Markov Chain Monte Carlo Methods

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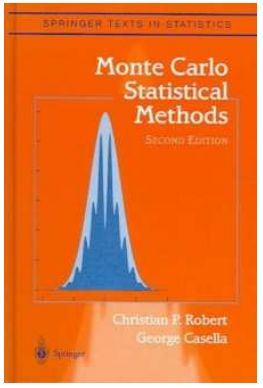
Textbook: *Monte Carlo Statistical Methods* by Christian. P. Robert and George Casella

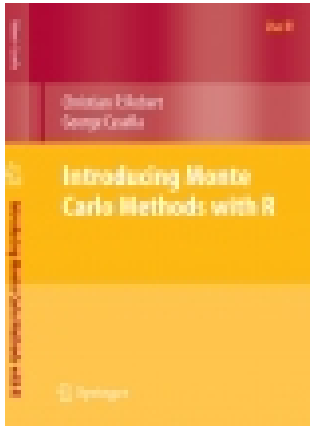


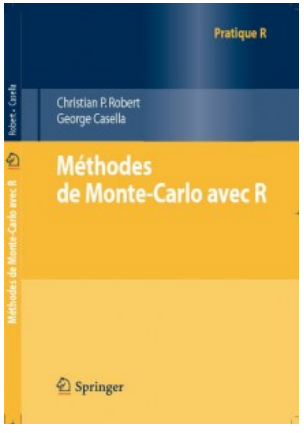
Slides: older slides on

`http://www.ceremade.dauphine.fr/~xian/coursBC.pdf`

Suggested reading

Introducing Monte Carlo Methods with R by Christian. P. Robert and George Casella [trad. française 2010; japonaise 2011]





Outline

Motivation and leading example

Latent structures make life harder!

Even simple models may lead to computational complications, as in **latent variable models**

$$f(x|\theta) = \int f^\star(x, x^\star|\theta)\, \mathrm{d}x^\star$$

If $(x, x^\star)$ observed, fine!
If only x observed, trouble!

Example (Mixture models)

Models of *mixtures of distributions*:

$$X \sim f_j \text{ with probability } p_j,$$

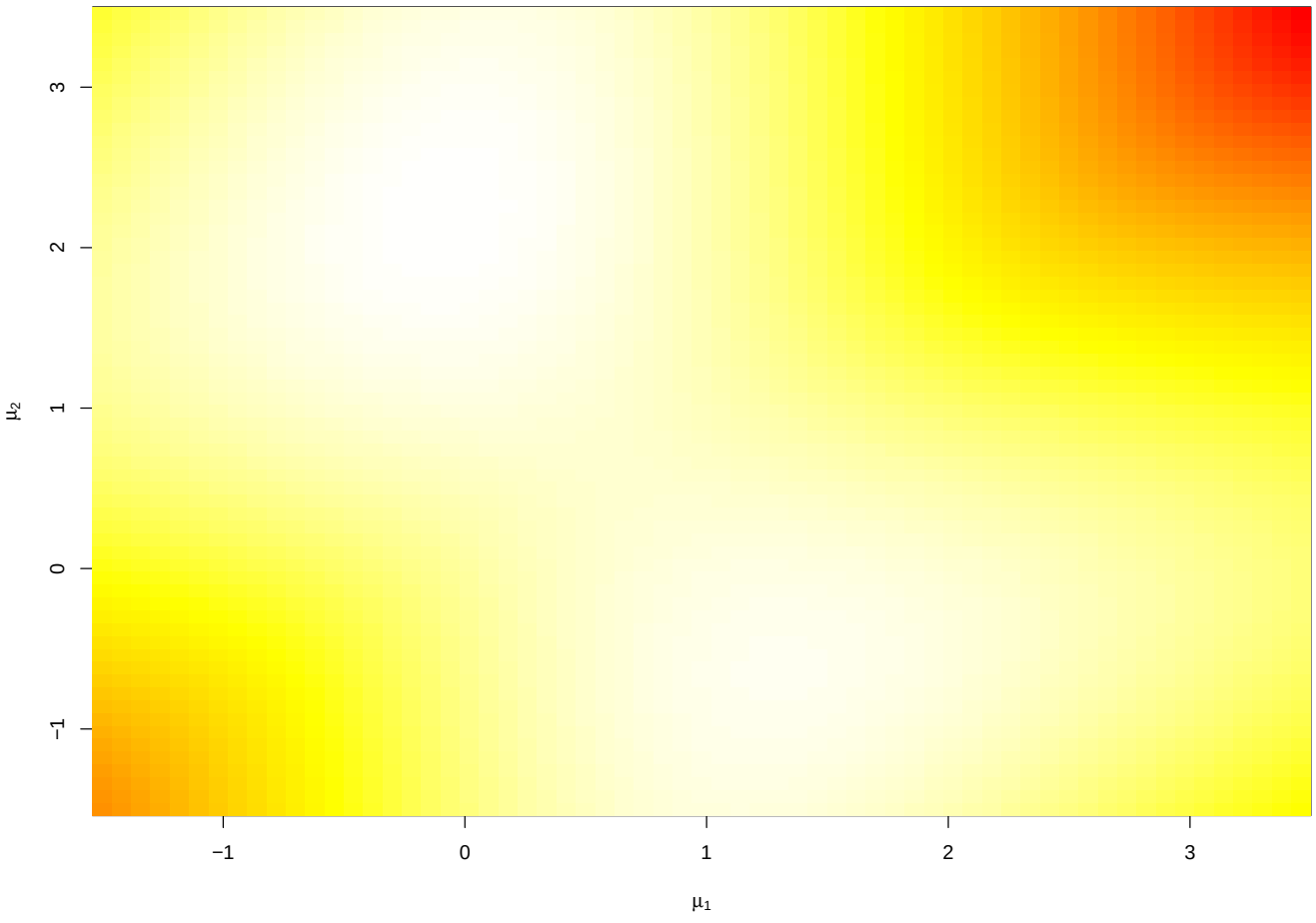
for $j = 1, 2, \ldots, k$, with overall density

$$X \sim p_1 f_1(x) + \cdots + p_k f_k(x) \ .$$

For a sample of independent random variables $(X_1, \cdots, X_n)$, sample density

$$\prod_{i=1}^{n} \{p_1 f_1(x_i) + \cdots + p_k f_k(x_i)\} \ .$$

Expanding this product involves k^n elementary terms: prohibitive to compute in large samples.



Case of the $0.3\mathcal{N}(\mu_1, 1) + 0.7\mathcal{N}(\mu_2, 1)$ likelihood

Maximum likelihood methods

▸ Go Bayes!!

- For an iid sample $X_1, \ldots, X_n$ from a population with density $f(x|\theta_1, \ldots, \theta_k)$, the *likelihood function* is

$$\begin{aligned} L(\boldsymbol{x}|\boldsymbol{\theta}) &= L(x_1, \ldots, x_n|\theta_1, \ldots, \theta_k) \\ &= \prod_{i=1}^{n} f(x_i|\theta_1, \ldots, \theta_k). \end{aligned}$$

$$\hat{\boldsymbol{\theta}}_{\boldsymbol{n}} = \arg\max_{\boldsymbol{\theta}} L(\boldsymbol{x}|\boldsymbol{\theta})$$

- Global justifications from asymptotics
- Computational difficulty depends on structure, eg latent variables

Example (Mixtures again)

For a mixture of two normal distributions,

$$p\mathcal{N}(\mu, \tau^2) + (1-p)\mathcal{N}(\theta, \sigma^2) \ ,$$

likelihood proportional to

$$\prod_{i=1}^{n} \left[p\tau^{-1}\varphi\left(\frac{x_i - \mu}{\tau}\right) + (1-p)\ \sigma^{-1}\ \varphi\left(\frac{x_i - \theta}{\sigma}\right) \right]$$

containing 2^n terms.

Standard maximization techniques often fail to find the global maximum because of multimodality or undesirable behavior (usually at the frontier of the domain) of the likelihood function.

Example

In the special case

$$f(x|\mu,\sigma) = (1-\epsilon)\exp\{(-1/2)x^2\} + \frac{\epsilon}{\sigma}\exp\{(-1/2\sigma^2)(x-\mu)^2\} \tag{1}$$

with $\epsilon > 0$ known, whatever n, the likelihood is unbounded:

$$\lim_{\sigma\to 0} L(x_1,\ldots,x_n|\mu = x_1,\sigma) = \infty$$

The special case of missing variable models

Consider again a latent variable representation

$$g(x|\theta) = \int_{\mathcal{Z}} f(x, z|\theta)\, dz$$

Define the completed (but unobserved) likelihood

$$L^c(\mathbf{x}, \mathbf{z}|\theta) = f(\mathbf{x}, \mathbf{z}|\theta)$$

Useful for optimisation algorithm

The EM Algorithm

▸ Gibbs connection ▸ Bayes rather than EM

Algorithm (Expectation–Maximisation)

Iterate (in m)

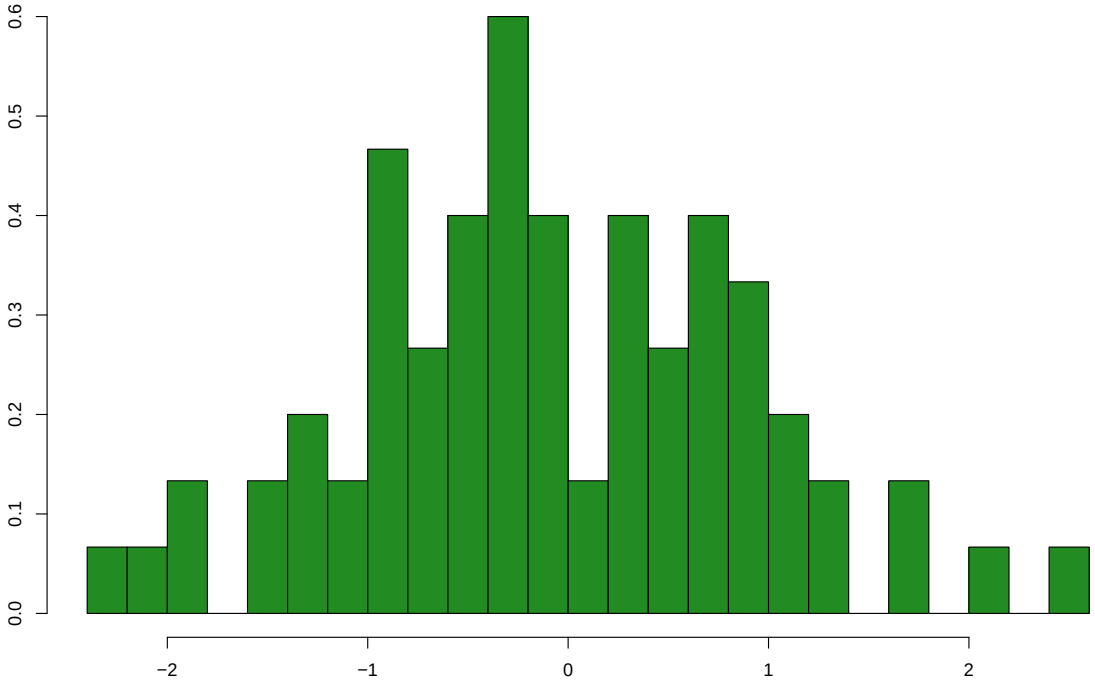
1. (*E step*) Compute

$$Q(\theta;\hat{\theta}_{(m)},\mathbf{x}) = \mathbb{E}[\log L^c(\mathbf{x},\mathbf{Z}|\theta)|\hat{\theta}_{(m)},\mathbf{x}]\,,$$

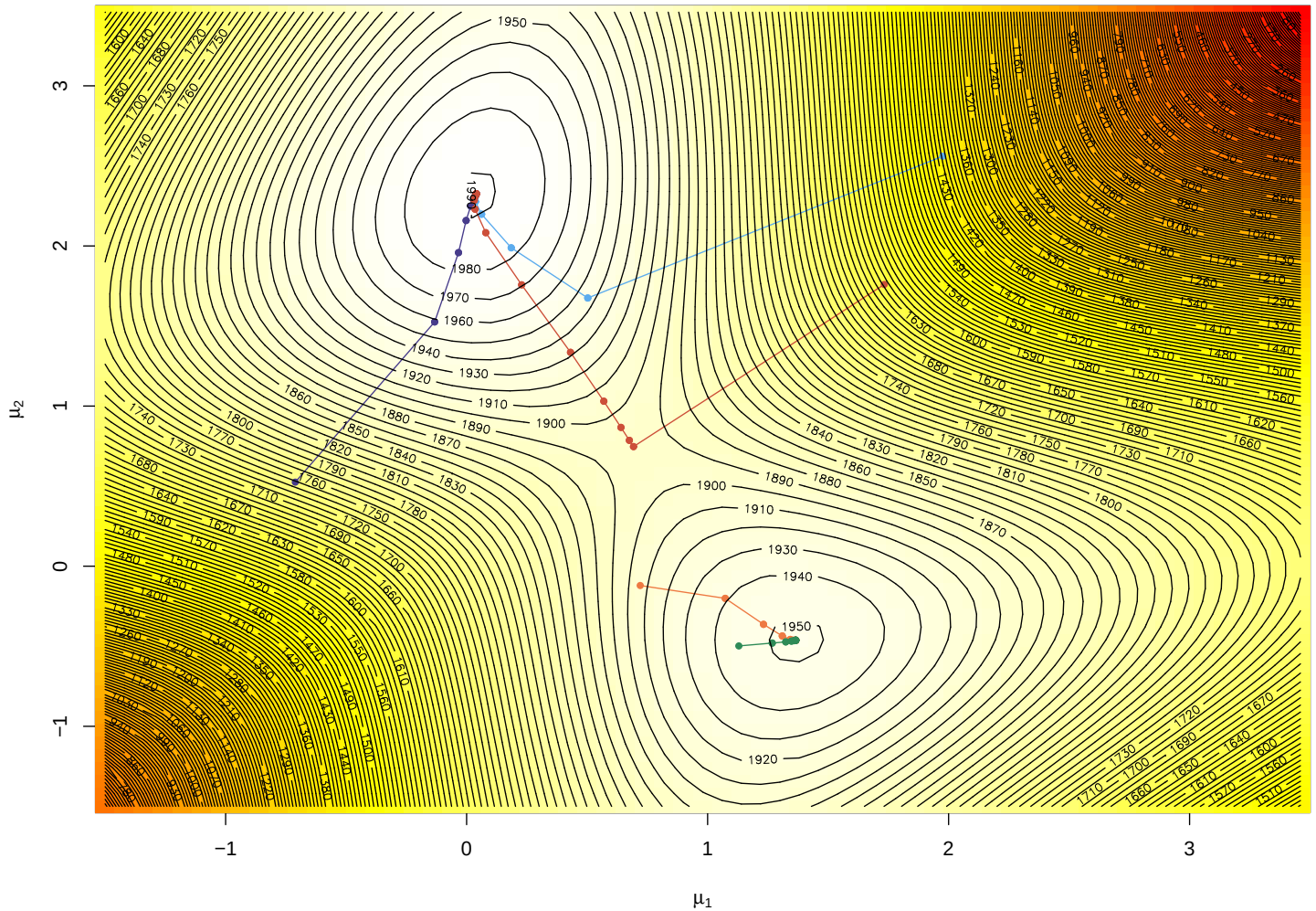
2. (*M step*) Maximise $Q(\theta;\hat{\theta}_{(m)},\mathbf{x})$ in θ and take

$$\hat{\theta}_{(m+1)} = \arg\max_{\theta}\ Q(\theta;\hat{\theta}_{(m)},\mathbf{x}).$$

until a fixed point [of Q] is reached



Sample from the mixture model



Likelihood of $.7\mathcal{N}(\mu_1, 1) + .3\mathcal{N}(\mu_2, 1)$ and EM steps

The Bayesian Perspective

In the Bayesian paradigm, the information brought by the data x, realization of

$$X \sim f(x|\theta),$$

is combined with **prior information** specified by *prior distribution* with density

$$\pi(\theta)$$

Central tool

Summary in a probability distribution, $\pi(\theta|x)$, called the **posterior distribution**

Derived from the *joint* distribution $f(x|\theta)\pi(\theta)$, according to

$$\pi(\theta|x) = \frac{f(x|\theta)\pi(\theta)}{\int f(x|\theta)\pi(\theta)d\theta},$$

[Bayes Theorem]

where

$$Z(x) = \int f(x|\theta)\pi(\theta)d\theta$$

is the *marginal density* of X also called the (Bayesian) evidence

Central tool... central to Bayesian inference

Posterior defined up to a constant as

$$\pi(\theta|x) \propto f(x|\theta)\,\pi(\theta)$$

- Operates conditional upon the observations
- Integrate simultaneously prior information and information brought by x
- Avoids averaging over the unobserved values of x
- Coherent updating of the information available on θ, independent of the order in which i.i.d. observations are collected
- Provides a complete inferential scope and a unique motor of inference

Conjugate bonanza...

Example (Binomial)

For an observation $X \sim \mathscr{B}(n, p)$ so-called **conjugate prior** is the family of beta $\mathscr{B}e(a, b)$ distributions
The classical Bayes estimator δ^π is the posterior mean

$$\frac{\Gamma(a+b+n)}{\Gamma(a+x)\Gamma(n-x+b)} \int_0^1 p\, p^{x+a-1}(1-p)^{n-x+b-1} dp$$
$$= \frac{x+a}{a+b+n}.$$

Conjugate Prior

Conjugacy

Given a likelihood function $L(y|\theta)$, the family Π of priors π_0 on Θ is conjugate if the posterior $\pi(\theta|y)$ also belong to Π

In this case, posterior inference is tractable and reduces to updating the hyperparameters* of the prior

*The *hyperparameters* are parameters of the priors; they are most often not treated as random variables

Discrete/Multinomial & Dirichlet

If the observations consist of positive counts $Y_1, \ldots, Y_d$ modelled by a Multinomial distribution

$$L(y|\theta, n) = \frac{n!}{\prod_{i=1}^{d} y_i!} \prod_{i=1}^{d} \theta_i^{y_i}$$

The conjugate family is the $\mathscr{D}(\alpha_1, \ldots, \alpha_d)$ distribution

$$\pi(\theta|\alpha) = \frac{\Gamma(\sum_{i=1}^{d} \alpha_i)}{\prod_{i=1}^{d} \Gamma(\alpha_i)} \prod_{i}^{d} \theta_i^{\alpha_i - 1}$$

defined on the probability simplex ($\theta_i \geq 0, \sum_{i=1}^{d} \theta_i = 1$), where Γ is the gamma function $\Gamma(\alpha) = \int_0^\infty t^{\alpha-1} \mathrm{e}^{-t} \mathrm{d}t$ ($\Gamma(k) = (k-1)!$ for integers k)

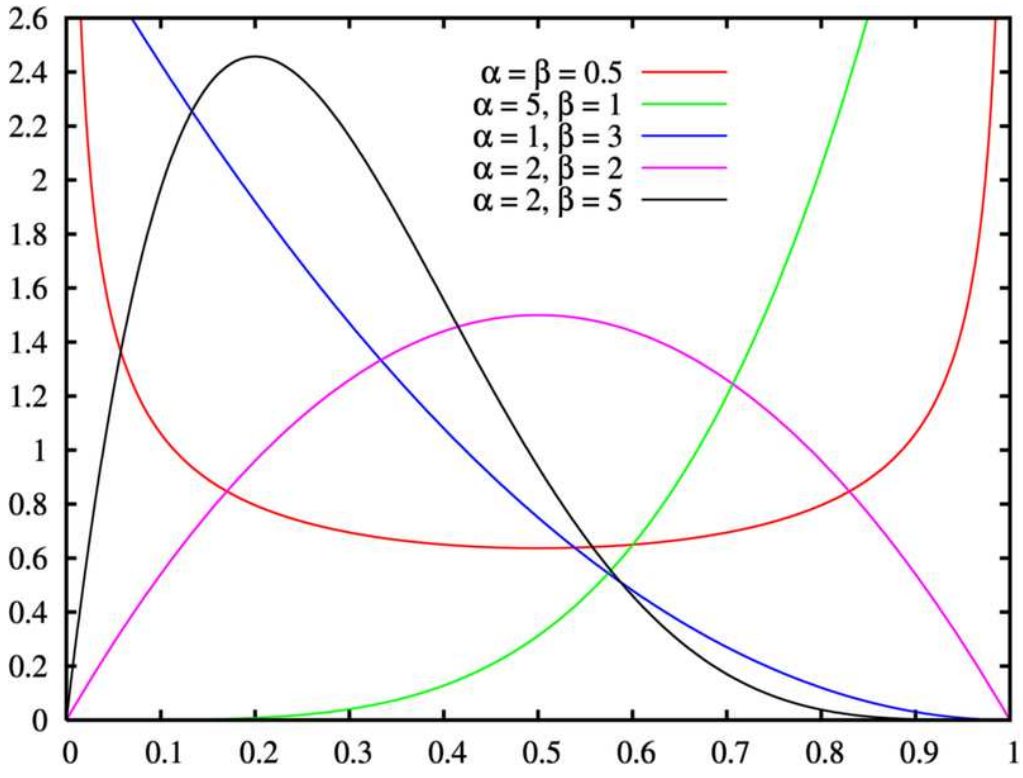


Figure: Dirichlet: 1D marginals

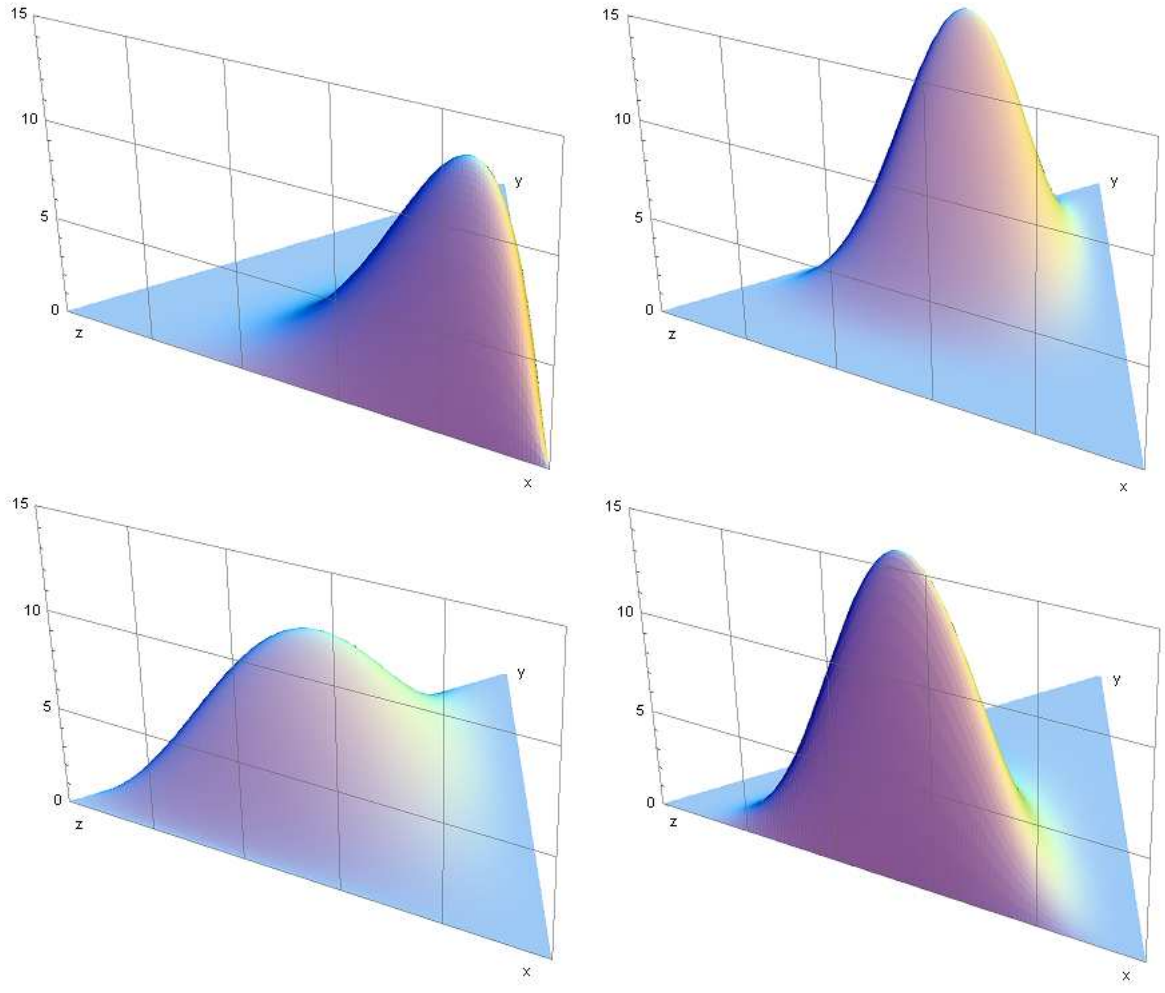


Figure: Dirichlet: 3D examples (projected on two dimensions)

