum_{s=t+1}^{T}\mathsf{Co}(Y_t, Y_s).$$

If the process is stationary, the covariances at lag k are the same regardless of the time index and the unconditional variance is constant.

Variance of sample average, redux

If a central limit theorem applies, the limiting variance of the sample mean simplifies to

$$\lim_{T\to\infty} T\mathsf{Va}\left(\overline{Y}_T\right) = \tau^2\left\{1+2\sum_{t=1}^{\infty}\gamma_t\right\}.$$

which is a function of

- the unconditional variance τ^2
- the lag-k autocorrelation $\mathsf{Cor}(Y_t, Y_{t+k}) = \gamma_k$

Correlogram

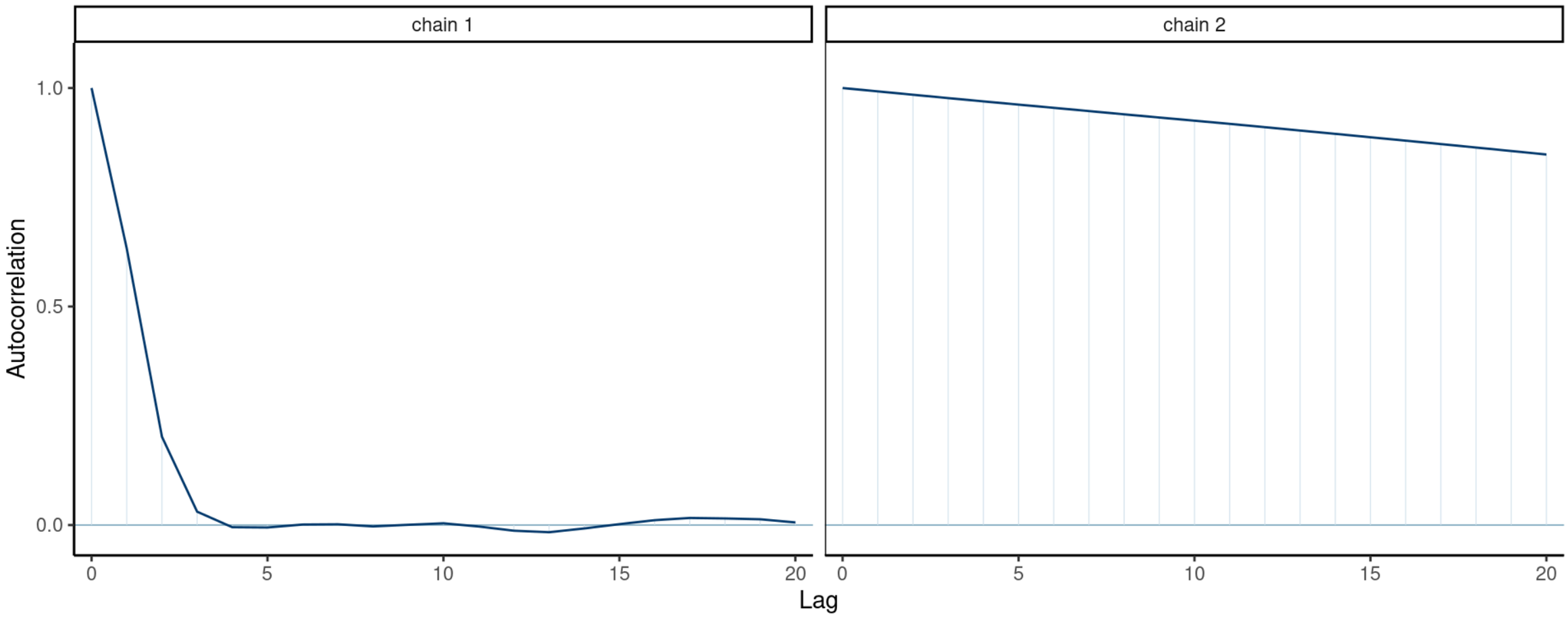


Figure 2: Correlogram of two Markov chains. These plots, often called acf or autocorrelation functions, show the lag-k sample autocorrelation against lag number.