Multinomial Posterior

Posterior

$$\pi(\theta|y) = \mathscr{D}(y_1 + \alpha_1, \ldots, y_d + \alpha_d)$$

Posterior Mean[†]

$$\left(\frac{y_i + \alpha_i}{\sum_{j=1}^{d} y_j + \alpha_j} \right)_{1 \leq i \leq d}$$

MAP

$$\left(\frac{y_i + \alpha_i - 1}{\sum_{j=1}^{d} y_j + \alpha_j - 1} \right)_{1 \leq i \leq d}$$

if $y_i + \alpha_i > 1$ for $i = 1, \ldots, d$

Evidence

$$Z(y) = \frac{\Gamma(\sum_{i=1}^{d} \alpha_i) \prod_{i=1}^{d} \Gamma(y_i + \alpha_i)}{\prod_{i=1}^{d} \Gamma(\alpha_i) \Gamma(\sum_{i=1}^{d} y_i + \alpha_i)}$$

[†] Also known as *Laplace smoothing* when $\alpha_i = 1$

Conjugate Priors for the Normal I

Conjugate Prior for the Normal Mean

For the $\mathcal{N}(y|\mu, w)$ distribution with iid observations $\boldsymbol{y_1}, \ldots, \boldsymbol{y_n}$, the conjugate prior for the mean $\boldsymbol{\mu}$ is Gaussian $\mathcal{N}(\mu|m_0, v_0)$:

$$\begin{aligned}\pi(\mu|y_{1:n}) &\propto \exp\left[-(\mu - m_0)^2/2v_0\right] \prod_{k=1}^{n} \exp\left[-(y_k - \mu)^2/2w\right] \\ &\propto \exp\left\{-\frac{1}{2}\left[\mu^2\left(\frac{1}{v_0} + \frac{n}{w}\right) - 2\mu\left(\frac{m_0}{v_0} + \frac{s_n}{w}\right)\right]\right\} \\ &= \mathcal{N}\left(\mu \,\middle|\, \frac{s_n + m_0 w/v_0}{n + w/v_0}, \frac{w}{n + w/v_0}\right)\end{aligned}$$

where $s_n = \sum_{k=1}^{n} y_k$[a]

[a] And $y_{1:n}$ denotes the collection $y_1, \ldots, y_n$

Conjugate Priors for the Normal II

Conjugate Priors for the Normal Variance

If w is to be estimated and μ is known, the conjugate prior for w is the inverse Gamma distribution $\mathscr{IG}(w|\alpha_0, \beta_0)$:

$$\pi_0(w|\beta_0, \alpha_0) = \frac{\beta_0^{\alpha_0}}{\Gamma(\alpha_0)} w^{-\alpha_0+1} \mathrm{e}^{-\beta_0/w}$$

and

$$\begin{aligned} \pi(w|y_{1:n}) &\propto w^{-(\alpha_0+1)} \mathrm{e}^{-\beta_0/w} \prod_{k=1}^{n} \frac{1}{\sqrt{w}} \exp\left[-(y_k-\mu)^2/2w\right] \\ &= w^{-(n/2+\alpha_0+1)} \exp\left[-(s_n^{(2)}/2 + \beta_0)/w\right] \end{aligned}$$

where $s_n^{(2)} = \sum_{k=1}^{n} (Y_k - \mu)^2$.

The Gamma, Chi-Square and Inverses

The Gamma Distribution[a]

[a] A different convention is to use `Gam*(a,b)`, where $b = 1/\beta$ is the scale parameter

$$\mathcal{G}a(\theta|\alpha,\beta) = \frac{\beta^\alpha}{\Gamma(\alpha)}\theta^{\alpha-1}\mathrm{e}^{-\beta\theta}$$

where α is the shape and β the inverse scale parameter
($\mathbb{E}(\theta) = \alpha/\beta$, $\mathrm{Var}(\theta) = \alpha/\beta^2$)

- $\theta \sim \mathcal{IG}(\theta|\alpha,\beta)$: $1/\theta \sim \mathcal{G}a(\theta|\alpha,\beta)$
- $\theta \sim \chi^2(\theta|\nu)$: $\theta \sim \mathcal{G}a(\theta|\nu/2, 1/2)$

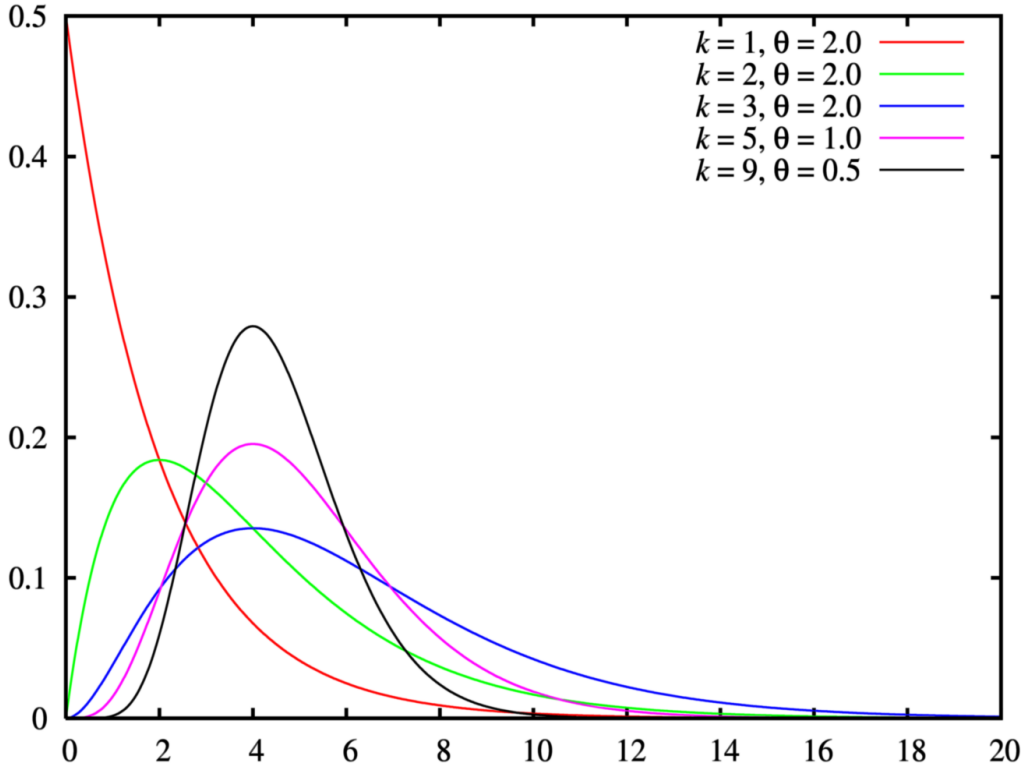


Figure: Gamma pdf ($k = \alpha, \theta = 1/\beta$)

Conjugate Priors for the Normal IV

Example (Normal)

In the normal $\mathcal{N}(\mu, w)$ case, with both μ and w unknown, conjugate prior on $\theta = (\mu, w)$ of the form

$$(w)^{-\lambda_w} \exp - \left\{\lambda_\mu(\mu - \xi)^2 + \alpha\right\}/w$$

since

$$\begin{aligned}
\pi((\mu, w)|x_1, \ldots, x_n) &\propto (w)^{-\lambda_w} \exp - \left\{\lambda_\mu(\mu - \xi)^2 + \alpha\right\}/w \\
&\quad \times (w)^{-n} \exp - \left\{n(\mu - \overline{x})^2 + s_x^2\right\}/w \\
&\propto (w)^{-\lambda_w + n} \exp - \left\{(\lambda_\mu + n)(\mu - \xi_x)^2 \right. \\
&\quad \left. + \alpha + s_x^2 + \frac{n\lambda_\mu}{n + \lambda_\mu}\right\}/w
\end{aligned}$$

Conjugate Priors for the Normal III

Conjugate Priors are However Available Only in Simple Cases

In the previous example the conjugate prior when both μ and w are unknown is not particularly useful.

- Hence, it is very common to resort to independent marginally conjugate priors: eg., in the Gaussian case, take $\mathscr{N}(\mu|m_0, v_0)\mathscr{IG}(w|\alpha_0, \beta_0)$ as prior, then $\pi(\mu|w, y)$ is Gaussian, $\pi(w|\mu, y)$ is inverse-gamma but $\pi(\mu, w|y)$ does not belong to a known family[‡]
- There nonetheless exists some important multivariate extensions : Bayesian normal linear model, inverse-Wishart distribution for covariance matrices

[‡] Although closed-form expressions for $\pi(\mu|y)$ and $\pi(w|y)$ are available

...and conjugate curse

Conjugate priors are very limited in scope

In addition, the use ofconjugate priors only for computational reasons

- implies a restriction on the modeling of the available prior information
- may be detrimental to the usefulness of the Bayesian approach
- gives an impression of subjective manipulation of the prior information disconnected from reality.

A typology of Bayes computational problems

(i). latent variable models in general

(ii). use of a complex parameter space, as for instance in constrained parameter sets like those resulting from imposing stationarity constraints in dynamic models;

(iii). use of a complex sampling model with an intractable likelihood, as for instance in some graphical models;

(iv). use of a huge dataset;

(v). use of a complex prior distribution (which may be the posterior distribution associated with an earlier sample);

Random variable generation

Random variable generation

- Rely on the possibility of producing (computer-wise) an endless flow of random variables (usually iid) from well-known distributions
- Given a uniform random number generator, illustration of methods that produce random variables from both standard and nonstandard distributions

The inverse transform method

For a function F on $\mathbb{R}$, the *generalized inverse* of F, F^-, is defined by

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

Definition (Probability Integral Transform)

If $U \sim \mathcal{U}_{[0,1]}$, then the random variable $F^-(U)$ has the distribution F.

The inverse transform method (2)

To generate a random variable $X \sim F$, simply generate

$$U \sim \mathcal{U}_{[0,1]}$$

and then make the transform

$$x = F^{-}(u)$$

Desiderata and limitations

skip Uniform

- Production of a *deterministic* sequence of values in $[0, 1]$ which imitates a sequence of *iid* uniform random variables $\mathcal{U}_{[0,1]}$.
- Can't use the physical imitation of a "random draw" [no guarantee of uniformity, no reproducibility]
- *Random* sequence in the sense: Having generated $(X_1, \cdots, X_n)$, knowledge of X_n [or of $(X_1, \cdots, X_n)$] imparts no discernible knowledge of the value of X_{n+1}.
- Deterministic: Given the initial value X_0, sample $(X_1, \cdots, X_n)$ always the same
- Validity of a random number generator based on a single sample $X_1, \cdots, X_n$ when n tends to $+\infty$, **not** on replications

$$(X_{11}, \cdots, X_{1n}), (X_{21}, \cdots, X_{2n}), \ldots (X_{k1}, \cdots, X_{kn})$$

where n fixed and k tends to infinity.

Uniform pseudo-random generator

Algorithm starting from an initial value $0 \leq u_0 \leq 1$ and a transformation D, which produces a sequence

$$(u_i) = (D^i(u_0))$$

in $[0, 1]$.
For all n,

$$(u_1, \cdots, u_n)$$

reproduces the behavior of an iid $\mathcal{U}_{[0,1]}$ sample $(V_1, \cdots, V_n)$ when compared through usual tests

Uniform pseudo-random generator (2)

- Validity means the sequence $U_1, \cdots, U_n$ leads to accept the hypothesis

$$\mathrm{H} : U_1, \cdots, U_n \quad \text{are iid} \quad \mathcal{U}_{[0,1]}.$$

- The set of tests used is generally of some consequence
  - Kolmogorov–Smirnov and other nonparametric tests
  - Time series methods, for correlation between U_i and $(U_{i-1}, \cdots, U_{i-k})$
  - Marsaglia's battery of tests called *Die Hard* (!)

Usual generators

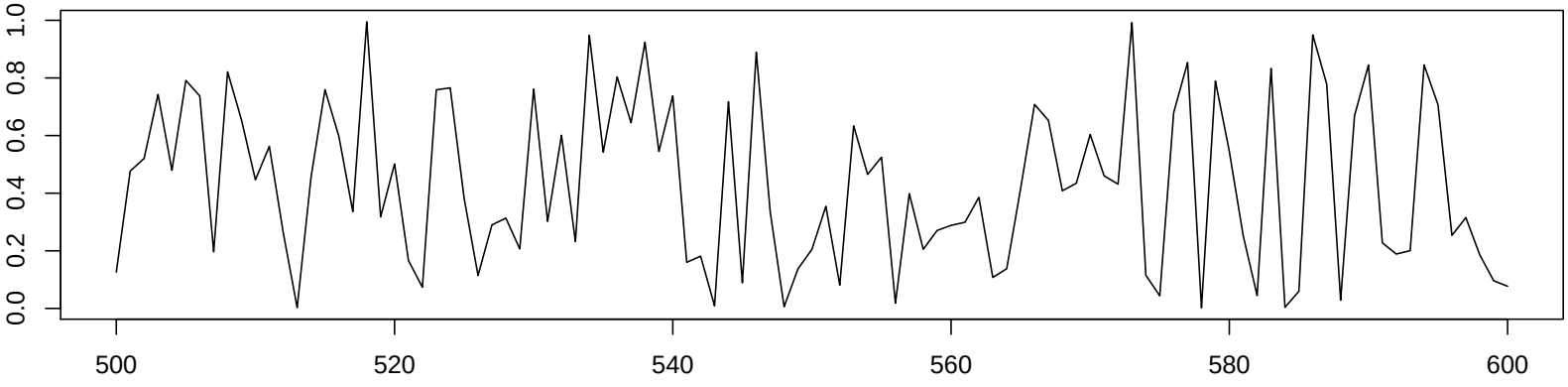
In R and S-plus, procedure `runif()`

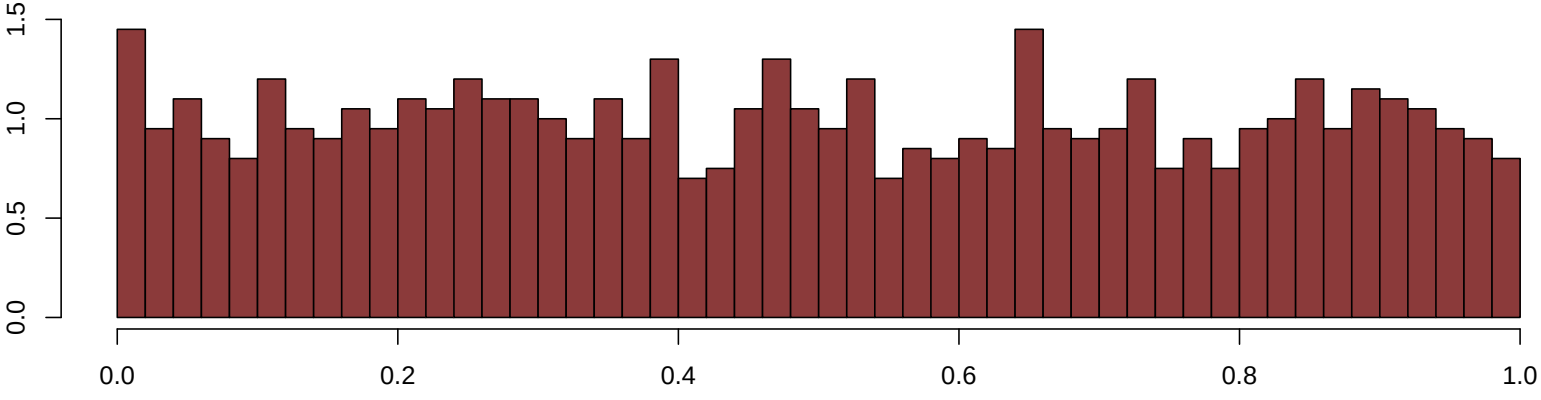
```
The Uniform Distribution

Description:
'runif' generates random deviates.

Example:
     u <- runif(20)

'.Random.seed' is an integer vector, containing
the random number generator state for random
number generation in R. It can be saved and
restored, but should not be altered by users.
```


0.0
0.2
0.4
0.6
0.8
1.0
500
520
540
560
580
600
uniform sample


0.0
0.5
1.0
1.5
0.0
0.2
0.4
0.6
0.8
1.0

Usual generators (2)

In C, procedure `rand()` or `random()`

```
SYNOPSIS
       #include <stdlib.h>
       long int random(void);
DESCRIPTION
The random() function uses a non-linear additive
feedback random number generator employing a
default table of size 31 long integers to return
successive pseudo-random numbers in the range
from 0 to RAND_MAX. The period of this random
generator is very large, approximately
16*((2**31)-1).
RETURN VALUE
random() returns a value between 0 and RAND_MAX.
```

Usual generators (3)

In Matlab and Octave, procedure `rand()`

```
RAND Uniformly distributed pseudorandom numbers.
   R = RAND(M,N) returns an M-by-N matrix containing
   pseudorandom values drawn from the standard uniform
   distribution on the open interval(0,1).

   The sequence of numbers produced by RAND is
   determined by the internal state of the uniform
   pseudorandom number generator that underlies RAND,
   RANDI, and RANDN.
```

Usual generators (4)

In Scilab, procedure `rand()`

```
rand()  :  with no arguments gives a scalar whose
value  changes  each  time  it  is referenced. By
default, random numbers are uniformly distributed
in the interval (0,1). rand('normal') switches to
a normal distribution with mean 0 and variance 1.

EXAMPLE
  x=rand(10,10,'uniform')
```

Beyond Uniform generators

- Generation of any sequence of random variables can be formally implemented through a uniform generator
  - Distributions with explicit F^- (for instance, exponential, and Weibull distributions), use the probability integral transform
    ◂ here
  - Case specific methods rely on properties of the distribution (for instance, normal distribution, Poisson distribution)
  - More generic methods (for instance, accept-reject)
- Simulation of the standard distributions is accomplished quite efficiently by many numerical and statistical programming packages.

Transformation methods

Case where a distribution F is linked in a simple way to another distribution easy to simulate.

Example (Exponential variables)

If $U \sim \mathcal{U}_{[0,1]}$, the random variable

$$X = -\log U/\lambda$$

has distribution

$$\begin{aligned} P(X \leq x) &= P(-\log U \leq \lambda x) \\ &= P(U \geq e^{-\lambda x}) = 1 - e^{-\lambda x}, \end{aligned}$$

the exponential distribution $\mathscr{E}xp(\lambda)$.

Other random variables that can be generated starting from an exponential include

$$Y = -2 \sum_{j=1}^{\nu} \log(U_j) \sim \chi^2_{2\nu}$$

$$Y = -\frac{1}{\beta} \sum_{j=1}^{a} \log(U_j) \sim \mathscr{G}a(a, \beta)$$

$$Y = \frac{\sum_{j=1}^{a} \log(U_j)}{\sum_{j=1}^{a+b} \log(U_j)} \sim \mathscr{B}e(a, b)$$

Points to note

- Transformation quite simple to use
- There are more efficient algorithms for gamma and beta random variables
- Cannot generate gamma random variables with a non-integer shape parameter
- For instance, cannot get a χ^2_1 variable, which would get us a $\mathcal{N}(0, 1)$ variable.

Box-Muller Algorithm

Example (Normal variables)

If r, θ polar coordinates of (X_1, X_2), then,

$$r^2 = X_1^2 + X_2^2 \sim \chi_2^2 = \mathscr{E}(1/2) \quad \text{and} \quad \theta \sim \mathscr{U}[0, 2\pi]$$

Consequence: If U_1, U_2 iid $\mathcal{U}_{[0,1]}$,

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

iid $\mathcal{N}(0, 1)$.

Box-Muller Algorithm (2)

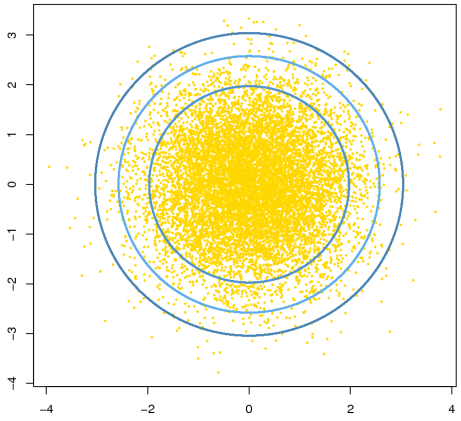
1. Generate U_1, U_2 iid $\mathcal{U}_{[0,1]}$;
2. Define

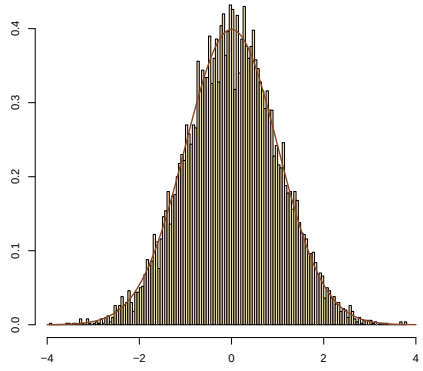
$$\begin{aligned} x_1 &= \sqrt{-2\log(u_1)}\cos(2\pi u_2) \ , \\ x_2 &= \sqrt{-2\log(u_1)}\sin(2\pi u_2) \ ; \end{aligned}$$

3. Take x_1 and x_2 as two independent draws from $\mathcal{N}(0,1)$.

Box-Muller Algorithm (3)

- Unlike algorithms based on the CLT, this algorithm is exact
- Get two normals for the price of two uniforms
- Drawback (in speed) in calculating log, cos and sin.





More transforms

Reject

Example (Poisson generation)

Poisson–exponential connection:
If $N \sim \mathcal{P}(\lambda)$ and $X_i \sim \mathcal{E}xp(\lambda)$, $i \in \mathbb{N}^*$,

$$P_\lambda(N = k) = P_\lambda(X_1 + \cdots + X_k \leq 1 < X_1 + \cdots + X_{k+1}) \,.$$

More Poisson

Skip Poisson

- A Poisson can be simulated by generating $\mathscr{E}xp(1)$ till their sum exceeds 1.
- This method is simple, but is really practical only for smaller values of λ.
- On average, the number of exponential variables required is λ.
- Other approaches are more suitable for large λ's.

Negative extension

- A generator of Poisson random variables can produce negative binomial random variables since,

$$Y \sim \mathcal{G}a(n, (1-p)/p) \quad X|y \sim \mathcal{P}(y)$$

implies

$$X \sim \mathcal{N}eg(n, p)$$

Mixture representation

- The representation of the negative binomial is a particular case of a *mixture distribution*
- The principle of a mixture representation is to represent a density f as the marginal of another distribution, for example

$$f(x) = \sum_{i \in \mathscr{Y}} p_i \, f_i(x) \, ,$$

- If the component distributions $f_i(x)$ can be easily generated, X can be obtained by first choosing f_i with probability p_i and then generating an observation from f_i.

Partitioned sampling

Special case of mixture sampling when

$$f_i(x) = f(x)\,\mathbb{I}_{A_i}(x) \Big/ \int_{A_i} f(x)\,dx$$

and

$$p_i = \mathsf{Pr}(X \in A_i)$$

for a partition $(A_i)_i$

Accept-Reject algorithm

- Many distributions from which it is difficult, or even impossible, to **directly** simulate.
- Another class of methods that only require us to know the functional form of the density f of interest **only** up to a multiplicative constant.
- The key to this method is to use a simpler (simulation-wise) density g, the *instrumental density*, from which the simulation from the *target density* f is actually done.

Fundamental theorem of simulation

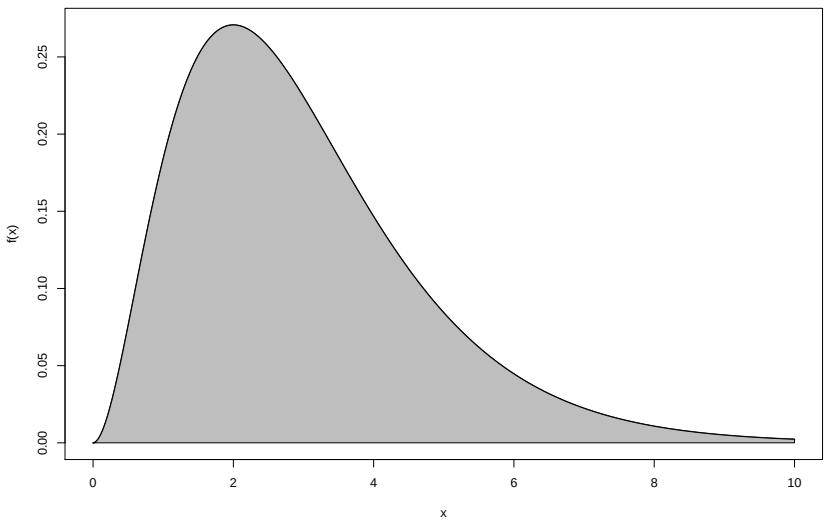
Lemma

Simulating

$$X \sim f(x)$$

equivalent to simulating

$$(X, U) \sim \mathcal{U}\{(x, u) : 0 < u < f(x)\}$$



The Accept-Reject algorithm

Given a density of interest f, find a density g and a constant M such that

$$f(x) \leq Mg(x)$$

on the support of f.

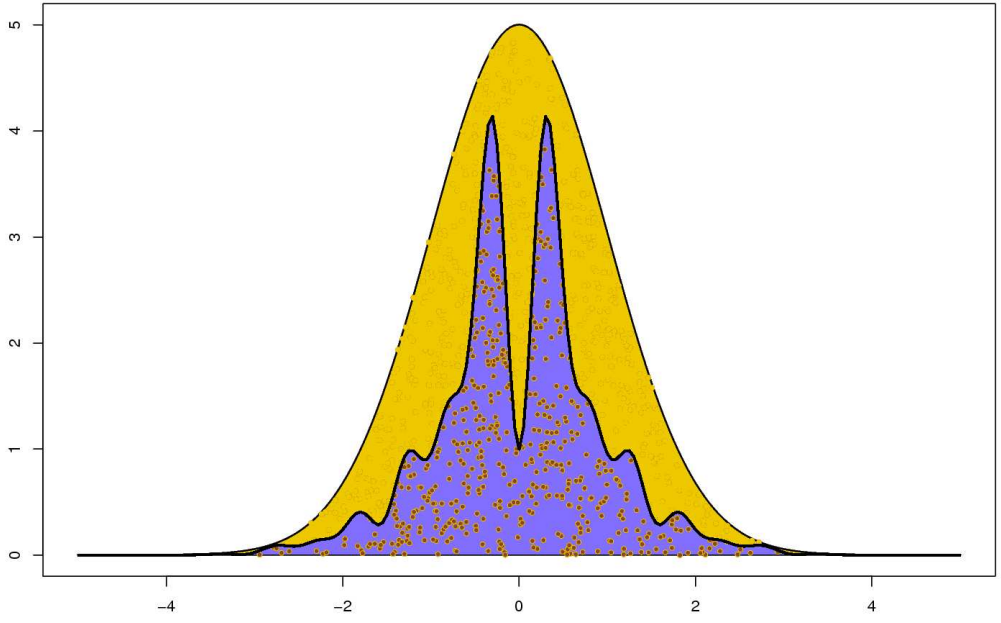
Accept-Reject Algorithm

1. Generate $X \sim g$, $U \sim \mathcal{U}_{[0,1]}$;
2. Accept $Y = X$ if $U \leq f(X)/Mg(X)$;
3. Return to 1. otherwise.

Validation of the Accept-Reject method

Warranty:

This algorithm produces a variable Y distributed according to f



Two interesting properties

- First, it provides a generic method to simulate from any density f that is known *up to a multiplicative factor* Property particularly important in Bayesian calculations where the posterior distribution

$$\pi(\theta|x) \propto \pi(\theta)\ f(x|\theta)\ .$$

  is specified up to a normalizing constant
- Second, the probability of acceptance in the algorithm is $1/M$, e.g., expected number of trials until a variable is accepted is M

More interesting properties

- In cases f and g both probability densities, the constant M is necessarily larger that 1.
- The size of M, and thus the efficiency of the algorithm, are functions of how closely g can imitate f, especially in the tails
- For f/g to remain bounded, necessary for g to have tails thicker than those of f.
  It is therefore impossible to use the A-R algorithm to simulate a Cauchy distribution f using a normal distribution g, however the reverse works quite well.

No Cauchy!

Example (Normal from a Cauchy)

Take

$$f(x) = \frac{1}{\sqrt{2\pi}} \exp(-x^2/2)$$

and

$$g(x) = \frac{1}{\pi} \frac{1}{1+x^2},$$

densities of the normal and Cauchy distributions.
Then

$$\frac{f(x)}{g(x)} = \sqrt{\frac{\pi}{2}}(1+x^2)\, e^{-x^2/2} \leq \sqrt{\frac{2\pi}{e}} = 1.52$$

attained at $x = \pm 1$.

Example (Normal from a Cauchy (2))

So probability of acceptance

$$1/1.52 = 0.66,$$

and, on the average, one out of every three simulated Cauchy variables is rejected.

No Double!

Example (Normal/Double Exponential)

Generate a $\mathcal{N}(0,1)$ by using a double-exponential distribution with density

$$g(x|\alpha) = (\alpha/2)\exp(-\alpha|x|)$$

Then

$$\frac{f(x)}{g(x|\alpha)} \leq \sqrt{\frac{2}{\pi}}\alpha^{-1}e^{-\alpha^2/2}$$

and minimum of this bound (in α) attained for

$$\alpha^\star = 1$$

Example (Normal/Double Exponential (2))

Probability of acceptance

$$\sqrt{\pi/2e} = .76$$

To produce one normal random variable requires on the average $1/.76 \approx 1.3$ uniform variables.

truncate

Example (Gamma generation)

Illustrates a real advantage of the Accept-Reject algorithm
The gamma distribution $\mathcal{G}a(\alpha, \beta)$ represented as the sum of α exponential random variables, only if α is an integer

Example (Gamma generation (2))

Can use the Accept-Reject algorithm with instrumental distribution

$$\mathcal{G}a(a, b), \text{ with } a = [\alpha], \quad \alpha \geq 0.$$

(Without loss of generality, $\beta = 1$.)
Up to a normalizing constant,

$$f/g_b = b^{-a} x^{\alpha - a} \exp\{-(1-b)x\} \leq b^{-a} \left(\frac{\alpha - a}{(1-b)e} \right)^{\alpha - a}$$

for $b \leq 1$.
The maximum is attained at $b = a/\alpha$.

Truncated Normal simulation

Example (Truncated Normal distributions)

Constraint $x \geq \underline{\mu}$ produces density proportional to

$$e^{-(x-\mu)^2/2\sigma^2}\ \mathbb{I}_{x \geq \underline{\mu}}$$

for a bound $\underline{\mu}$ large compared with μ
There exists alternatives far superior to the naïve method of generating a $\mathcal{N}(\mu, \sigma^2)$ until exceeding $\underline{\mu}$, which requires an average number of

$$1/\Phi((\mu - \underline{\mu})/\sigma)$$

simulations from $\mathcal{N}(\mu, \sigma^2)$ for a single acceptance.

Example (Truncated Normal distributions (2))

Instrumental distribution: translated exponential distribution, $\mathscr{E}(\alpha, \underline{\mu})$, with density

$$g_\alpha(z) = \alpha e^{-\alpha(z-\underline{\mu})}\, \mathbb{I}_{z \geq \underline{\mu}}\,.$$

The ratio f/g_α is bounded by

$$f/g_\alpha \leq \begin{cases} 1/\alpha\ \exp(\alpha^2/2 - \alpha\underline{\mu}) & \text{if } \alpha > \underline{\mu}\,, \\ 1/\alpha\ \exp(-\underline{\mu}^2/2) & \text{otherwise.} \end{cases}$$

Log-concave densities (1)

move to next chapter Densities f whose logarithm is concave, for instance Bayesian posterior distributions such that

$$\log\ \pi(\theta|x) = \log\ \pi(\theta) + \log\ f(x|\theta) + c$$

concave

Log-concave densities (2)

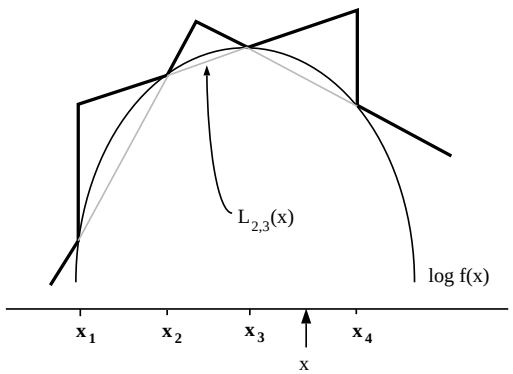
Take

$$\mathfrak{S}_n = \{x_i, i = 0, 1, \ldots, n+1\} \subset \text{supp}(f)$$

such that $h(x_i) = \log f(x_i)$ known up to the same constant.

By concavity of h, line $L_{i,i+1}$ through $(x_i, h(x_i))$ and $(x_{i+1}, h(x_{i+1}))$

- below h in $[x_i, x_{i+1}]$ and
- above this graph outside this interval



Log-concave densities (3)

For $x \in [x_i, x_{i+1}]$, if

$$\overline{h}_n(x) = \min\{L_{i-1,i}(x), L_{i+1,i+2}(x)\} \quad \text{and} \quad \underline{h}_n(x) = L_{i,i+1}(x)\,,$$

the envelopes are

$$\underline{h}_n(x) \le h(x) \le \overline{h}_n(x)$$

uniformly on the support of f, with

$$\underline{h}_n(x) = -\infty \quad \text{and} \quad \overline{h}_n(x) = \min(L_{0,1}(x), L_{n,n+1}(x))$$

on $[x_0, x_{n+1}]^c$.

Log-concave densities (4)

Therefore, if

$$\underline{f}_n(x) = \exp \underline{h}_n(x) \text{ and } \overline{f}_n(x) = \exp \overline{h}_n(x)$$

then

$$\underline{f}_n(x) \le f(x) \le \overline{f}_n(x) = \varpi_n \, g_n(x) \, ,$$

where ϖ_n normalizing constant of f_n

ARS Algorithm

1. Initialize n and $\mathfrak{S}_n$.
2. Generate $X \sim g_n(x)$, $U \sim \mathcal{U}_{[0,1]}$.
3. If $U \leq \underline{f}_n(X)/\varpi_n \, g_n(X)$, accept X;
   otherwise, if $U \leq f(X)/\varpi_n \, g_n(X)$, accept X

▸ kill ducks

Example (Northern Pintail ducks)

Ducks captured at time i with both probability p_i and size N of the population unknown.
Dataset

$$(n_1, \ldots, n_{11}) = (32, 20, 8, 5, 1, 2, 0, 2, 1, 1, 0)$$

Number of recoveries over the years 1957–1968 of 1612 Northern Pintail ducks banded in 1956

Example (Northern Pintail ducks (2))

Corresponding conditional likelihood

$$L(n_1, \ldots, n_I | N, p_1, \ldots, p_I) \propto \prod_{i=1}^{I} p_i^{n_i} (1 - p_i)^{N - n_i},$$

where I number of captures, n_i number of captured animals during the ith capture, and r is the total number of different captured animals.

Example (Northern Pintail ducks (3))

Prior selection

If

$$N \sim \mathscr{P}(\lambda)$$

and

$$\alpha_i = \log\left(\frac{p_i}{1-p_i}\right) \sim \mathcal{N}(\mu_i, \sigma^2),$$

[Normal logistic]

Example (Northern Pintail ducks (4))

Posterior distribution

$$\pi(\alpha, N|, n_1, \ldots, n_I) \propto \frac{N!}{(N-r)!}\frac{\lambda^N}{N!}\prod_{i=1}^{I}(1+e^{\alpha_i})^{-N} \prod_{i=1}^{I}\exp\left\{\alpha_i n_i - \frac{1}{2\sigma^2}(\alpha_i-\mu_i)^2\right\}$$

Example (Northern Pintail ducks (5))

For the conditional posterior distribution

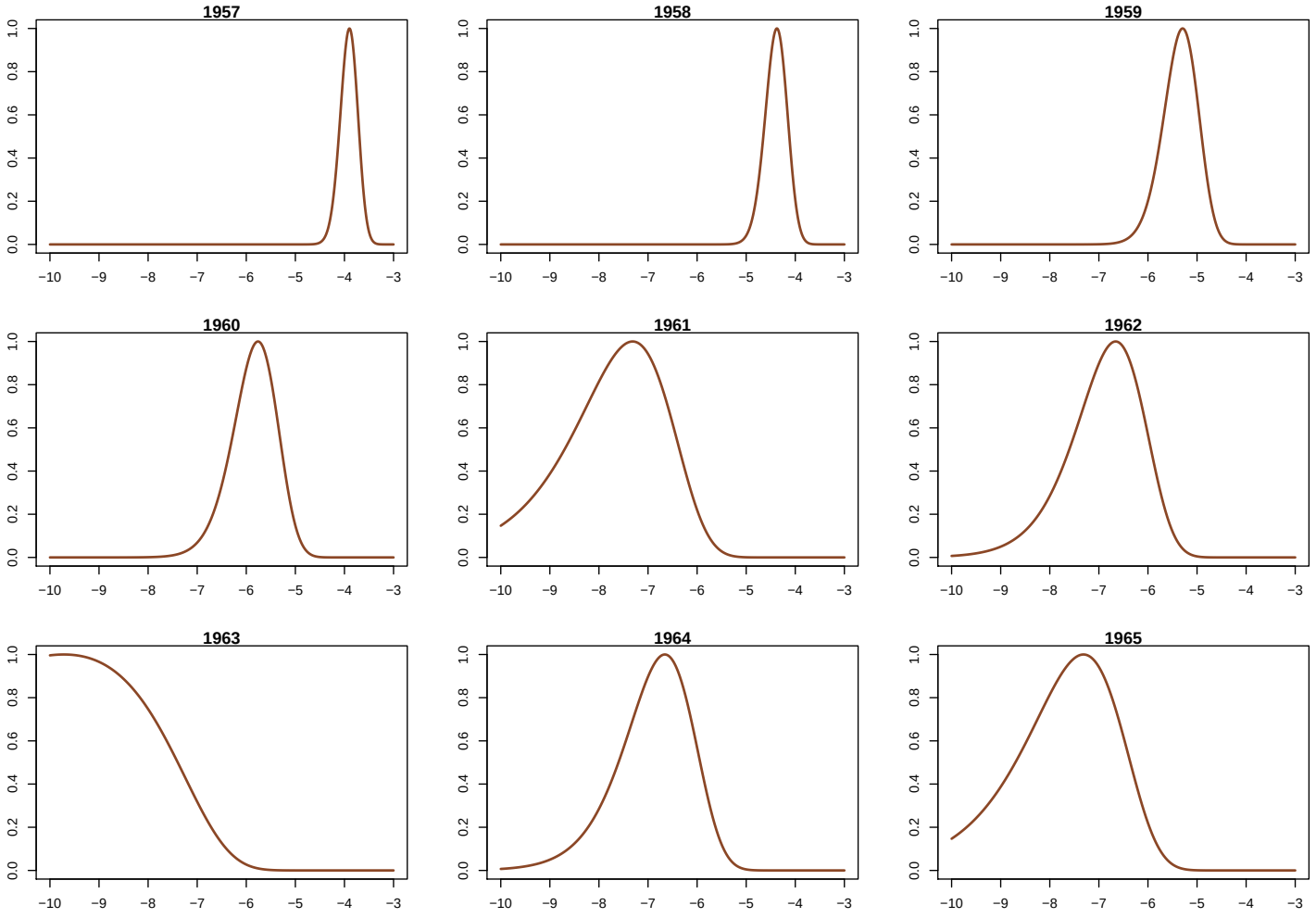
$$\pi(\alpha_i|N, n_1, \ldots, n_I) \propto \exp\left\{\alpha_i n_i - \frac{1}{2\sigma^2}(\alpha_i - \mu_i)^2\right\} \Big/ (1+e^{\alpha_i})^N ,$$

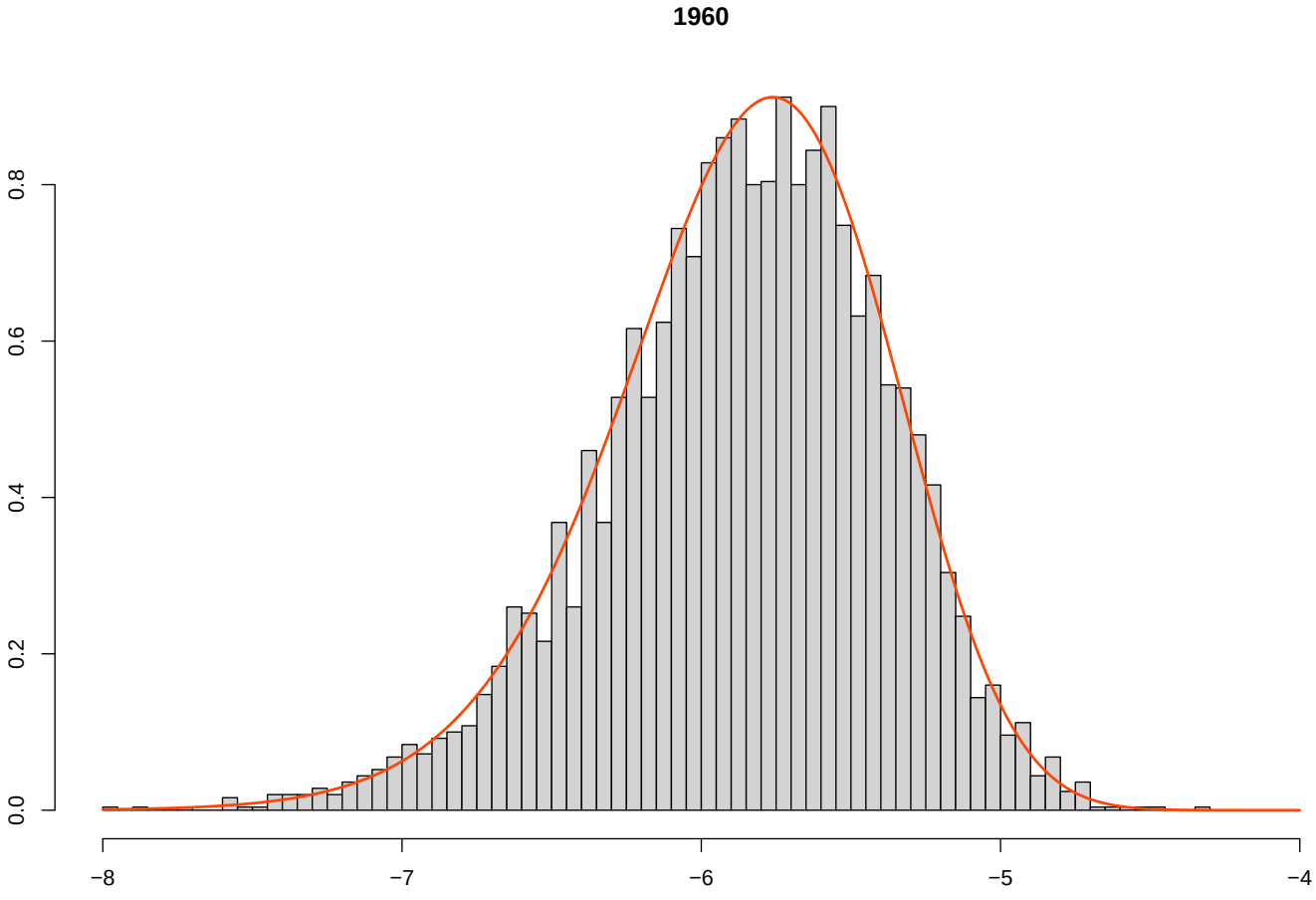
the ARS algorithm can be implemented since

$$\alpha_i n_i - \frac{1}{2\sigma^2}\,(\alpha_i - \mu_i)^2 - N\,\log(1 + e^{\alpha_i})$$

is concave in α_i.