Variance of sample mean of AR(1)

The lag-k correlation of the stationary autoregressive process of order 1 is ϕ^k, so

$$T\mathsf{Va}\left(\overline{Y}_T\right) = \sigma^2(1+\phi)/(1-\phi).$$

For an independent sample, we have

$$T\mathsf{Va}\left(\overline{Y}_T\right) = \sigma^2/(1-\phi^2).$$

Inefficiency curve for AR(1)

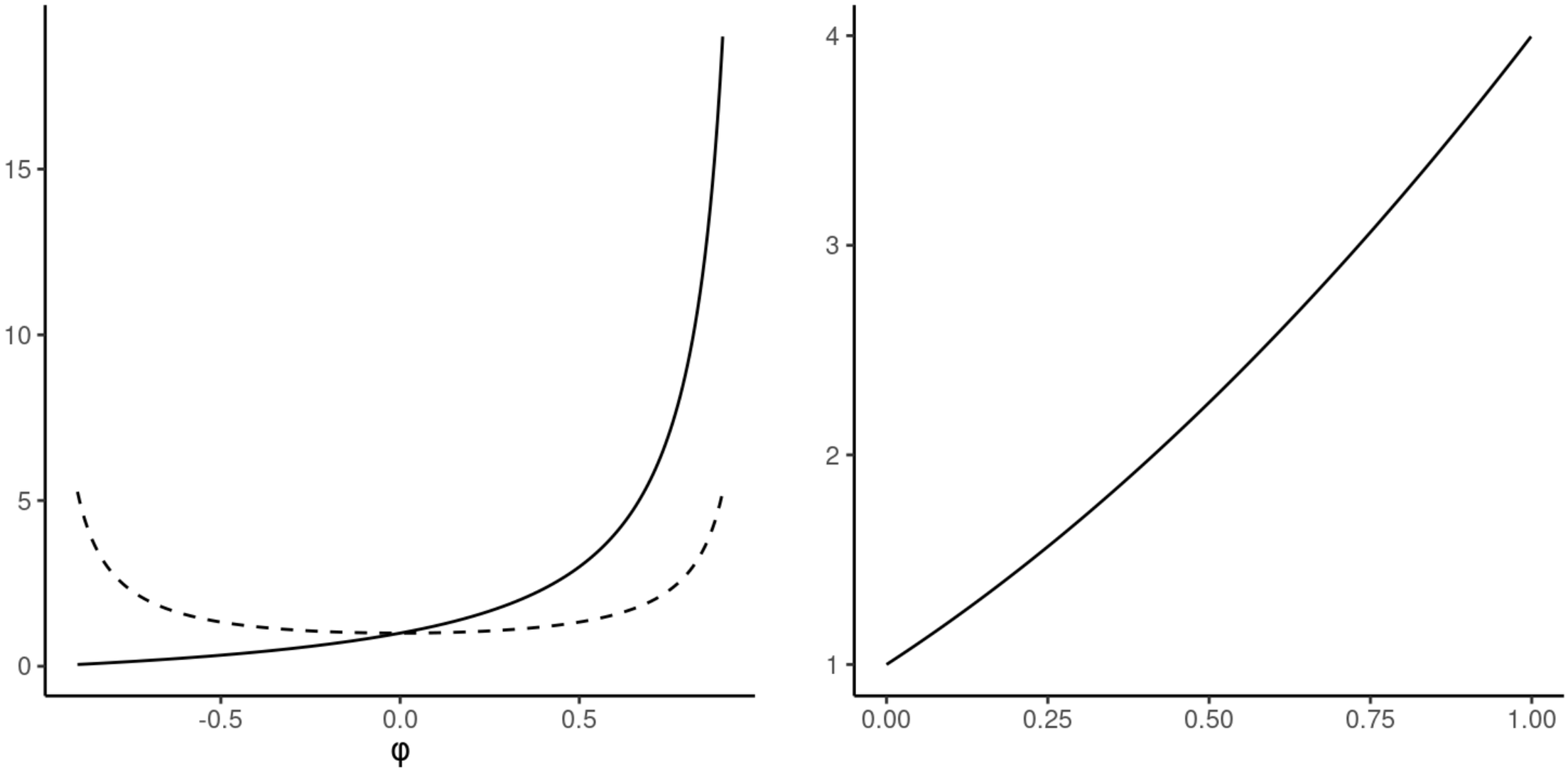


Figure 3: Left: scaled asymptotic variance of the sample mean for AR(1) (full line) and independent observations with the same marginal variance (dashed). Right: variance ratio for positive correlations.

To get the same precision for the mean of $\mathsf{AR}(1)$ process with $\phi \approx 0.75$ than with i.i.d. data, we would need 9 times as many observations.

Morale of the story

The price to pay for having correlated samples is

inefficiency

The higher the autocorrelation, the larger the variability of our estimators.

When can we use Markov chains?

If a Markov chain is irreducible and acyclic, it has a unique stationary distribution.

- irreducibility: means that the chain can move from anywhere to anywhere, so it doesn't get stuck in part of the space forever.
- acyclic: cyclical chains loop around and visit periodically a state

Ergodic theorem is our guarantee of convergence.

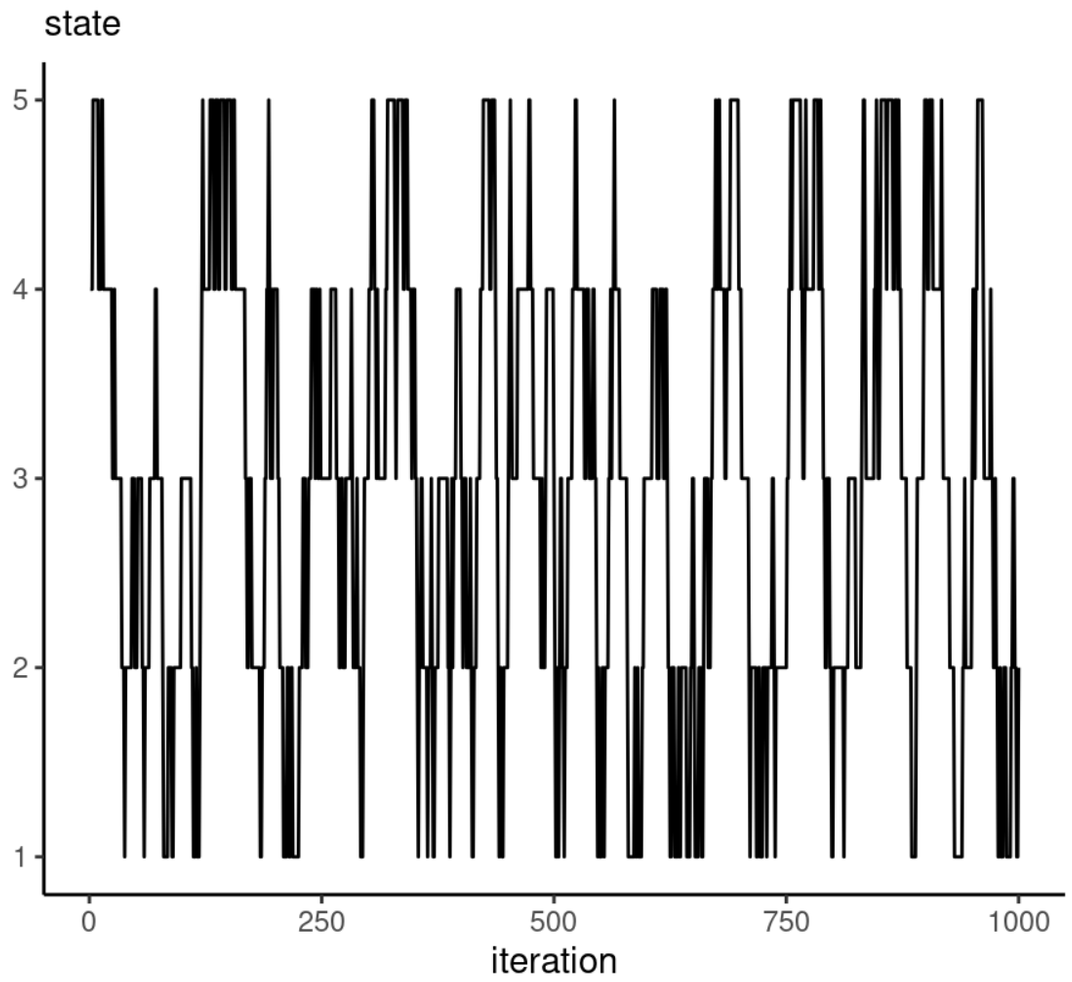
Examples

Consider discrete Markov chains over the integers $1, 2, 3$ with transition matrices

$$P_1 = \begin{pmatrix} 0.5 & 0.3 & 0.2 \\ 0 & 0.4 & 0.6 \\ 0 & 0.5 & 0.5 \end{pmatrix}, \quad P_2 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

Chain 1 is reducible to $\{2, 3\}$, chain 2 is cyclical.