Posterior distributions of capture log-odds ratios for the years 1957–1965.





True distribution versus histogram of simulated sample

Monte Carlo integration

Quick reminder

Two major classes of numerical problems that arise in statistical inference

- **Optimization** - generally associated with the likelihood approach
- **Integration**- generally associated with the Bayesian approach

skip Example!

Example (Bayesian decision theory)

Bayes estimators are not always posterior expectations, but rather solutions of the minimization problem

$$\min_{\delta} \int_{\Theta} \mathrm{L}(\theta, \delta)\, \pi(\theta)\, f(x|\theta)\, d\theta\ .$$

Proper loss:
For $\mathrm{L}(\theta, \delta) = (\theta - \delta)^2$, the Bayes estimator is the **posterior mean**
Absolute error loss:
For $\mathrm{L}(\theta, \delta) = |\theta - \delta|$, the Bayes estimator is the **posterior median**
With no loss function
use the maximum a posteriori (MAP) estimator

$$\arg\max_{\theta} \ell(\theta|x)\pi(\theta)$$

Monte Carlo integration

Theme:

Generic problem of evaluating the integral

$$\mathfrak{I} = \mathbb{E}_f[h(X)] = \int_{\mathscr{X}} h(x)\ f(x)\ dx$$

where $\mathscr{X}$ is uni- or multidimensional, f is a closed form, partly closed form, or implicit density, and h is a function

Monte Carlo integration (2)

Monte Carlo solution

First use a sample $(X_1, \ldots, X_m)$ from the density f to approximate the integral $\mathfrak{I}$ by the empirical average

$$\overline{h}_m = \frac{1}{m} \sum_{j=1}^{m} h(x_j)$$

which converges

$$\overline{h}_m \longrightarrow \mathbb{E}_f[h(X)]$$

by the **Strong Law of Large Numbers**

Monte Carlo precision

Estimate the variance with

$$v_m = \frac{1}{m-1} \sum_{j=1}^{m} [h(x_j) - \overline{h}_m]^2,$$

and for m large,

$$\frac{\overline{h}_m - \mathbb{E}_f[h(X)]}{\sqrt{v_m}} \sim \mathcal{N}(0,1).$$

Note: This can lead to the construction of a convergence test and of confidence bounds on the approximation of $\mathbb{E}_f[h(X)]$.

Example (Cauchy prior/normal sample)

For estimating a normal mean, a *robust* prior is a Cauchy prior

$$X \sim \mathcal{N}(\theta, 1), \quad \theta \sim \mathcal{C}(0, 1).$$

Under squared error loss, posterior mean

$$\delta^\pi(x) = \frac{\displaystyle\int_{-\infty}^{\infty} \frac{\theta}{1+\theta^2} e^{-(x-\theta)^2/2} d\theta}{\displaystyle\int_{-\infty}^{\infty} \frac{1}{1+\theta^2} e^{-(x-\theta)^2/2} d\theta}$$

Example (Cauchy prior/normal sample (2))

Form of δ^π suggests simulating iid variables

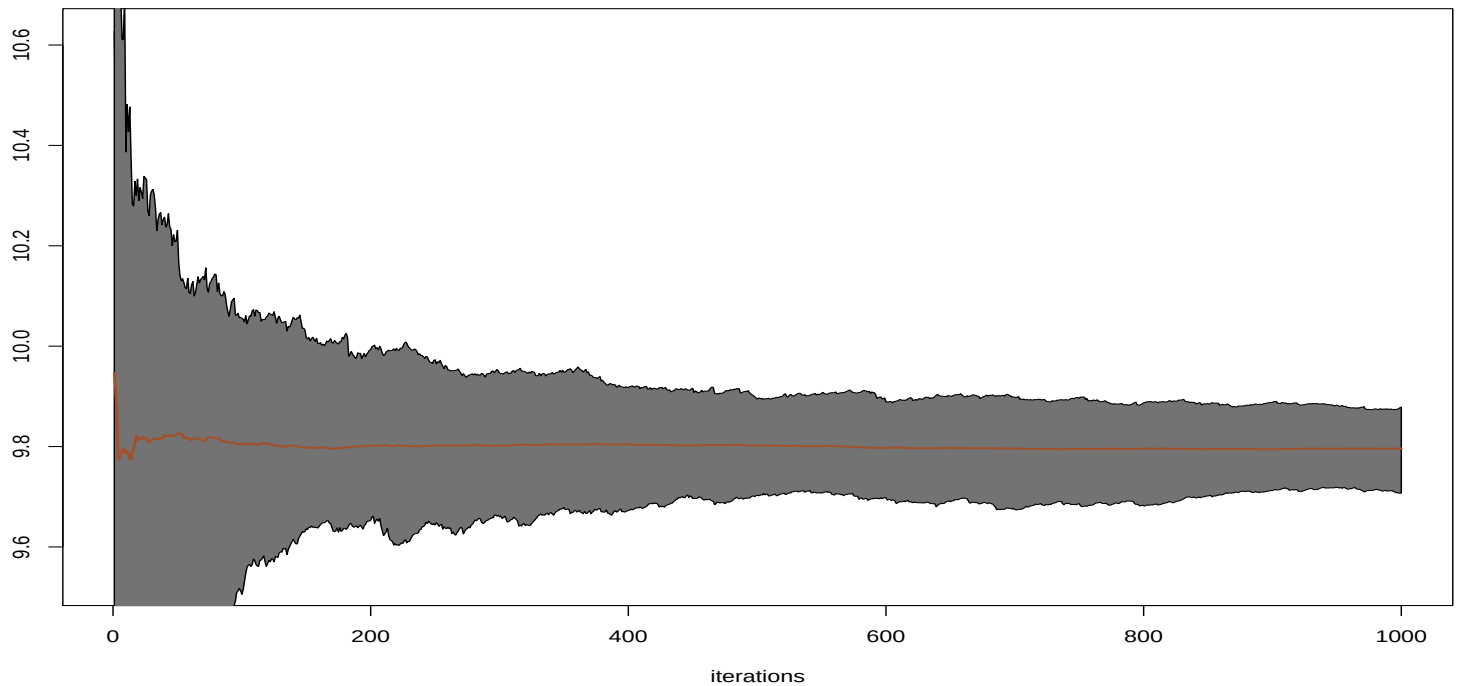
$$\theta_1, \cdots, \theta_m \sim \mathcal{N}(x, 1)$$

and calculating

$$\hat{\delta}_m^\pi(x) = \sum_{i=1}^m \frac{\theta_i}{1+\theta_i^2} \Big/ \sum_{i=1}^m \frac{1}{1+\theta_i^2} \ .$$

The Law of Large Numbers implies

$$\hat{\delta}_m^\pi(x) \longrightarrow \delta^\pi(x) \text{ as } m \longrightarrow \infty.$$



Range of estimators δ_m^π for 100 runs and $x = 10$

Importance sampling

Paradox

Simulation from f (the true density) is not necessarily **optimal**

Alternative to direct sampling from f is **importance sampling**, based on the alternative representation

$$\mathbb{E}_f[h(X)] = \int_{\mathcal{X}} \left[h(x) \, \frac{f(x)}{g(x)} \right] \, g(x) \, dx \, .$$

which allows us to use **other** distributions than f

Importance sampling algorithm

Evaluation of

$$\mathbb{E}_f[h(X)] = \int_{\mathscr{X}} h(x)\, f(x)\, dx$$

by

1. Generate a sample $X_1, \ldots, X_n$ from a distribution g
2. Use the approximation

$$\frac{1}{m} \sum_{j=1}^{m} \frac{f(X_j)}{g(X_j)}\, h(X_j)$$

Same thing as before!!!

Convergence of the estimator

$$\frac{1}{m}\sum_{j=1}^{m}\frac{f(X_j)}{g(X_j)}\,h(X_j)\longrightarrow\int_{\mathscr{X}}h(x)\,f(x)\,dx$$

converges for any choice of the distribution g
[as long as $supp(g)\supset supp(f)$**]**

Important details

- Instrumental distribution g chosen from distributions easy to simulate
- The same sample (generated from g) can be used repeatedly, not only for different functions h, but also for different densities f
- Even dependent proposals can be used, as seen later

▸ PMC chapter

Although g can be any density, some choices are better than others:

- Finite variance only when

$$\mathbb{E}_f \left[h^2(X) \frac{f(X)}{g(X)} \right] = \int_{\mathcal{X}} h^2(x) \, \frac{f^2(X)}{g(X)} \, dx < \infty \, .$$

- Instrumental distributions with tails lighter than those of f (that is, with $\sup f/g = \infty$) not appropriate.
- If $\sup f/g = \infty$, the weights $f(x_j)/g(x_j)$ vary widely, giving too much importance to a few values x_j.
- If $\sup f/g = M < \infty$, the accept-reject algorithm can be used as well to simulate f directly.

Example (Cauchy target)

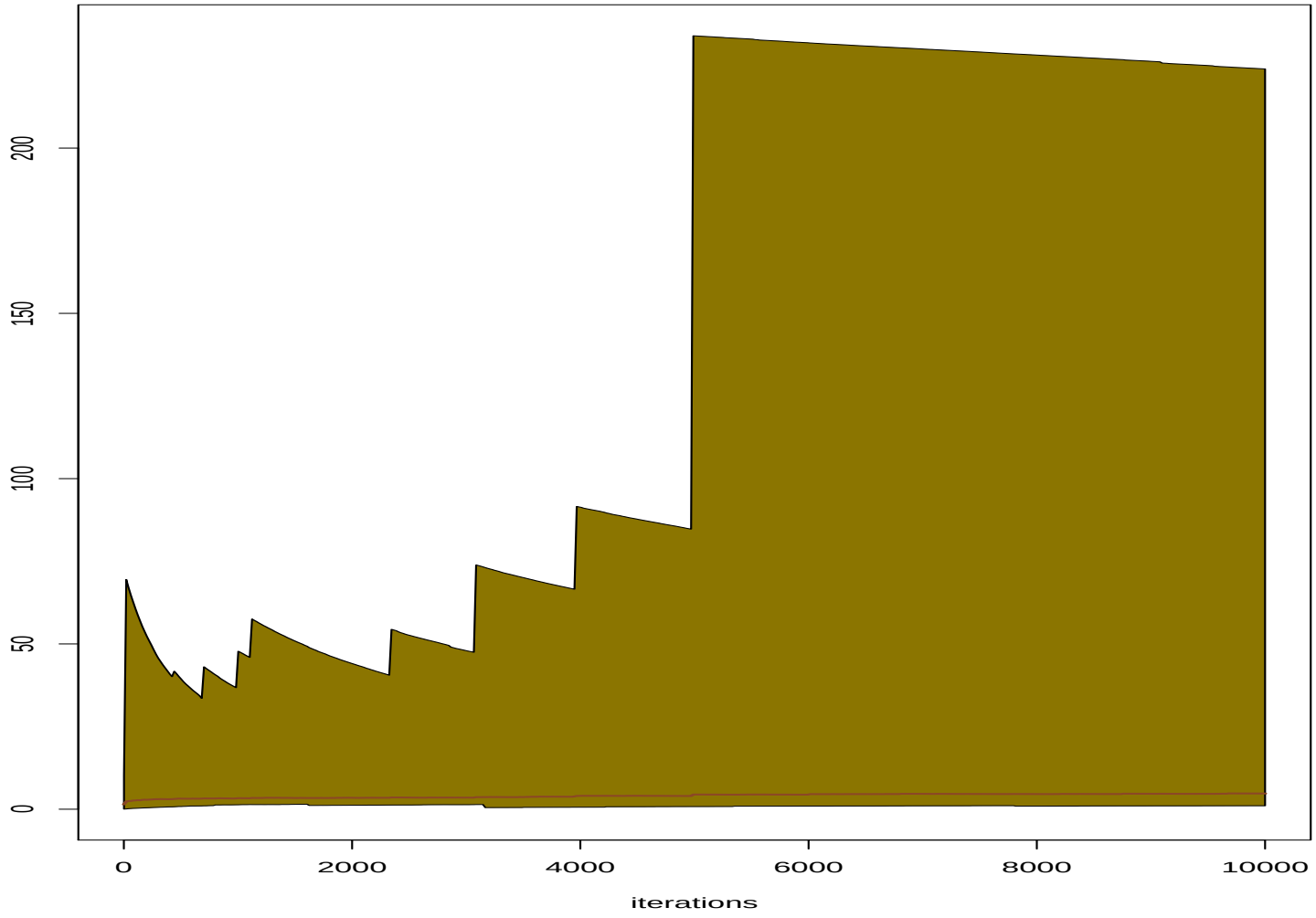
Case of Cauchy distribution $\mathrm{C}(0,1)$ when importance function is Gaussian $\mathcal{N}(0,1)$.
Ratio of the densities

$$\varrho(x) = \frac{p^\star(x)}{p_0(x)} = \sqrt{2\pi}\,\frac{\exp x^2/2}{\pi\,(1+x^2)}$$

very badly behaved: e.g.,

$$\int_{-\infty}^{\infty} \varrho(x)^2 p_0(x) dx = \infty\,.$$

Poor performances of the associated importance sampling estimator



Range and average of 500 replications of IS estimate of $\mathbb{E}[\exp -X]$ over $10,000$ iterations.

Optimal importance function

The choice of g that minimizes the variance of the importance sampling estimator is

$$g^*(x) = \frac{|h(x)|\ f(x)}{\int_{\mathcal{Z}} |h(z)|\ f(z)\ dz}\ .$$

Rather formal optimality result since optimal choice of $g^*(x)$ requires the knowledge of $\mathfrak{I}$, the integral of interest!

Practical impact

$$\frac{\sum_{j=1}^{m} h(X_j)\ f(X_j)/g(X_j)}{\sum_{j=1}^{m} f(X_j)/g(X_j)},$$

where f and g are known up to constants.

- Also converges to $\mathfrak{I}$ by the Strong Law of Large Numbers.
- Biased, but the bias is quite small
- In some settings beats the unbiased estimator in squared error loss.
- Using the 'optimal' solution does not always work:

$$\frac{\sum_{j=1}^{m} h(x_j)\ f(x_j)/|h(x_j)|\ f(x_j)}{\sum_{j=1}^{m} f(x_j)/|h(x_j)|\ f(x_j)} = \frac{\#\text{positive } h - \#\text{negative } h}{\sum_{j=1}^{m} 1/|h(x_j)|}$$

Selfnormalised importance sampling

For ratio estimator

$$\delta_h^n = \sum_{i=1}^{n} \omega_i \, h(x_i) \Big/ \sum_{i=1}^{n} \omega_i$$

with $X_i \sim g(y)$ and W_i such that

$$\mathbb{E}[W_i | X_i = x] = \kappa f(x)/g(x)$$

Selfnormalised variance

then

$$\mathrm{var}(\delta_h^n) \approx \frac{1}{n^2\kappa^2}\left(\mathrm{var}(S_h^n) - 2\mathbb{E}^\pi[h]\,\mathrm{cov}(S_h^n, S_1^n) + \mathbb{E}^\pi[h]^2\,\mathrm{var}(S_1^n)\right) .$$

for

$$S_h^n = \sum_{i=1}^n W_i h(X_i)\,, \quad S_1^n = \sum_{i=1}^n W_i$$

Rough approximation

$$\mathrm{var}\delta_h^n \approx \frac{1}{n}\,\mathrm{var}^\pi(h(X))\,\{1 + \mathrm{var}_g(W)\}$$

Example (Student's t distribution)

$X \sim \mathcal{T}(\nu, \theta, \sigma^2)$, with density

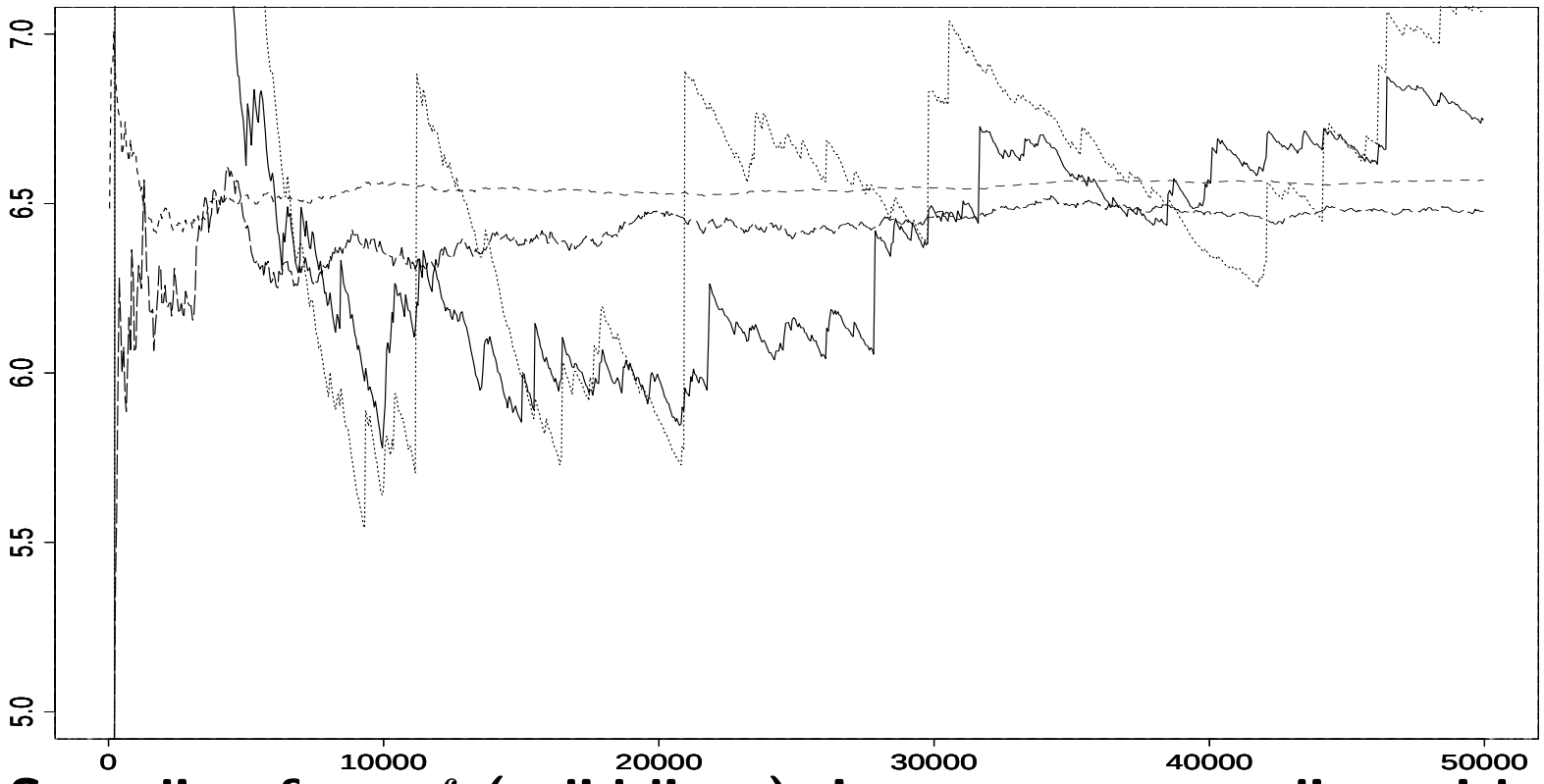
$$f_\nu(x) = \frac{\Gamma((\nu+1)/2)}{\sigma\sqrt{\nu\pi}\,\Gamma(\nu/2)} \left(1 + \frac{(x-\theta)^2}{\nu\sigma^2}\right)^{-(\nu+1)/2}.$$

Without loss of generality, take $\theta = 0$, $\sigma = 1$.
Problem: Calculate the integral

$$\int_{2.1}^{\infty} \left(\frac{\sin(x)}{x}\right)^n f_\nu(x)dx.$$

Example (Student's t distribution (2))

- Simulation possibilities
  - Directly from f_ν, since $f_\nu = \frac{\mathcal{N}(0,1)}{\sqrt{\chi^2_\nu}}$
  - Importance sampling using Cauchy $\mathcal{C}(0,1)$
  - Importance sampling using a normal $\mathcal{N}(0,1)$ (expected to be nonoptimal)
  - Importance sampling using a $\mathcal{U}([0,1/2.1])$ change of variables



Sampling from f (solid lines), importance sampling with Cauchy instrumental (short dashes), $\mathscr{U}([0, 1/2.1])$ instrumental (long dashes) and normal instrumental (dots).

IS suffers from curse of dimensionality

As dimension increases, discrepancy between importance and target worsens

skip explanation

Explanation:

Take target distribution μ and instrumental distribution ν
Simulation of a sample of iid samples of size n $x_{1:n}$ from $\mu_n = \mu^{\otimes n}$
Importance sampling estimator for $\mu_n(f_n) = \int f_n(x_{1:n})\mu_n(dx_{1:n})$

$$\widehat{\mu_n(f_n)} = \frac{\sum_{i=1}^N f_n(\xi_{1:n}^i) \prod_{j=1}^N W_j^i}{\sum_{j=1}^N \prod_{j=1}^N W_j},$$

where $W_k^i = \frac{d\mu}{d\nu}(\xi_k^i)$, and ξ_j^i are iid with distribution ν.
For $\{V_k\}_{k\geq 0}$, sequence of iid nonnegative random variables and for $n \geq 1$, $\mathcal{F}_n = \sigma(V_k; k \leq n)$, set

$$U_n = \prod_{k=1}^n V_k$$

IS suffers (2)

Since $\mathbb{E}[V_{n+1}] = 1$ and V_{n+1} independent from $\mathcal{F}_n$,

$$\mathbb{E}(U_{n+1} \mid \mathcal{F}_n) = U_n \mathbb{E}(V_{n+1} \mid \mathcal{F}_n) = U_n,$$

and thus $\{U_n\}_{n \geq 0}$ **martingale**
Since $x \mapsto \sqrt{x}$ concave, by Jensen's inequality,

$$\mathbb{E}(\sqrt{U_{n+1}} \mid \mathcal{F}_n) \leq \sqrt{\mathbb{E}(U_{n+1} \mid \mathcal{F}_n)} \leq \sqrt{U_n}$$

and thus $\{\sqrt{U_n}\}_{n \geq 0}$ **supermartingale**
Assume $\mathbb{E}(\sqrt{V_{n+1}}) < 1$. Then

$$\mathbb{E}(\sqrt{U_n}) = \prod_{k=1}^{n} \mathbb{E}(\sqrt{V_k}) \to 0, \quad n \to \infty.$$

IS suffers (3)

But $\{\sqrt{U_n}\}_{n\geq 0}$ is a nonnegative supermartingale and thus $\sqrt{U_n}$ converges a.s. to a random variable $Z \geq 0$. By **Fatou's lemma**,

$$\mathbb{E}(Z) = \mathbb{E}\left(\lim_{n\to\infty} \sqrt{U_n}\right) \leq \liminf_{n\to\infty} \mathbb{E}(\sqrt{U_n}) = 0.$$

Hence, $Z = 0$ and $U_n \to 0$ a.s., which implies that the martingale $\{U_n\}_{n\geq 0}$ is not regular.
Apply these results to $V_k = \frac{d\mu}{d\nu}(\xi_k^i)$, $i \in \{1, \ldots, N\}$:

$$\mathbb{E}\left[\sqrt{\frac{d\mu}{d\nu}(\xi_k^i)}\right] \leq \mathbb{E}\left[\frac{d\mu}{d\nu}(\xi_k^i)\right] = 1.$$

with equality iff $\frac{d\mu}{d\nu} = 1$, ν-a.e., i.e. $\mu = \nu$.

Thus all importance weights converge to 0

▸ too volatile!

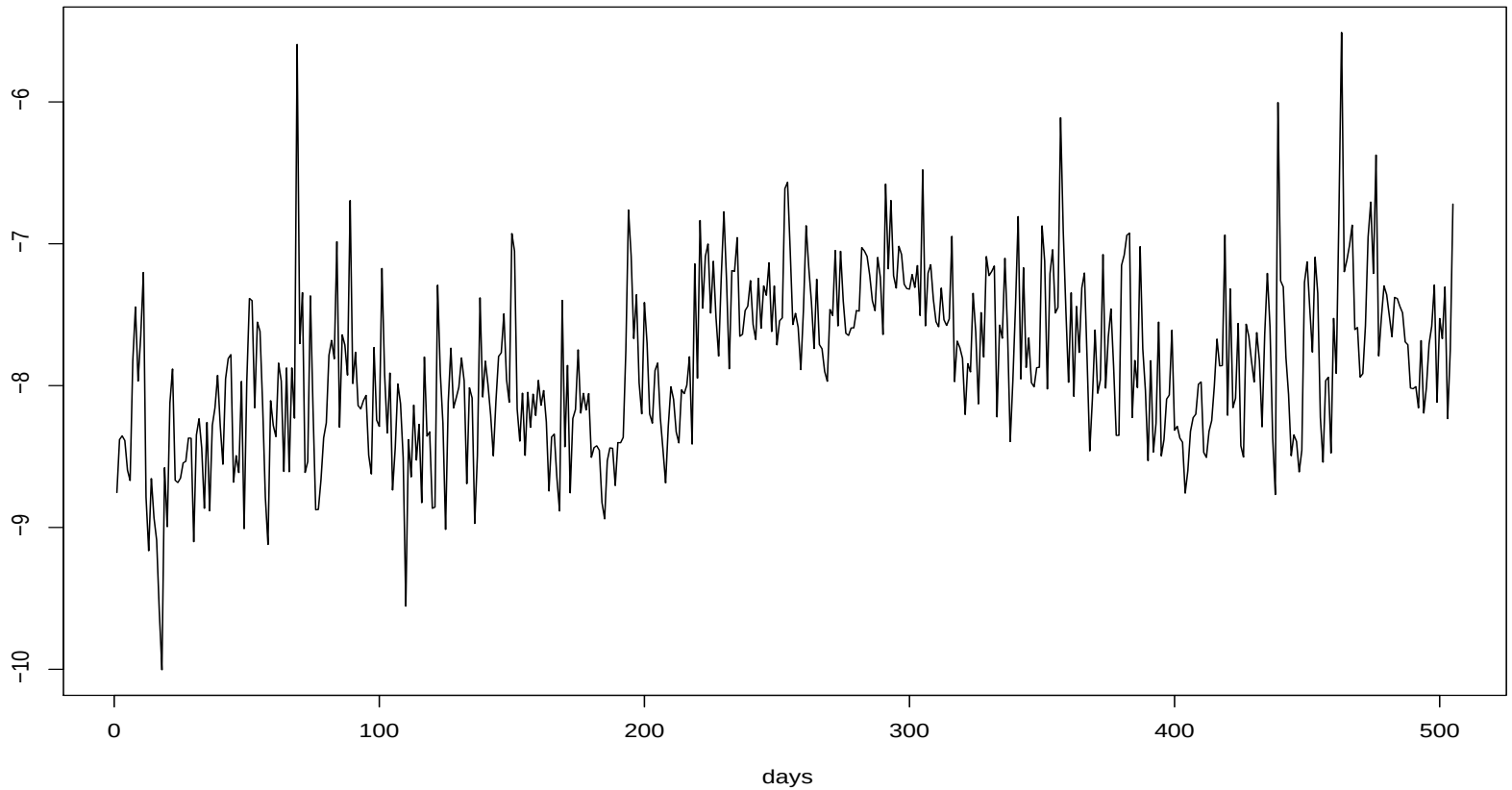
Example (Stochastic volatility model)

$$y_t = \beta \exp(x_t/2)\, \epsilon_t\,, \qquad \epsilon_t \sim \mathcal{N}(0,1)$$

with AR(1) log-variance process (or *volatility*)

$$x_{t+1} = \varphi x_t + \sigma u_t\,, \quad u_t \sim \mathcal{N}(0,1)$$

Evolution of IBM stocks (corrected from trend and log-ratio-ed)



Example (Stochastic volatility model (2))

Observed likelihood unavailable in closed from.
Joint posterior (or conditional) distribution of the hidden state sequence $\{X_k\}_{1\leq k\leq K}$ can be evaluated explicitly

$$\prod_{k=2}^{K} \exp - \left\{\sigma^{-2}(x_k - \phi x_{k-1})^2 + \beta^{-2}\exp(-x_k)y_k^2 + x_k\right\}/2\,, \quad (2)$$

up to a normalizing constant.

Computational problems

Example (Stochastic volatility model (3))

Direct simulation from this distribution impossible because of

(a) dependence among the X_k's,

(b) dimension of the sequence $\{X_k\}_{1 \leq k \leq K}$, and

(c) exponential term $\exp(-x_k)y_k^2$ within (2).

Importance sampling

Example (Stochastic volatility model (4))

Natural candidate: replace the exponential term with a quadratic approximation to preserve Gaussianity.
E.g., expand $\exp(-x_k)$ around its conditional expectation ϕx_{k-1} as

$$\exp(-x_k) \approx \exp(-\phi x_{k-1}) \left\{ 1 - (x_k - \phi x_{k-1}) + \frac{1}{2}(x_k - \phi x_{k-1})^2 \right\}$$

Example (Stochastic volatility model (5))

Corresponding Gaussian importance distribution with mean

$$\mu_k = \frac{\phi x_{k-1}\{\sigma^{-2} + y_k^2 \exp(-\phi x_{k-1})/2\} - \{1 - y_k^2 \exp(-\phi x_{k-1})\}/2}{\sigma^{-2} + y_k^2 \exp(-\phi x_{k-1})/2}$$

and variance

$$\tau_k^2 = (\sigma^{-2} + y_k^2 \exp(-\phi x_{k-1})/2)^{-1}$$

Prior proposal on X_1,

$$X_1 \sim \mathcal{N}(0, \sigma^2)$$

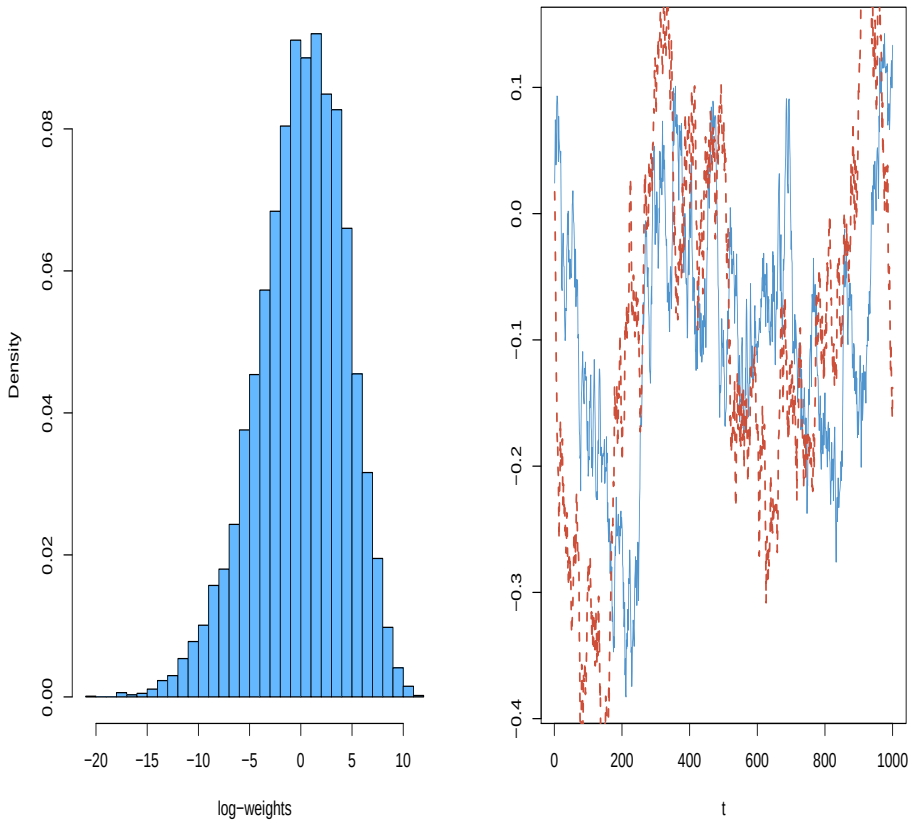
Example (Stochastic volatility model (6))

Simulation starts with X_1 and proceeds forward to X_n, each X_k being generated conditional on Y_k and the previously generated X_{k-1}.

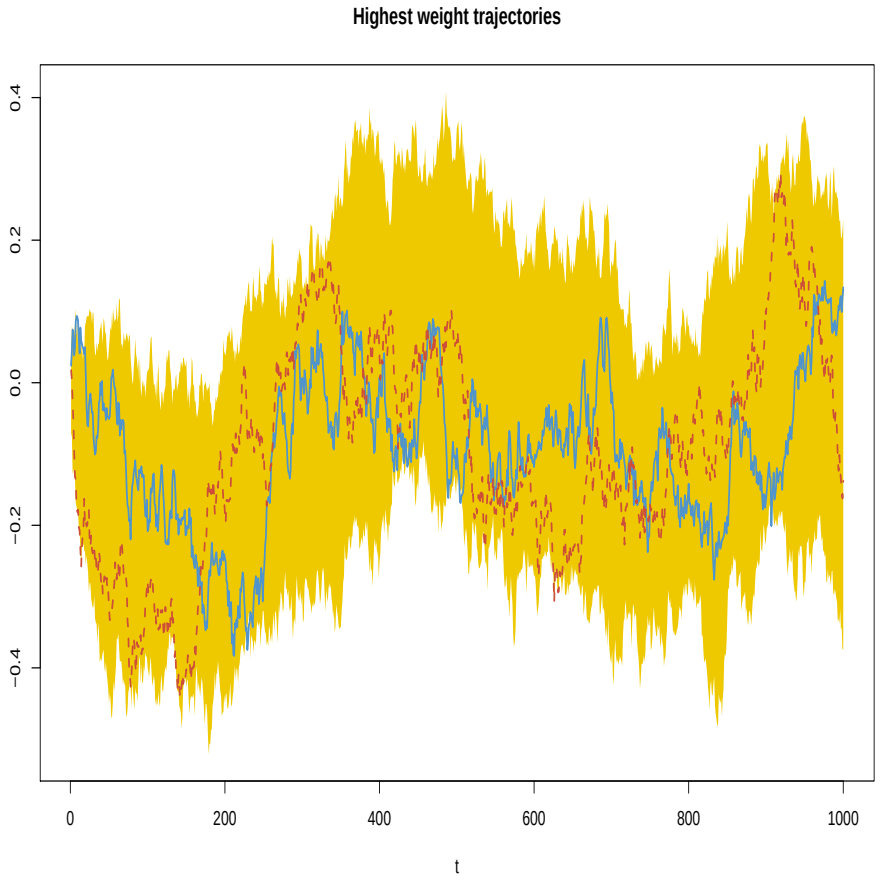
Importance weight computed sequentially as the product of

$$\frac{\exp - \left\{ \sigma^{-2}(x_k - \phi x_{k-1})^2 + \exp(-x_k) y_k^2 + x_k \right\} / 2}{\exp - \left\{ \tau_k^{-2}(x_k - \mu_k)^2 \right\} \tau_k^{-1}} .$$

$(1 \leq k \leq K)$



Histogram of the logarithms of the importance weights (left) and comparison between the true volatility and the best fit, based on $10,000$ simulated importance samples.



Corresponding range of the simulated $\{X_k\}_{1 \leq k \leq 100}$, compared with the true value.

Correlated simulations

Negative correlation reduces variance

Special technique — but efficient when it applies

Two samples $(X_1, \ldots, X_m)$ and $(Y_1, \ldots, Y_m)$ from f to estimate

$$\mathfrak{I} = \int_{\mathbb{R}} h(x) f(x) dx$$

by

$$\widehat{\mathfrak{I}}_1 = \frac{1}{m} \sum_{i=1}^{m} h(X_i) \quad \text{and} \quad \widehat{\mathfrak{I}}_2 = \frac{1}{m} \sum_{i=1}^{m} h(Y_i)$$

with mean $\mathfrak{I}$ and variance σ^2

Variance reduction

Variance of the average

$$\mathrm{var}\left(\frac{\widehat{\mathfrak{I}}_1 + \widehat{\mathfrak{I}}_2}{2}\right) = \frac{\sigma^2}{2} + \frac{1}{2}\mathrm{cov}(\widehat{\mathfrak{I}}_1, \widehat{\mathfrak{I}}_2).$$

If the two samples are **negatively correlated**,

$$\mathrm{cov}(\widehat{\mathfrak{I}}_1, \widehat{\mathfrak{I}}_2) \leq 0\,,$$

they improve on two independent samples of same size

Antithetic variables

- If f symmetric about μ, take $Y_i = 2\mu - X_i$
- If $X_i = F^{-1}(U_i)$, take $Y_i = F^{-1}(1 - U_i)$
- If $(A_i)_i$ partition of $\mathcal{X}$, **partitioned sampling** by sampling X_j's in each A_i (requires to know $\Pr(A_i)$)

Control variates

out of control!

For

$$\mathfrak{I} = \int h(x) f(x) dx$$

unknown and

$$\mathfrak{I}_0 = \int h_0(x) f(x) dx$$

known,

$\mathfrak{I}_0$ estimated by $\widehat{\mathfrak{I}}_0$ and

$\mathfrak{I}$ estimated by $\widehat{\mathfrak{I}}$

Control variates (2)

Combined estimator

$$\widehat{\mathfrak{I}}^* = \widehat{\mathfrak{I}} + \beta(\widehat{\mathfrak{I}}_0 - I_0)$$

$\widehat{\mathfrak{I}}^*$ is unbiased for $\mathfrak{I}$ and

$$\mathrm{var}(\widehat{\mathfrak{I}}^*) = \mathrm{var}(\widehat{\mathfrak{I}}) + \beta^2 \mathrm{var}(\widehat{\mathfrak{I}}) + 2\beta \mathrm{cov}(\widehat{\mathfrak{I}}, \widehat{\mathfrak{I}}_0)$$

Optimal control

Optimal choice of β

$$\beta^\star = -\frac{\mathrm{cov}(\widehat{\mathfrak{I}}, \widehat{\mathfrak{I}}_0)}{\mathrm{var}(\widehat{\mathfrak{I}}_0)} \ ,$$

with

$$\mathrm{var}(\widehat{\mathfrak{I}}^\star) = (1 - \rho^2)\ \mathrm{var}(\widehat{\mathfrak{I}}) \ ,$$

where ρ correlation between $\widehat{\mathfrak{I}}$ and $\widehat{\mathfrak{I}}_0$
Usual solution: **regression coefficient of $h(x_i)$ over $h_0(x_i)$**

Example (Quantile Approximation)

Evaluate

$$\varrho = \mathsf{Pr}(X > a) = \int_a^\infty f(x)dx$$

by

$$\widehat{\varrho} = \frac{1}{n}\sum_{i=1}^{n} \mathbb{I}(X_i > a),$$

with X_i iid f.
If $\mathsf{Pr}(X > \mu) = \frac{1}{2}$ known

Example (Quantile Approximation (2))

Control variate

$$\tilde{\varrho} = \frac{1}{n}\sum_{i=1}^{n} \mathbb{I}(X_i > a) + \beta\left(\frac{1}{n}\sum_{i=1}^{n} \mathbb{I}(X_i > \mu) - \mathsf{Pr}(X > \mu)\right)$$

improves upon $\widehat{\varrho}$ if

$$\beta < 0 \quad \text{and} \quad |\beta| < 2\frac{\mathrm{cov}(\widehat{\varrho}, \widehat{\varrho}_0)}{\mathrm{var}(\widehat{\varrho}_0)} 2\frac{\mathsf{Pr}(X > a)}{\mathsf{Pr}(X > \mu)}.$$

Integration by conditioning

Use **Rao-Blackwell Theorem**

$$\mathbf{var}(\mathbb{E}[\delta(\mathbf{X})|\mathbf{Y}]) \leq \mathbf{var}(\delta(\mathbf{X}))$$

Consequence

If $\widehat{\mathfrak{I}}$ unbiased estimator of $\mathfrak{I} = \mathbb{E}_f[h(X)]$, with X simulated from a joint density $\tilde{f}(x, y)$, where

$$\int \tilde{f}(x, y)dy = f(x),$$

the estimator

$$\widehat{\mathfrak{I}}^* = \mathbb{E}_{\tilde{f}}[\widehat{\mathfrak{I}}|Y_1, \ldots, Y_n]$$

dominate $\widehat{\mathfrak{I}}(X_1, \ldots, X_n)$ variance-wise (and is unbiased)

skip expectation

Example (Student's t expectation)

For

$$\mathbb{E}[h(x)] = \mathbb{E}[\exp(-x^2)] \quad \text{with} \quad X \sim \mathscr{T}(\nu, 0, \sigma^2)$$

a Student's t distribution can be simulated as

$$X|y \sim \mathcal{N}(\mu, \sigma^2 y) \qquad \text{and} \qquad Y^{-1} \sim \chi^2_\nu.$$

Example (Student's t expectation (2))

Empirical distribution

$$\frac{1}{m}\sum_{j=1}^{m}\exp(-X_j^2)\,,$$

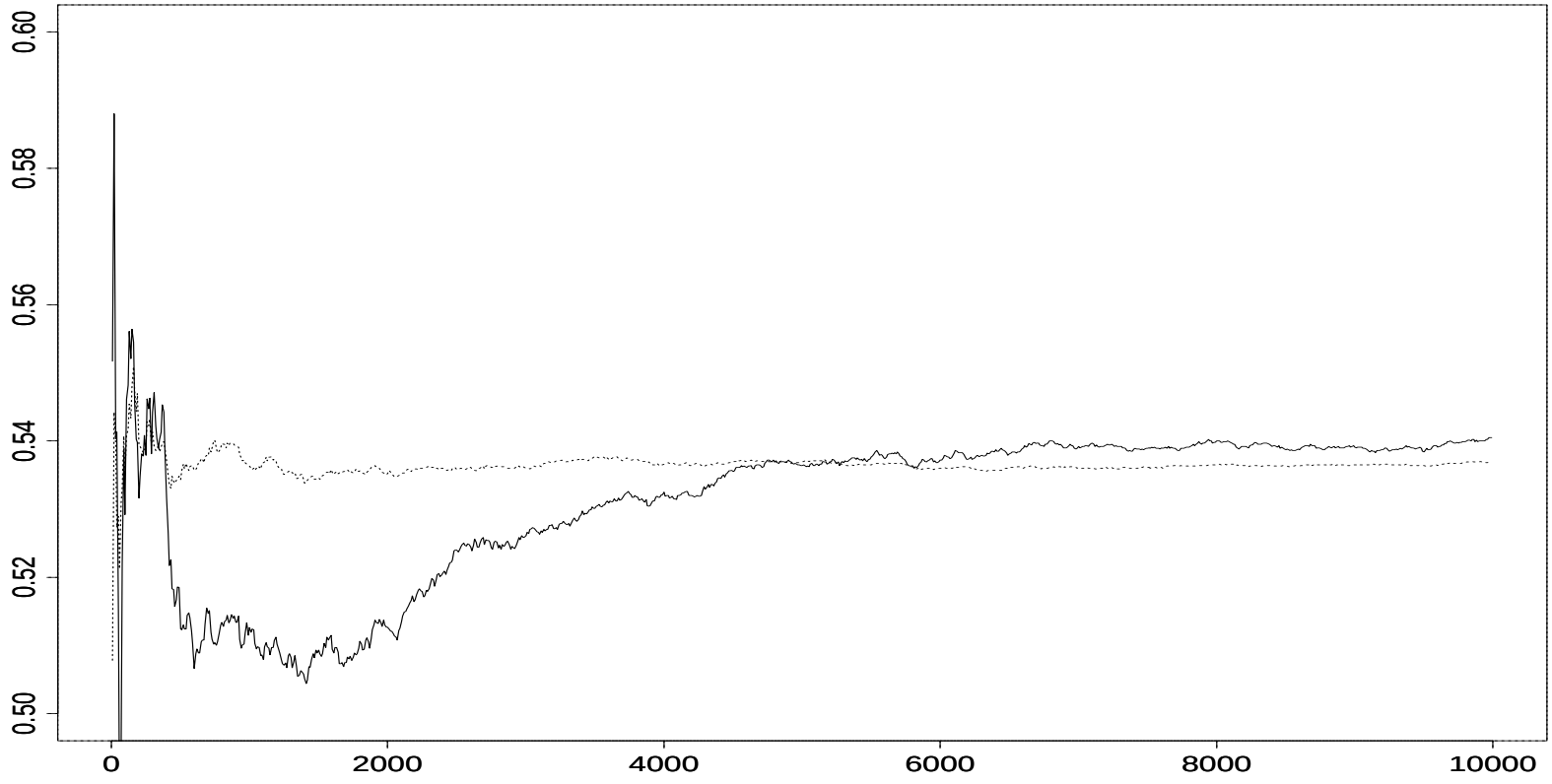
can be improved from the joint sample

$$((X_1,Y_1),\ldots,(X_m,Y_m))$$

since

$$\frac{1}{m}\sum_{j=1}^{m}\mathbb{E}[\exp(-X^2)|Y_j]=\frac{1}{m}\sum_{j=1}^{m}\frac{1}{\sqrt{2\sigma^2Y_j+1}}$$

is the conditional expectation.
In this example, precision **ten times** better



Estimators of $\mathbb{E}[\exp(-X^2)]$: empirical average (full) and conditional expectation (dotted) for $(\nu, \mu, \sigma) = (4.6, 0, 1)$.