Convergence of Markov chains



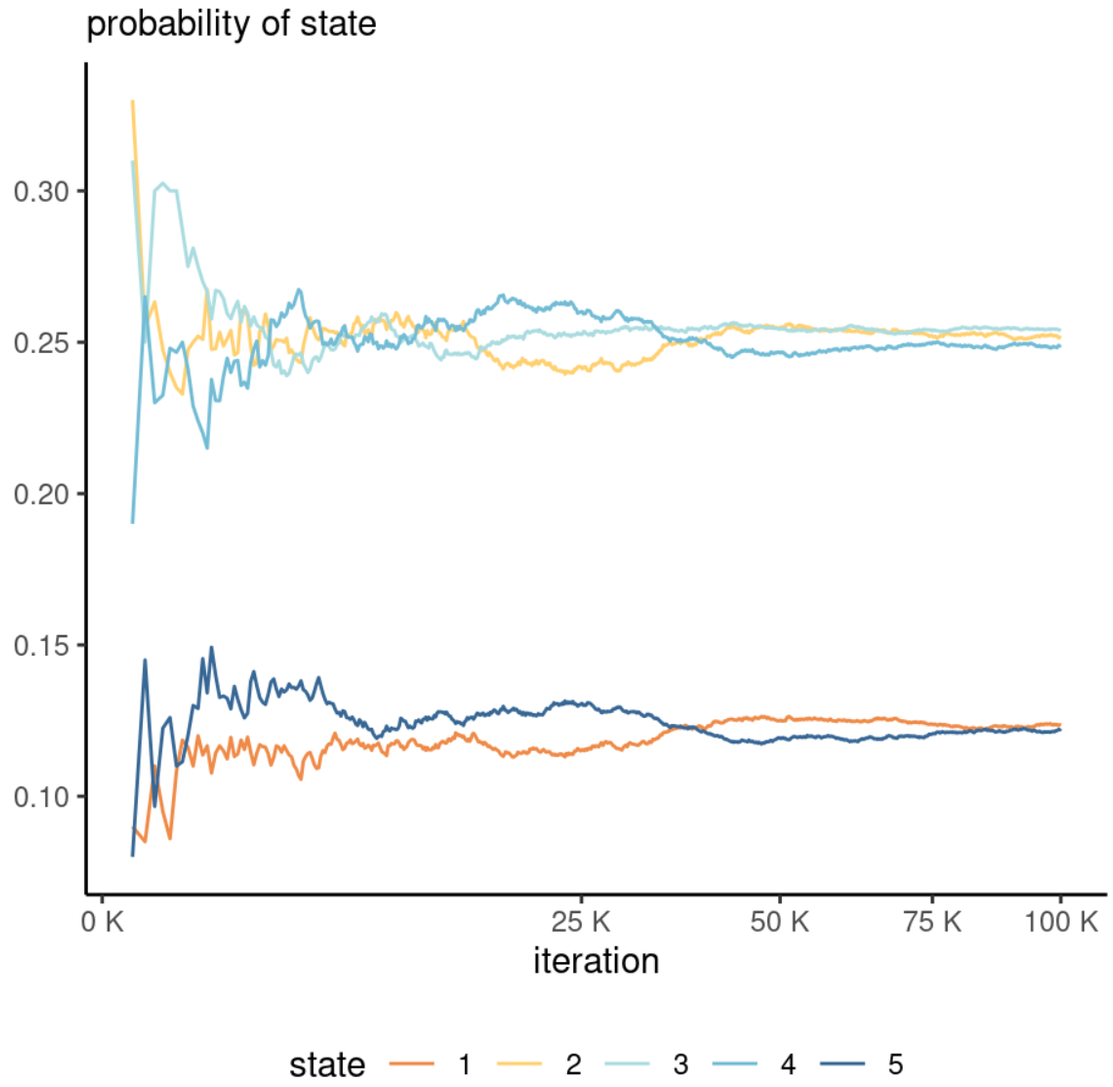


Figure 4: Discrete Markov chain on integers from 1 to 5, with traceplot of 1000 first iterations (left) and running mean plots of sample proportion of each state visited (right).

Markov chain Monte Carlo

We consider simulating from a distribution with associated density function $\propto p(\boldsymbol{\theta})$.

- known up to a normalizing factor not depending on $\boldsymbol{\theta}$.

We use $q(\boldsymbol{\theta} \mid \boldsymbol{\theta}^*)$ as transition kernel to generate proposals.

Metropolis–Hastings algorithm

Starting from an initial value $\boldsymbol{\theta}_0$:

1. draw a proposal value $\boldsymbol{\theta}_t^\star \sim q(\boldsymbol{\theta} \mid \boldsymbol{\theta}_{t-1})$.
2. Compute the acceptance ratio

$$R = \frac{p(\boldsymbol{\theta}_t^\star)}{p(\boldsymbol{\theta}_{t-1})} \frac{q(\boldsymbol{\theta}_{t-1} \mid \boldsymbol{\theta}_t^\star)}{q(\boldsymbol{\theta}_t^\star \mid \boldsymbol{\theta}_{t-1})}$$

3. With probability $\min\{R, 1\}$, accept the proposal and set $\boldsymbol{\theta}_t \leftarrow \boldsymbol{\theta}_t^\star$, otherwise set the value to the previous state, $\boldsymbol{\theta}_t \leftarrow \boldsymbol{\theta}_{t-1}$.

Interpretation

- If $R > 1$, the proposal has higher density and we always accept the move.
- If we reject the move, the Markov chain stays at the current value, which induces autocorrelation.
- Since the acceptance probability depends only on the density through ratios, normalizing factors of p and q cancel out.

Symmetric proposals and random walk

If the proposal is symmetric, the ratio of proposal densities is

$$q(\boldsymbol{\theta}_{t-1} \mid \boldsymbol{\theta}_t^\star)/q(\boldsymbol{\theta}_t^\star \mid \boldsymbol{\theta}_{t-1}) = 1.$$

Common examples include random walk proposals

$$\boldsymbol{\theta}_t^\star \leftarrow \boldsymbol{\theta}_{t-1} + \tau Z, \qquad Z$$

where Z is a mean zero, variance one random variable.

Independent proposals

- If we pick instead a global proposal, we must ensure that q samples in far regions (recall rejection sampling), otherwise …
- Good proposals include heavy tailed distribution such as Student-t with small degrees of freedom, centered at the maximum a posteriori $\widehat{\boldsymbol{\theta}}$ and with scale matrix $-\mathbf{H}^{-1}(\boldsymbol{\theta}_t^\star)$, where $\mathbf{H}(\cdot)$ is the Hessian of the log posterior.