Bayesian model choice

directly Markovian

Probabilise the entire model/parameter space

- allocate probabilities p_i to all models $\mathfrak{M}_i$
- define priors $\pi_i(\theta_i)$ for each parameter space Θ_i
- compute

$$\pi(\mathfrak{M}_i|x) = \frac{p_i \int_{\Theta_i} f_i(x|\theta_i)\pi_i(\theta_i)\mathrm{d}\theta_i}{\sum_j p_j \int_{\Theta_j} f_j(x|\theta_j)\pi_j(\theta_j)\mathrm{d}\theta_j}$$

- take largest $\pi(\mathfrak{M}_i|x)$ to determine "best" model,

Bayes factor

Definition (Bayes factors)

For testing hypotheses $H_0 : \theta \in \Theta_0$ vs. $H_{\mathsf{a}} : \theta \notin \Theta_0$, under prior

$$\pi(\Theta_0)\pi_0(\theta) + \pi(\Theta_0^c)\pi_1(\theta)\,,$$

central quantity

$$B_{01} = \frac{\pi(\Theta_0|x)}{\pi(\Theta_0^c|x)} \Big/ \frac{\pi(\Theta_0)}{\pi(\Theta_0^c)} = \frac{\displaystyle\int_{\Theta_0} f(x|\theta)\pi_0(\theta)\mathrm{d}\theta}{\displaystyle\int_{\Theta_0^c} f(x|\theta)\pi_1(\theta)\mathrm{d}\theta}$$

[Jeffreys, 1939]

Evidence

Problems using a similar quantity, the *evidence*

$$\mathfrak{E}_k = \int_{\Theta_k} \pi_k(\theta_k) L_k(\theta_k) \, \mathrm{d}\theta_k,$$

aka the marginal likelihood.

[Jeffreys, 1939]

Bayes factor approximation

When approximating the Bayes factor

$$B_{01} = \frac{\int_{\Theta_0} f_0(x|\theta_0)\pi_0(\theta_0)\mathrm{d}\theta_0}{\int_{\Theta_1} f_1(x|\theta_1)\pi_1(\theta_1)\mathrm{d}\theta_1}$$

use of importance functions ϖ_0 and ϖ_1 and

$$\widehat{B}_{01} = \frac{n_0^{-1}\sum_{i=1}^{n_0} f_0(x|\theta_0^i)\pi_0(\theta_0^i)/\varpi_0(\theta_0^i)}{n_1^{-1}\sum_{i=1}^{n_1} f_1(x|\theta_1^i)\pi_1(\theta_1^i)/\varpi_1(\theta_1^i)}$$

Diabetes in Pima Indian women

Example (R benchmark)

"A population of women who were at least 21 years old, of Pima Indian heritage and living near Phoenix (AZ), was tested for diabetes according to WHO criteria. The data were collected by the US National Institute of Diabetes and Digestive and Kidney Diseases."

200 Pima Indian women with observed variables

- plasma glucose concentration in oral glucose tolerance test
- diastolic blood pressure
- diabetes pedigree function
- presence/absence of diabetes

Probit modelling on Pima Indian women

Probability of diabetes function of above variables

$$\mathbb{P}(y = 1|x) = \Phi(x_1\beta_1 + x_2\beta_2 + x_3\beta_3)\,,$$

Test of $H_0 : \beta_3 = 0$ for 200 observations of Pima.tr based on a g-prior modelling:

$$\beta \sim \mathcal{N}_3(0, n\left(\mathbf{X}^{\mathsf{T}}\mathbf{X}\right)^{-1}\right)$$

MCMC 101 for probit models

Use of either a random walk proposal

$$\beta' = \beta + \epsilon$$

in a Metropolis-Hastings algorithm (since the likelihood is available)
or of a Gibbs sampler that takes advantage of the missing/latent variable

$$z|y, x, \beta \sim \mathcal{N}(x^{\mathsf{T}}\beta, 1) \left\{ \mathbb{I}^{y}_{z\geq 0} \times \mathbb{I}^{1-y}_{z\leq 0} \right\}$$

(since $\beta|y, X, z$ is distributed as a standard normal)

[Gibbs three times faster]

Importance sampling for the Pima Indian dataset

Use of the importance function inspired from the MLE estimate distribution

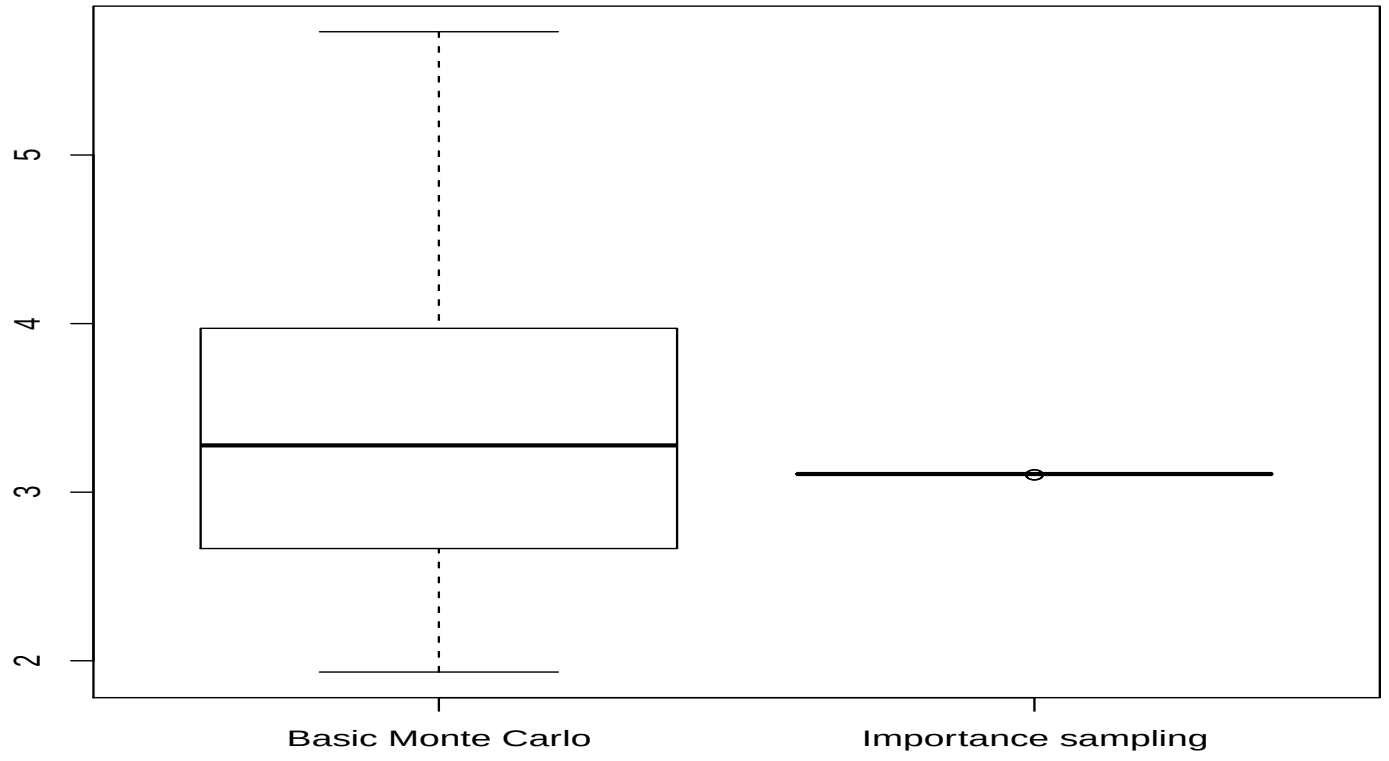
$$\beta \sim \mathcal{N}(\hat{\beta}, \hat{\Sigma})$$

R Importance sampling code

```
model1=summary(glm(y~-1+X1,family=binomial(link="probit")))
is1=rmvnorm(Niter,mean=model1$coeff[,1],sigma=2*model1$cov.unscaled)
is2=rmvnorm(Niter,mean=model2$coeff[,1],sigma=2*model2$cov.unscaled)
bfis=mean(exp(probitlpost(is1,y,X1)-dmvlnorm(is1,mean=model1$coeff[,1],
     sigma=2*model1$cov.unscaled))) / mean(exp(probitlpost(is2,y,X2)-
     dmvlnorm(is2,mean=model2$coeff[,1],sigma=2*model2$cov.unscaled)))
```

Diabetes in Pima Indian women

Comparison of the variation of the Bayes factor approximations based on 100 replicas for $20,000$ simulations from the prior and the above MLE importance sampler



Bridge sampling

Special case:
If

$$\begin{aligned} \pi_1(\theta_1|x) &\propto \tilde{\pi}_1(\theta_1|x) \\ \pi_2(\theta_2|x) &\propto \tilde{\pi}_2(\theta_2|x) \end{aligned}$$

live on the same space ($\Theta_1 = \Theta_2$), then

$$B_{12} \approx \frac{1}{n} \sum_{i=1}^{n} \frac{\tilde{\pi}_1(\theta_i|x)}{\tilde{\pi}_2(\theta_i|x)} \qquad \theta_i \sim \pi_2(\theta|x)$$

[Gelman & Meng, 1998; Chen, Shao & Ibrahim, 2000]

Bridge sampling variance

The bridge sampling estimator does poorly if

$$\frac{\text{var}(\widehat{B}_{12})}{B_{12}^2} \approx \frac{1}{n}\,\mathbb{E}\left[\left(\frac{\pi_1(\theta)-\pi_2(\theta)}{\pi_2(\theta)}\right)^2\right]$$

is large, i.e. if π_1 and π_2 have little overlap...

(Further) bridge sampling

General identity:

$$B_{12} = \frac{\int \tilde{\pi}_2(\theta|x)\alpha(\theta)\pi_1(\theta|x)d\theta}{\int \tilde{\pi}_1(\theta|x)\alpha(\theta)\pi_2(\theta|x)d\theta} \qquad \forall\ \alpha(\cdot)$$

$$\approx \frac{\frac{1}{n_1}\sum_{i=1}^{n_1} \tilde{\pi}_2(\theta_{1i}|x)\alpha(\theta_{1i})}{\frac{1}{n_2}\sum_{i=1}^{n_2} \tilde{\pi}_1(\theta_{2i}|x)\alpha(\theta_{2i})} \qquad \theta_{ji} \sim \pi_j(\theta|x)$$

Optimal bridge sampling

The optimal choice of auxiliary function is

$$\alpha^\star = \frac{n_1 + n_2}{n_1\pi_1(\theta|x) + n_2\pi_2(\theta|x)}$$

leading to

$$\widehat{B}_{12} \approx \frac{\dfrac{1}{n_1}\displaystyle\sum_{i=1}^{n_1} \dfrac{\tilde{\pi}_2(\theta_{1i}|x)}{n_1\pi_1(\theta_{1i}|x) + n_2\pi_2(\theta_{1i}|x)}}{\dfrac{1}{n_2}\displaystyle\sum_{i=1}^{n_2} \dfrac{\tilde{\pi}_1(\theta_{2i}|x)}{n_1\pi_1(\theta_{2i}|x) + n_2\pi_2(\theta_{2i}|x)}}$$

Back later!

Optimal bridge sampling (2)

Reason:

$$\frac{\mathrm{Var}(\widehat{B}_{12})}{B_{12}^2} \approx \frac{1}{n_1 n_2} \left\{ \frac{\int \pi_1(\theta)\pi_2(\theta)[n_1\pi_1(\theta) + n_2\pi_2(\theta)]\alpha(\theta)^2 \,\mathrm{d}\theta}{\left(\int \pi_1(\theta)\pi_2(\theta)\alpha(\theta)\,\mathrm{d}\theta\right)^2} - 1 \right\}$$

(by the δ method)

Drawback: Dependence on the unknown normalising constants solved iteratively

Extension to varying dimensions

When $\dim(\Theta_1) \neq \dim(\Theta_2)$, e.g. $\theta_2 = (\theta_1, \psi)$, introduction of a *pseudo-posterior density*, $\omega(\psi|\theta_1, x)$, augmenting $\pi_1(\theta_1|x)$ into joint distribution

$$\pi_1(\theta_1|x) \times \omega(\psi|\theta_1, x)$$

on Θ_2 so that

$$B_{12} = \frac{\int \tilde{\pi}_1(\theta_1|x)\alpha(\theta_1,\psi)\pi_2(\theta_1,\psi|x)\mathrm{d}\theta_1\omega(\psi|\theta_1,x)\,\mathrm{d}\psi}{\int \tilde{\pi}_2(\theta_1,\psi|x)\alpha(\theta_1,\psi)\pi_1(\theta_1|x)\mathrm{d}\theta_1\,\omega(\psi|\theta_1,x)\,\mathrm{d}\psi}$$

$$= \mathbb{E}_{\pi_2}\left[\frac{\tilde{\pi}_1(\theta_1)\omega(\psi|\theta_1)}{\tilde{\pi}_2(\theta_1,\psi)}\right] = \frac{\mathbb{E}_\varphi\left[\tilde{\pi}_1(\theta_1)\omega(\psi|\theta_1)/\varphi(\theta_1,\psi)\right]}{\mathbb{E}_\varphi\left[\tilde{\pi}_2(\theta_1,\psi)/\varphi(\theta_1,\psi)\right]}$$

for any conditional density $\omega(\psi|\theta_1)$ and any joint density φ.

Illustration for the Pima Indian dataset

Use of the MLE induced conditional of β_3 given (β_1, β_2) as a pseudo-posterior and mixture of both MLE approximations on β_3 in bridge sampling estimate

R bridge sampling code

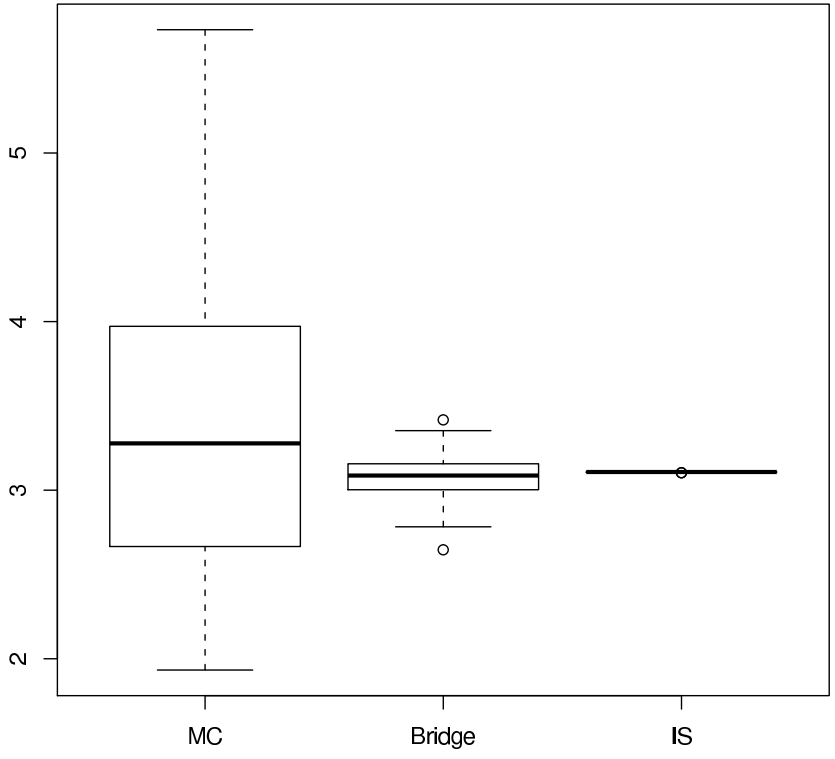
```
cova=model2$cov.unscaled
expecta=model2$coeff[,1]
covw=cova[3,3]-t(cova[1:2,3])%*%ginv(cova[1:2,1:2])%*%cova[1:2,3]

probit1=hmprobit(Niter,y,X1)
probit2=hmprobit(Niter,y,X2)
pseudo=rnorm(Niter,meanw(probit1),sqrt(covw))
probit1p=cbind(probit1,pseudo)

bfbs=mean(exp(probitlpost(probit2[,1:2],y,X1)+dnorm(probit2[,3],meanw(probit2[,1:2]),
     sqrt(covw),log=T))/ (dmvnorm(probit2,expecta,cova)+dnorm(probit2[,3],expecta[3],
     cova[3,3])))/ mean(exp(probitlpost(probit1p,y,X2))/(dmvnorm(probit1p,expecta,cova)+
     dnorm(pseudo,expecta[3],cova[3,3])))
```

Diabetes in Pima Indian women (cont'd)

Comparison of the variation of the Bayes factor approximations based on $100 \times 20,000$ simulations from the prior (MC), the above bridge sampler and the above importance sampler



The original harmonic mean estimator

When $\theta_{ki} \sim \pi_k(\theta|x)$,

$$\frac{1}{T}\sum_{t=1}^{T}\frac{1}{L(\theta_{kt}|x)}$$

is an unbiased estimator of $1/m_k(x)$

[Newton & Raftery, 1994]

Highly dangerous: Most often leads to an infinite variance!!!

"The Worst Monte Carlo Method Ever"

"The good news is that the Law of Large Numbers guarantees that this estimator is consistent ie, it will very likely be very close to the correct answer if you use a sufficiently large number of points from the posterior distribution.
The bad news is that the number of points required for this estimator to get close to the right answer will often be greater than the number of atoms in the observable universe. The even worse news is that it's easy for people to not realize this, and to naïvely accept estimates that are nowhere close to the correct value of the marginal likelihood."

[Radford Neal's blog, Aug. 23, 2008]

Approximating $\mathfrak{Z}_k$ from a posterior sample

Use of the [harmonic mean] identity

$$\mathbb{E}^{\pi_k}\left[\left.\frac{\varphi(\theta_k)}{\pi_k(\theta_k)L_k(\theta_k)}\right| x\right] = \int \frac{\varphi(\theta_k)}{\pi_k(\theta_k)L_k(\theta_k)}\,\frac{\pi_k(\theta_k)L_k(\theta_k)}{\mathfrak{Z}_k}\,\mathrm{d}\theta_k = \frac{1}{\mathfrak{Z}_k}$$

no matter what the proposal $\varphi(\cdot)$ is.

[Gelfand & Dey, 1994; Bartolucci et al., 2006]

Direct exploitation of the MCMC output

Comparison with regular importance sampling

Harmonic mean: Constraint opposed to usual importance sampling constraints: $\varphi(\theta)$ must have lighter (rather than fatter) tails than $\pi_k(\theta_k)L_k(\theta_k)$ for the approximation

$$\widehat{\mathfrak{Z}_{1k}} = 1 \Big/ \frac{1}{T} \sum_{t=1}^{T} \frac{\varphi(\theta_k^{(t)})}{\pi_k(\theta_k^{(t)})L_k(\theta_k^{(t)})}$$

to have a finite variance.
E.g., use finite support kernels (like Epanechnikov's kernel) for φ

Comparison with regular importance sampling (cont'd)

Compare $\widehat{\mathfrak{Z}_{1k}}$ with a standard importance sampling approximation

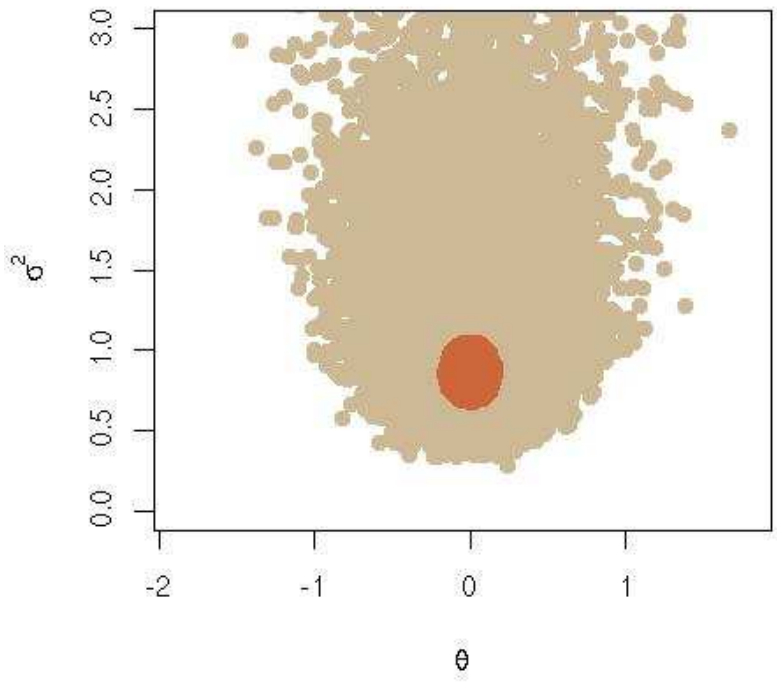
$$\widehat{\mathfrak{Z}_{2k}} = \frac{1}{T} \sum_{t=1}^{T} \frac{\pi_k(\theta_k^{(t)}) L_k(\theta_k^{(t)})}{\varphi(\theta_k^{(t)})}$$

where the $\theta_k^{(t)}$'s are generated from the density $\varphi(\cdot)$ (with fatter tails like t's)

HPD indicator as φ

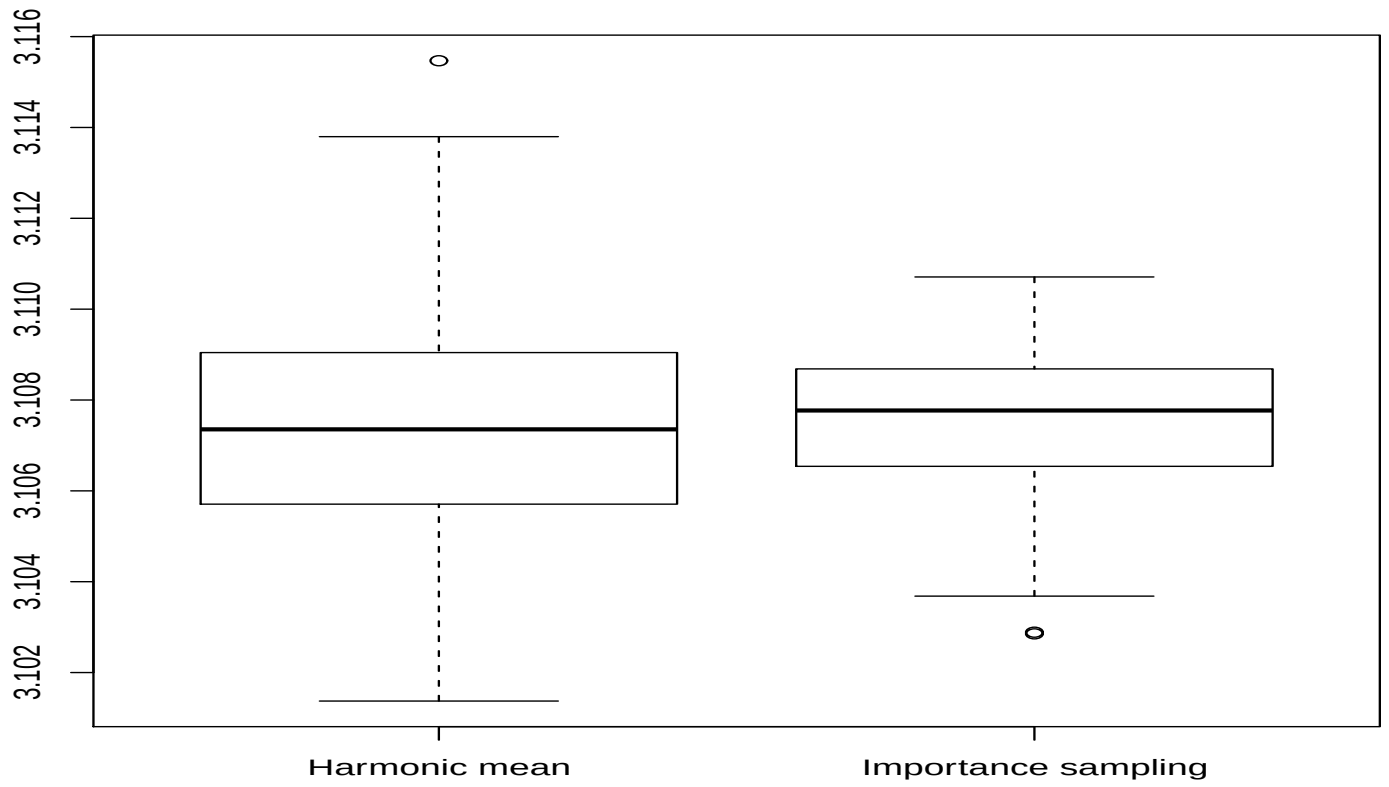
Use the convex hull of MCMC simulations corresponding to the 10% HPD region (easily derived!) and φ as indicator:

$$\varphi(\theta) = \frac{10}{T} \sum_{t \in \text{HPD}} \mathbb{I}_{d(\theta,\theta^{(t)}) \leq \epsilon}$$



Diabetes in Pima Indian women (cont'd)

Comparison of the variation of the Bayes factor approximations based on 100 replicas for $20,000$ simulations for a simulation from the above harmonic mean sampler and importance samplers



Approximating $\mathfrak{Z}_k$ using a mixture representation

◂ Bridge sampling redux

Design a specific mixture for simulation [importance sampling] purposes, with density

$$\widetilde{\varphi}_k(\theta_k) \propto \omega_1 \pi_k(\theta_k) L_k(\theta_k) + \varphi(\theta_k)\,,$$

where $\varphi(\cdot)$ is arbitrary (but normalised)
Note: ω_1 is not a probability weight

Approximating $\mathfrak{Z}$ using a mixture representation (cont'd)

Corresponding MCMC (=Gibbs) sampler

At iteration t

1. Take $\delta^{(t)} = 1$ with probability

$$\omega_1 \pi_k(\theta_k^{(t-1)}) L_k(\theta_k^{(t-1)}) \Big/ \left(\omega_1 \pi_k(\theta_k^{(t-1)}) L_k(\theta_k^{(t-1)}) + \varphi(\theta_k^{(t-1)})\right)$$

   and $\delta^{(t)} = 2$ otherwise;

2. If $\delta^{(t)} = 1$, generate $\theta_k^{(t)} \sim \text{MCMC}(\theta_k^{(t-1)}, \theta_k)$ where $\text{MCMC}(\theta_k, \theta_k')$ denotes an arbitrary MCMC kernel associated with the posterior $\pi_k(\theta_k|x) \propto \pi_k(\theta_k) L_k(\theta_k)$;

3. If $\delta^{(t)} = 2$, generate $\theta_k^{(t)} \sim \varphi(\theta_k)$ independently

Evidence approximation by mixtures

Rao-Blackwellised estimate

$$\hat{\xi} = \frac{1}{T}\sum_{t=1}^{T} \omega_1 \pi_k(\theta_k^{(t)}) L_k(\theta_k^{(t)}) \Big/ \omega_1 \pi_k(\theta_k^{(t)}) L_k(\theta_k^{(t)}) + \varphi(\theta_k^{(t)}) \,,$$

converges to $\omega_1 \mathfrak{Z}_k / \{\omega_1 \mathfrak{Z}_k + 1\}$
Deduce $\hat{\mathfrak{Z}}_{3k}$ from $\omega_1 \hat{\mathfrak{E}}_{3k} / \{\omega_1 \hat{\mathfrak{E}}_{3k} + 1\} = \hat{\xi}$ ie

$$\hat{\mathfrak{E}}_{3k} = \frac{\sum_{t=1}^{T} \omega_1 \pi_k(\theta_k^{(t)}) L_k(\theta_k^{(t)}) \Big/ \omega_1 \pi(\theta_k^{(t)}) L_k(\theta_k^{(t)}) + \varphi(\theta_k^{(t)})}{\sum_{t=1}^{T} \varphi(\theta_k^{(t)}) \Big/ \omega_1 \pi_k(\theta_k^{(t)}) L_k(\theta_k^{(t)}) + \varphi(\theta_k^{(t)})}$$

[Bridge sampler]

Chib's representation

Direct application of Bayes' theorem: given $\mathbf{x} \sim f_k(\mathbf{x}|\theta_k)$ and $\theta_k \sim \pi_k(\theta_k)$,

$$\mathfrak{E}_k = m_k(\mathbf{x}) = \frac{f_k(\mathbf{x}|\theta_k)\,\pi_k(\theta_k)}{\pi_k(\theta_k|\mathbf{x})}$$

Use of an approximation to the posterior

$$\widehat{\mathfrak{E}}_k = \widehat{m_k}(\mathbf{x}) = \frac{f_k(\mathbf{x}|\theta_k^*)\,\pi_k(\theta_k^*)}{\hat{\pi}_k(\theta_k^*|\mathbf{x})}\,.$$

Case of latent variables

For missing variable $\mathbf{z}$ as in mixture models, natural Rao-Blackwell estimate

$$\widehat{\pi_k}(\theta_k^*|\mathbf{x}) = \frac{1}{T}\sum_{t=1}^{T} \pi_k(\theta_k^*|\mathbf{x}, \mathbf{z}_k^{(t)})\,,$$

where the $\mathbf{z}_k^{(t)}$'s are Gibbs sampled latent variables

Label switching

A mixture model [special case of missing variable model] is invariant under permutations of the indices of the components. E.g., mixtures

$$0.3\mathcal{N}(0,1) + 0.7\mathcal{N}(2.3,1)$$

and

$$0.7\mathcal{N}(2.3,1) + 0.3\mathcal{N}(0,1)$$

are **exactly** the same!

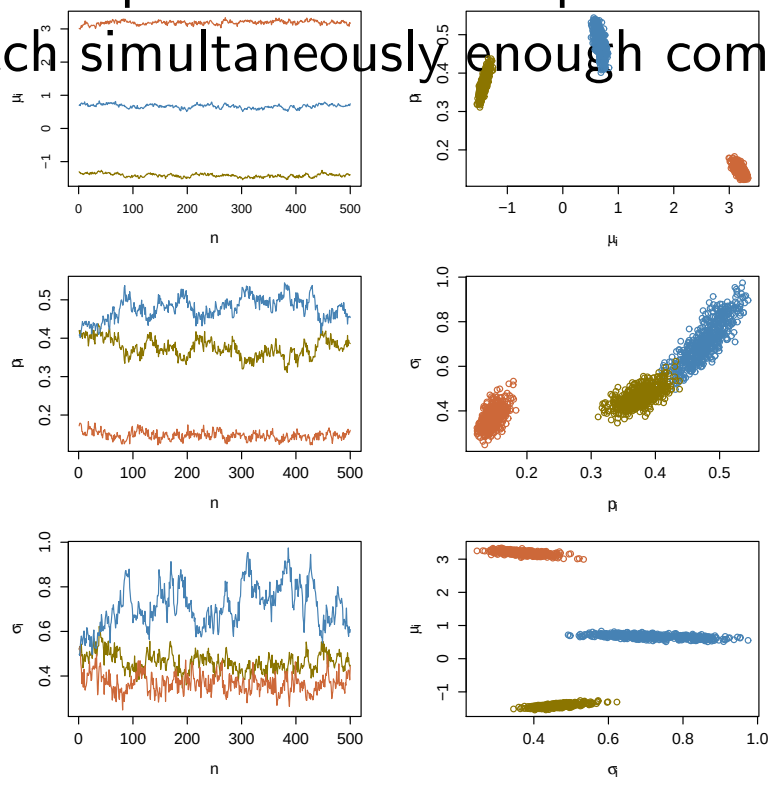
© **The component parameters θ_i are not identifiable marginally since they are exchangeable**

Connected difficulties

1. Number of modes of the likelihood of order $\mathrm{O}(k!)$:
   © Maximization and even [MCMC] exploration of the posterior surface harder
2. Under exchangeable priors on $(\theta, \mathbf{p})$ *[prior invariant under permutation of the indices]*, all posterior marginals are identical:
   © Posterior expectation of θ_1 equal to posterior expectation of θ_2

License

Since Gibbs output does not produce exchangeability, the Gibbs sampler has not explored the whole parameter space: it lacks energy to switch simultaneously enough component allocations at once



Label switching paradox

We should observe the exchangeability of the components [label switching] to conclude about convergence of the Gibbs sampler.
If we observe it, then we do not know how to estimate the parameters.
If we do not, then we are uncertain about the convergence!!!

Compensation for label switching

For mixture models, $\mathbf{z}_k^{(t)}$ usually fails to visit all configurations in a balanced way, despite the symmetry predicted by the theory

$$\pi_k(\theta_k|\mathbf{x}) = \pi_k(\sigma(\theta_k)|\mathbf{x}) = \frac{1}{k!}\sum_{\sigma\in\mathfrak{S}} \pi_k(\sigma(\theta_k)|\mathbf{x})$$

for all σ's in $\mathfrak{S}_k$, set of all permutations of $\{1,\ldots,k\}$.
Consequences on numerical approximation, biased by an order $k!$
Recover the theoretical symmetry by using

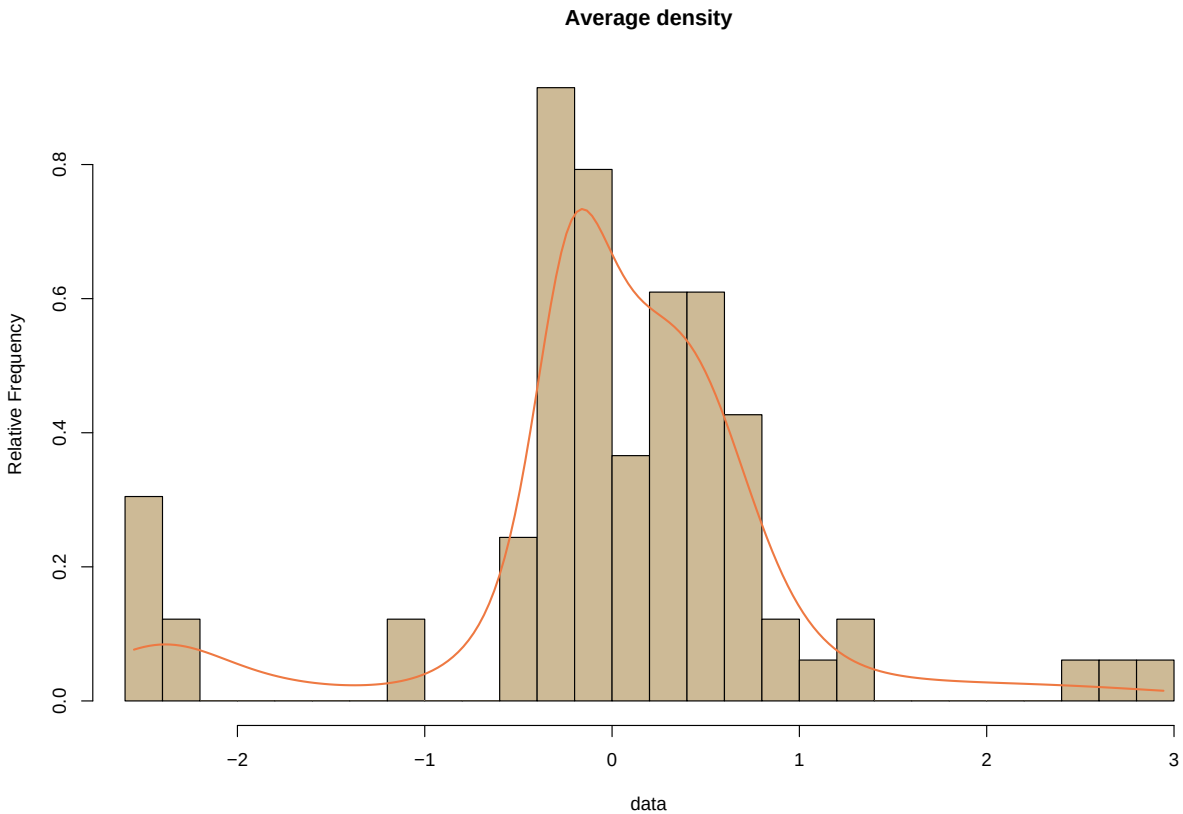
$$\widetilde{\pi_k}(\theta_k^*|\mathbf{x}) = \frac{1}{T\,k!}\sum_{\sigma\in\mathfrak{S}_k}\sum_{t=1}^{T} \pi_k(\sigma(\theta_k^*)|\mathbf{x},\mathbf{z}_k^{(t)})\,.$$

[Berkhof, Mechelen, & Gelman, 2003]

Galaxy dataset

$n = 82$ galaxies as a mixture of k normal distributions with both mean and variance unknown.

[Roeder, 1992]



Galaxy dataset (k)

Using only the original estimate, with θ_k^* as the MAP estimator,

$$\log(\hat{m}_k(\mathbf{x})) = -105.1396$$

for $k = 3$ (based on 10^3 simulations), while introducing the permutations leads to

$$\log(\hat{m}_k(\mathbf{x})) = -103.3479$$

Note that

$$-105.1396 + \log(3!) = -103.3479$$

k	2	3	4	5	6	7	8
$m_k(\mathbf{x})$	-115.68	-103.35	-102.66	-101.93	-102.88	-105.48	-108.44

Estimations of the marginal likelihoods by the symmetrised Chib's approximation (based on 10^5 Gibbs iterations and, for $k > 5$, 100 permutations selected at random in $\mathfrak{S}_k$).

[Lee, Marin, Mengersen & Robert, 2008]

Case of the probit model

For the completion by z,

$$\hat{\pi}(\theta|x) = \frac{1}{T} \sum_t \pi(\theta|x, z^{(t)})$$

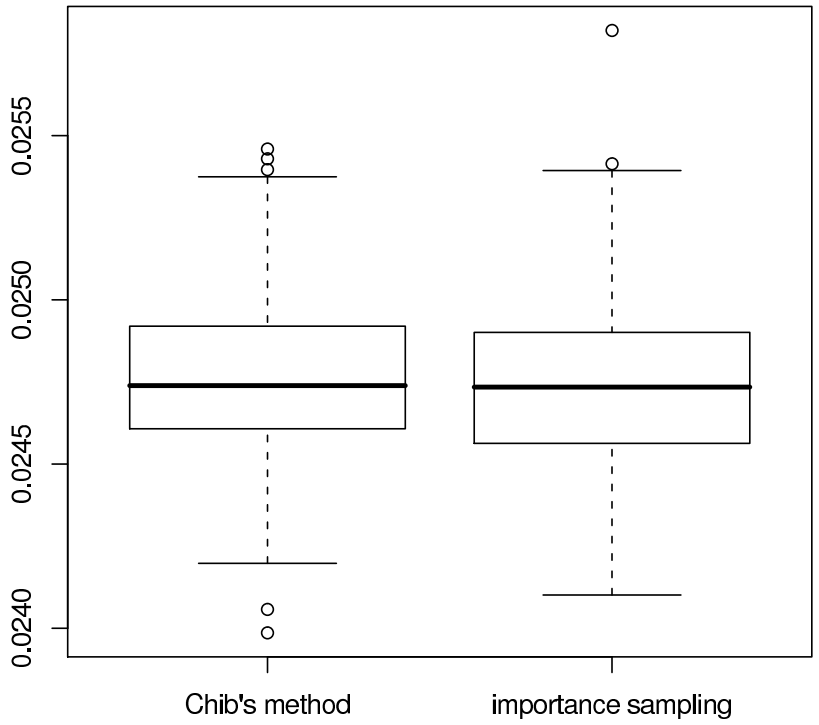
is a simple average of normal densities

R Bridge sampling code

```
gibbs1=gibbsprobit(Niter,y,X1)
gibbs2=gibbsprobit(Niter,y,X2)
bfchi=mean(exp(dmvlnorm(t(t(gibbs2$mu)-model2$coeff[,1]),mean=rep(0,3),
        sigma=gibbs2$Sigma2)-probitlpost(model2$coeff[,1],y,X2)))/
      mean(exp(dmvlnorm(t(t(gibbs1$mu)-model1$coeff[,1]),mean=rep(0,2),
        sigma=gibbs1$Sigma2)-probitlpost(model1$coeff[,1],y,X1)))
```

Diabetes in Pima Indian women (cont'd)

Comparison of the variation of the Bayes factor approximations based on 100 replicas for $20,000$ simulations for a simulation from the above Chib's and importance samplers



The Savage–Dickey ratio

Special representation of the Bayes factor used for simulation
Given a test $H_0 : \theta = \theta_0$ in a model $f(x|\theta, \psi)$ with a nuisance parameter ψ, under priors $\pi_0(\psi)$ and $\pi_1(\theta, \psi)$ such that

$$\pi_1(\psi|\theta_0) = \pi_0(\psi)$$

then

$$B_{01} = \frac{\pi_1(\theta_0|x)}{\pi_1(\theta_0)}\,,$$

with the obvious notations

$$\pi_1(\theta) = \int \pi_1(\theta, \psi)\mathrm{d}\psi\,, \quad \pi_1(\theta|x) = \int \pi_1(\theta, \psi|x)\mathrm{d}\psi\,,$$

[Dickey, 1971; Verdinelli & Wasserman, 1995]

Measure-theoretic difficulty

The representation depends on the choice of versions of conditional densities:

$$
\begin{aligned}
B_{01} &= \frac{\int \pi_0(\psi) f(x|\theta_0,\psi)\,\mathrm{d}\psi}{\int \pi_1(\theta,\psi) f(x|\theta,\psi)\,\mathrm{d}\psi\mathrm{d}\theta} && \text{[by definition]}\\
&= \frac{\int \pi_1(\psi|\theta_0) f(x|\theta_0,\psi)\,\mathrm{d}\psi\,\pi_1(\theta_0)}{\int \pi_1(\theta,\psi) f(x|\theta,\psi)\,\mathrm{d}\psi\mathrm{d}\theta\,\pi_1(\theta_0)} && \text{[specific version of } \pi_1(\psi|\theta_0)\text{]}\\
&= \frac{\int \pi_1(\theta_0,\psi) f(x|\theta_0,\psi)\,\mathrm{d}\psi}{m_1(x)\pi_1(\theta_0)} && \text{[specific version of } \pi_1(\theta_0,\psi)\text{]}\\
&= \frac{\pi_1(\theta_0|x)}{\pi_1(\theta_0)}
\end{aligned}
$$