Upworthy data example

We model the Poisson rates for headlines with questions or not. Our model is

$$
\begin{aligned}
Y_i &\sim \mathsf{Po}(n_i \lambda_i), \qquad (i = 1, 2) \\
\lambda_1 &= \exp(\beta + \kappa) \\
\lambda_2 &= \exp(\beta) \\
\beta &\sim \mathsf{No}(\log 0.01, 1.5) \\
\kappa &\sim \mathsf{No}(0, 1)
\end{aligned}
$$

Implementation details: data and containers

In regression models, scale inputs if possible.

```
data(upworthy_question, package = "hecbayes")
# Compute sufficient statistics
data <- upworthy_question |>
  dplyr::group_by(question) |>
  dplyr::summarize(ntot = sum(impressions),
                   y = sum(clicks))
# Create containers for MCMC
niter <- 1e4L
chain <- matrix(0, nrow = niter, ncol = 2L)
colnames(chain) <- c("beta","kappa")
```

Implementation details: log posterior function

Perform all calculations on the log scale to avoid numerical overflow!

```r
# Code log posterior as sum of log likelihood and log prior
loglik <- function(par, counts = data$y, offset = data$ntot, ...){
  lambda <- exp(c(par[1] + log(offset[1]), par[1] + par[2] + log(offset[2])))
 sum(dpois(x = counts, lambda = lambda, log = TRUE))
}
# Note common signature of function
logprior <- function(par, ...){
  dnorm(x = par[1], mean = log(0.01), sd = 1.5, log = TRUE) +
    dnorm(x = par[2], log = TRUE)
}
logpost <- function(par, ...){
  loglik(par, ...) + logprior(par, ...)
}
```

Implementation details: proposals

Use good starting values for your Markov chains, such as maximum a posteriori.

```
# Compute maximum a posteriori (MAP)
map <- optim(
  par = c(-4, 0.07),
  fn = logpost,
  control = list(fnscale = -1),
  offset = data$ntot,
  counts = data$y,
  hessian = TRUE)
# Use MAP as starting value
cur <- map$par
# Compute logpost_cur - we can keep track of this to reduce calculations
logpost_cur <- logpost(cur)
# Proposal covariance
cov_map <- -2*solve(map$hessian)
chol <- chol(cov_map)
```

Implementation details: Metropolis–Hastings algorithm

Use seed for reproducibility, do not compute posterior twice, compute log of acceptance ratio.

```
set.seed(80601)
naccept <- 0L
for(i in seq_len(niter)){
  # Multivariate normal proposal - symmetric random walk
  prop <- c(rnorm(n = 2) %*% chol + cur)
  logpost_prop <- logpost(prop)
  logR <- logpost_prop - logpost_cur
  if(logR > -rexp(1)){
    cur <- prop
    logpost_cur <- logpost_prop
    naccept <- naccept + 1L
  }
  chain[i,] <- cur
}
```

Implementation details: analysis of output

Need specialized methods to compute standard errors of the posterior mean.

```
# Posterior summaries
summary(coda::as.mcmc(chain))
# Computing standard errors using batch means
sqrt(diag(mcmc::olbm(chain, batch.length = niter/40)))
```

```
1. Empirical mean and standard deviation for each variable,
   plus standard error of the mean:

          Mean       SD  Naive SE Time-series SE
beta  -4.51268 0.001697 1.697e-05      6.176e-05
kappa  0.07075 0.002033 2.033e-05      9.741e-05

2. Quantiles for each variable:

          2.5%      25%      50%      75%    97.5%
beta  -4.51591 -4.51385 -4.51273 -4.51154 -4.50929
kappa  0.06673  0.06933  0.07077  0.07212  0.07463
```

References

Botev, Z., & L'Écuyer, P. (2017). Simulation from the normal distribution truncated to an interval in the tail. *Proceedings of the 10th EAI International Conference on Performance Evaluation Methodologies and Tools on 10th EAI International Conference on Performance Evaluation Methodologies and Tools*, 23–29. https://doi.org/10.4108/eai.25-10-2016.2266879

Devroye, L. (1986). *Non-Uniform Random Variate Generation*. Springer. http://www.nrbook.com/devroye/