© Dickey's (1971) condition is not a condition

Similar measure-theoretic difficulty

Verdinelli-Wasserman extension:

$$B_{01} = \frac{\pi_1(\theta_0|x)}{\pi_1(\theta_0)} \, \mathbb{E}^{\pi_1(\psi|x,\theta_0,x)} \left[\frac{\pi_0(\psi)}{\pi_1(\psi|\theta_0)} \right]$$

depends on similar choices of versions

Monte Carlo implementation relies on continuous versions of all densities *without making mention of it*

[Chen, Shao & Ibrahim, 2000]

Computational implementation

Starting from the (new) prior

$$\tilde{\pi}_1(\theta, \psi) = \pi_1(\theta)\pi_0(\psi)$$

define the associated posterior

$$\tilde{\pi}_1(\theta, \psi|x) = \pi_0(\psi)\pi_1(\theta)f(x|\theta, \psi)/\tilde{m}_1(x)$$

and impose

$$\frac{\tilde{\pi}_1(\theta_0|x)}{\pi_0(\theta_0)} = \frac{\int \pi_0(\psi)f(x|\theta_0, \psi)\,\mathrm{d}\psi}{\tilde{m}_1(x)}$$

to hold.
Then

$$B_{01} = \frac{\tilde{\pi}_1(\theta_0|x)}{\pi_1(\theta_0)}\,\frac{\tilde{m}_1(x)}{m_1(x)}$$

First ratio

If $(\theta^{(1)}, \psi^{(1)}), \ldots, (\theta^{(T)}, \psi^{(T)}) \sim \tilde{\pi}(\theta, \psi|x)$, then

$$\frac{1}{T} \sum_t \tilde{\pi}_1(\theta_0|x, \psi^{(t)})$$

converges to $\tilde{\pi}_1(\theta_0|x)$ (if the right version is used in θ_0). When $\tilde{\pi}_1(\theta_0|x, \psi$ unavailable, replace with

$$\frac{1}{T} \sum_{t=1}^{T} \tilde{\pi}_1(\theta_0|x, z^{(t)}, \psi^{(t)})$$

Bridge revival (1)

Since $\tilde{m}_1(x)/m_1(x)$ is unknown, apparent failure!
Use of the identity

$$\mathbb{E}^{\tilde{\pi}_1(\theta,\psi|x)}\left[\frac{\pi_1(\theta,\psi)f(x|\theta,\psi)}{\pi_0(\psi)\pi_1(\theta)f(x|\theta,\psi)}\right] = \mathbb{E}^{\tilde{\pi}_1(\theta,\psi|x)}\left[\frac{\pi_1(\psi|\theta)}{\pi_0(\psi)}\right] = \frac{m_1(x)}{\tilde{m}_1(x)}$$

to (biasedly) estimate $\tilde{m}_1(x)/m_1(x)$ by

$$T/\sum_{t=1}^{T}\frac{\pi_1(\psi^{(t)}|\theta^{(t)})}{\pi_0(\psi^{(t)})}$$

based on the same sample from $\tilde{\pi}_1$.

Bridge revival (2)

Alternative identity

$$\mathbb{E}^{\pi_1(\theta,\psi|x)}\left[\frac{\pi_0(\psi)\pi_1(\theta)f(x|\theta,\psi)}{\pi_1(\theta,\psi)f(x|\theta,\psi)}\right] = \mathbb{E}^{\pi_1(\theta,\psi|x)}\left[\frac{\pi_0(\psi)}{\pi_1(\psi|\theta)}\right] = \frac{\tilde{m}_1(x)}{m_1(x)}$$

suggests using a second sample $(\bar{\theta}^{(1)}, \bar{\psi}^{(1)}, z^{(1)}), \ldots,$ $(\bar{\theta}^{(T)}, \bar{\psi}^{(T)}, z^{(T)}) \sim \pi_1(\theta, \psi|x)$ and

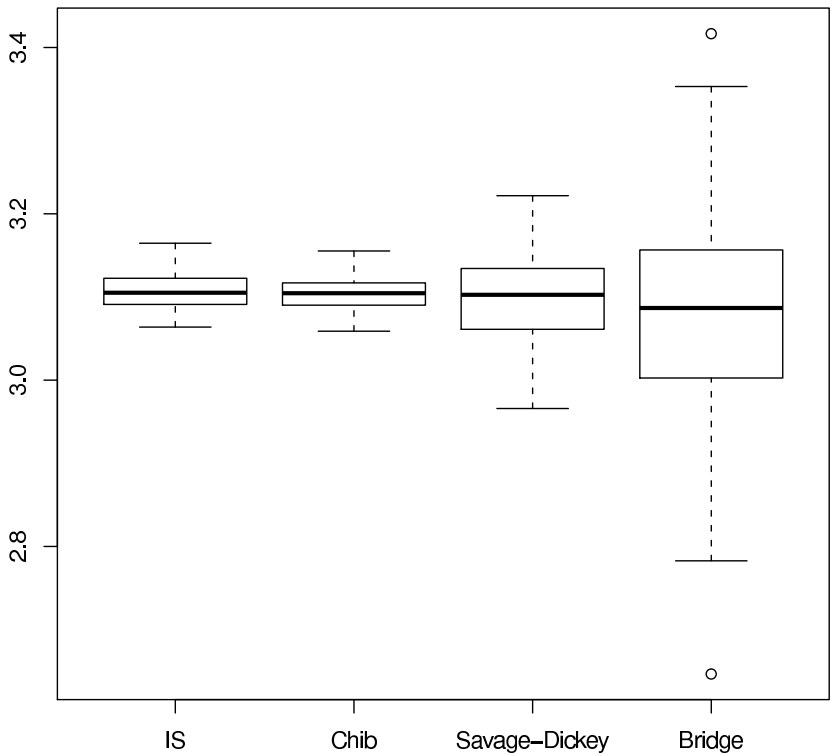
$$\frac{1}{T}\sum_{t=1}^{T}\frac{\pi_0(\bar{\psi}^{(t)})}{\pi_1(\bar{\psi}^{(t)}|\bar{\theta}^{(t)})}$$

Resulting estimate:

$$\widehat{B_{01}} = \frac{1}{T}\frac{\sum_t \tilde{\pi}_1(\theta_0|x, z^{(t)}, \psi^{(t)})}{\pi_1(\theta_0)}\,\frac{1}{T}\sum_{t=1}^{T}\frac{\pi_0(\bar{\psi}^{(t)})}{\pi_1(\bar{\psi}^{(t)}|\bar{\theta}^{(t)})}$$

Diabetes in Pima Indian women (cont'd)

Comparison of the variation of the Bayes factor approximations based on 100 replicas for $20,000$ simulations for a simulation from the above importance, Chib's, Savage–Dickey's and bridge samplers



Nested sampling: Goal

Skilling's (2007) technique using the one-dimensional representation:

$$\mathfrak{E} = \mathbb{E}^{\pi}[L(\theta)] = \int_0^1 \varphi(x)\,\mathrm{d}x$$

with

$$\varphi^{-1}(l) = P^{\pi}(L(\theta) > l).$$

Note; $\varphi(\cdot)$ is intractable in most cases.

Nested sampling: First approximation

Approximate $\mathfrak{E}$ by a Riemann sum:

$$\widehat{\mathfrak{E}} = \sum_{i=1}^{j} (x_{i-1} - x_i)\varphi(x_i)$$

where the x_i's are either:

- deterministic: $x_i = e^{-i/N}$
- or random:

$$x_0 = 1, \quad x_{i+1} = t_i x_i, \quad t_i \sim \mathcal{B}e(N, 1)$$

so that $\mathbb{E}[\log x_i] = -i/N$.

Extraneous white noise

Take

$$\mathfrak{E} = \int e^{-\theta}\,\mathrm{d}\theta = \int \frac{1}{\delta}\, e^{-(1-\delta)\theta}\, e^{-\delta\theta} = \mathbb{E}_\delta\left[\frac{1}{\delta}\, e^{-(1-\delta)\theta}\right]$$

$$\hat{\mathfrak{E}} = \frac{1}{N}\sum_{i=1}^{N} \delta^{-1}\, e^{-(1-\delta)\theta_i}(x_{i-1} - x_i)\,, \quad \theta_i \sim \mathcal{E}(\delta)\,\mathbb{I}(\theta_i \le \theta_{i-1})$$

N	deterministic	random
50	4.64	10.5
	4.65	10.5
100	2.47	4.9
	2.48	5.02
500	.549	1.01
	.550	1.14

Comparison of variances and MSEs

Nested sampling: Second approximation

Replace (intractable) $\varphi(x_i)$ by φ_i, obtained by

Nested sampling

Start with N values $\theta_1, \ldots, \theta_N$ sampled from π
At iteration i,

1. Take $\varphi_i = L(\theta_k)$, where θ_k is the point with smallest likelihood in the pool of θ_i's
2. Replace θ_k with a sample from the prior constrained to $L(\theta) > \varphi_i$: the current N points are sampled from prior constrained to $L(\theta) > \varphi_i$.

Nested sampling: Third approximation

Iterate the above steps until a given stopping iteration j is reached: e.g.,

- observe very small changes in the approximation $\widehat{\mathfrak{Z}}$;
- reach the maximal value of $L(\theta)$ when the likelihood is bounded and its maximum is known;
- truncate the integral $\mathfrak{E}$ at level ϵ, i.e. replace

$$\int_0^1 \varphi(x)\,\mathrm{d}x \qquad \text{with} \qquad \int_\epsilon^1 \varphi(x)\,\mathrm{d}x$$

Approximation error

$$\text{Error} = \widehat{\mathfrak{E}} - \mathfrak{E}$$

$$= \sum_{i=1}^{j}(x_{i-1} - x_i)\varphi_i - \int_0^1 \varphi(x)\,\mathrm{d}x = -\int_0^\epsilon \varphi(x)\,\mathrm{d}x$$

$$+ \left[\sum_{i=1}^{j}(x_{i-1} - x_i)\varphi(x_i) - \int_\epsilon^1 \varphi(x)\,\mathrm{d}x\right] \quad \text{(Quadrature Error)}$$

$$+ \left[\sum_{i=1}^{j}(x_{i-1} - x_i)\left\{\varphi_i - \varphi(x_i)\right\}\right] \quad \text{(Stochastic Error)}$$

[Dominated by Monte Carlo!]

A CLT for the Stochastic Error

The (dominating) stochastic error is $O_P(N^{-1/2})$:

$$N^{1/2}\left\{\text{Stochastic Error}\right\} \xrightarrow{\mathcal{D}} \mathcal{N}\left(0, V\right)$$

with

$$V = -\int_{s,t\in[\epsilon,1]} s\varphi'(s)t\varphi'(t)\log(s\vee t)\,\mathrm{d}s\,\mathrm{d}t.$$

[Proof based on Donsker's theorem]

The number of simulated points equals the number of iterations j, and is a multiple of N: if one stops at first iteration j such that $e^{-j/N} < \epsilon$, then: $j = N\lceil -\log\epsilon\rceil$.

Curse of dimension

For a simple Gaussian-Gaussian model of dimension $\dim(\theta) = d$, the following 3 quantities are $\mathrm{O}(d)$:

1. asymptotic variance of the NS estimator;
2. number of iterations (necessary to reach a given truncation error);
3. cost of one simulated sample.

Therefore, CPU time necessary for achieving error level e is

$$\mathrm{O}(d^3/e^2)$$

Sampling from constr'd priors

Exact simulation from the constrained prior is intractable in most cases!

Skilling (2007) proposes to use MCMC, but:

- this introduces a bias (stopping rule).
- if MCMC stationary distribution is unconst'd prior, more and more difficult to sample points such that $L(\theta) > l$ as l increases.

If implementable, then slice sampler can be devised at the same cost!

A IS variant of nested sampling

Consider instrumental prior $\widetilde{\pi}$ and likelihood $\tilde{L}$, weight function

$$w(\theta) = \frac{\pi(\theta)L(\theta)}{\widetilde{\pi}(\theta)\widetilde{L}(\theta)}$$

and weighted NS estimator

$$\widehat{\mathfrak{E}} = \sum_{i=1}^{j}(x_{i-1} - x_i)\varphi_i w(\theta_i).$$

Then choose $(\widetilde{\pi}, \widetilde{L})$ so that sampling from $\widetilde{\pi}$ constrained to $\widetilde{L}(\theta) > l$ is easy; e.g. $\mathcal{N}(c, I_d)$ constrained to $\|c - \theta\| < r$.

Benchmark: Target distribution

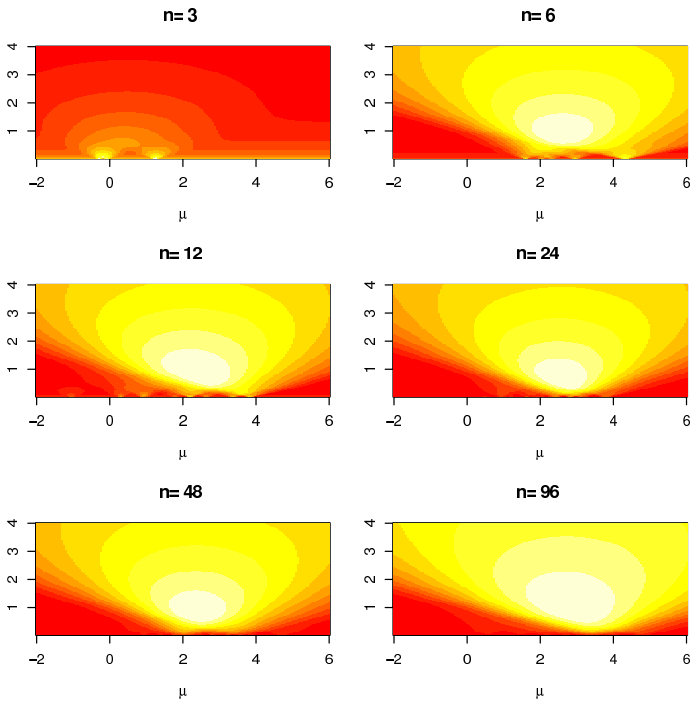
Posterior distribution on (μ, σ) associated with the mixture

$$p\mathcal{N}(0,1) + (1-p)\mathcal{N}(\mu,\sigma)\,,$$

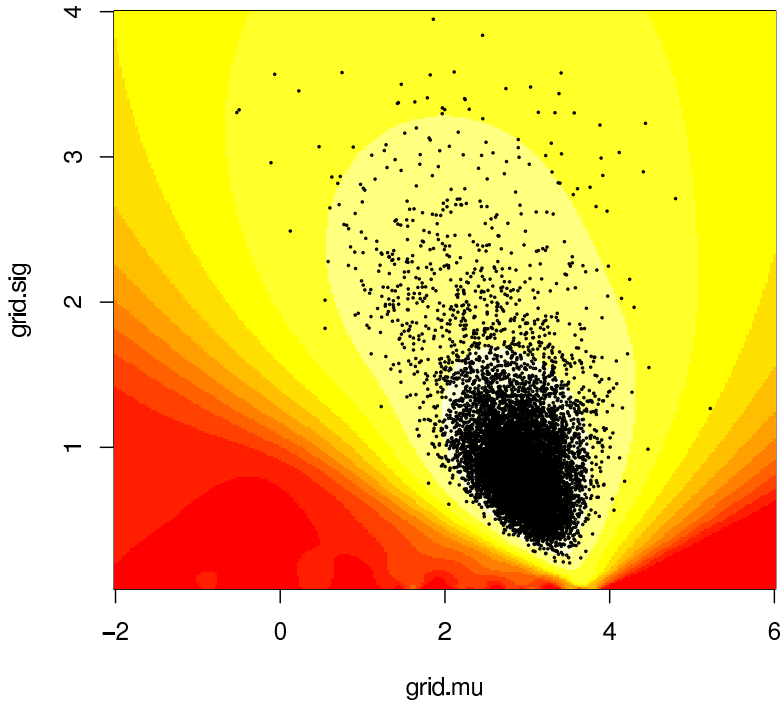
when p is known

Experiment

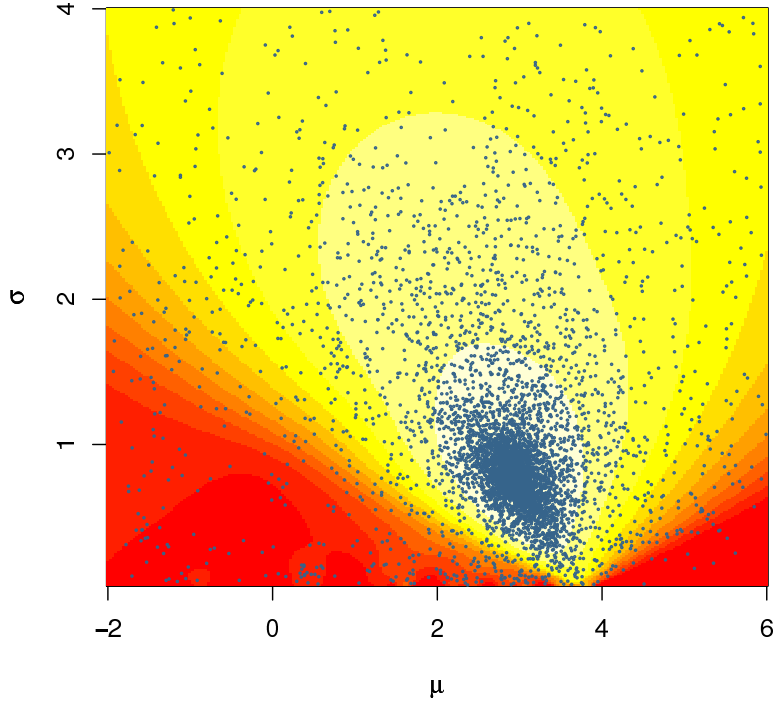
- n observations with $\mu = 2$ and $\sigma = 3/2$,
- Use of a uniform prior both on $(-2, 6)$ for μ and on $(.001, 16)$ for $\log \sigma^2$.
- occurrences of posterior bursts for $\mu = x_i$
- computation of the various estimates of $\mathfrak{E}$



Experiment (cont'd)

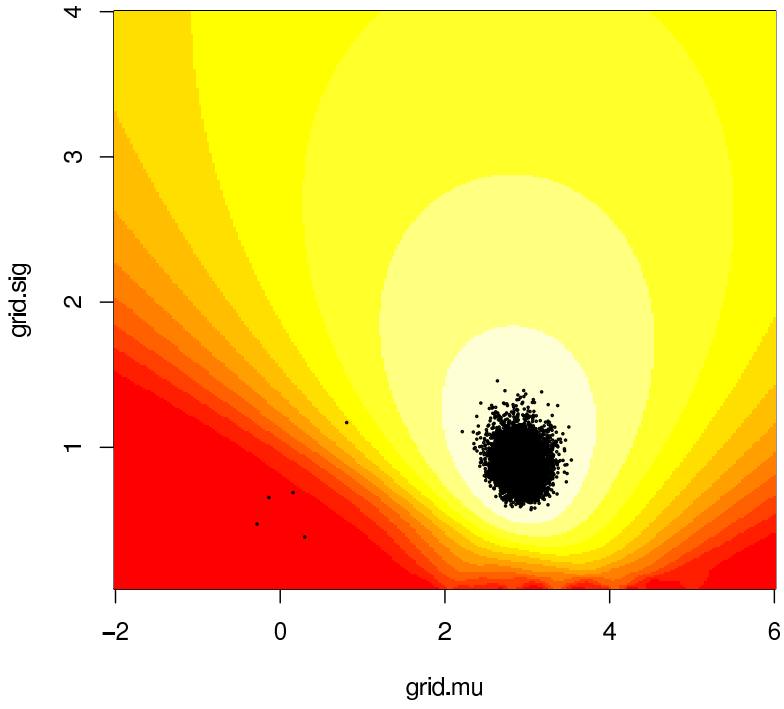


MCMC sample for $n = 16$ observations from the mixture.

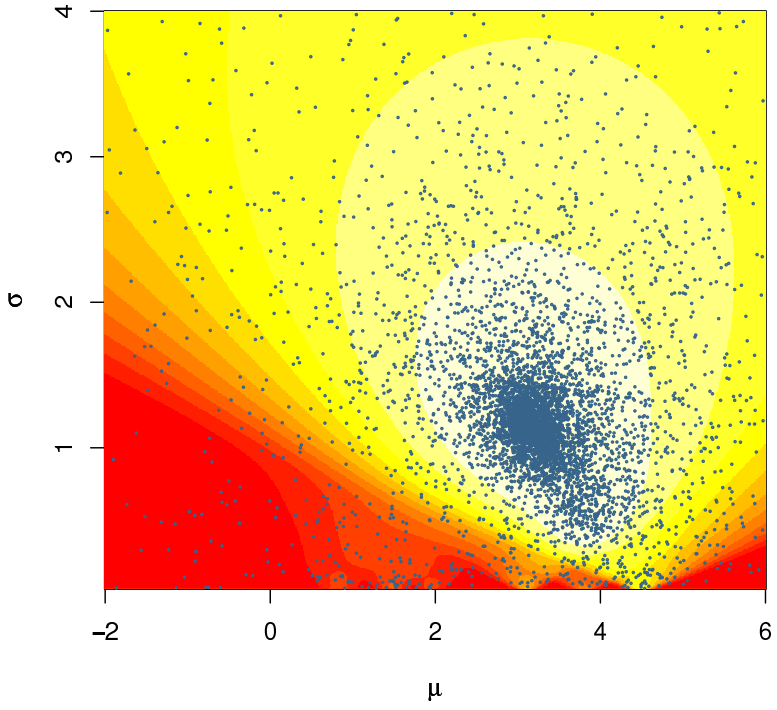


Nested sampling sequence with $M = 1000$ starting points.

Experiment (cont'd)



MCMC sample for $n = 50$ observations from the mixture.

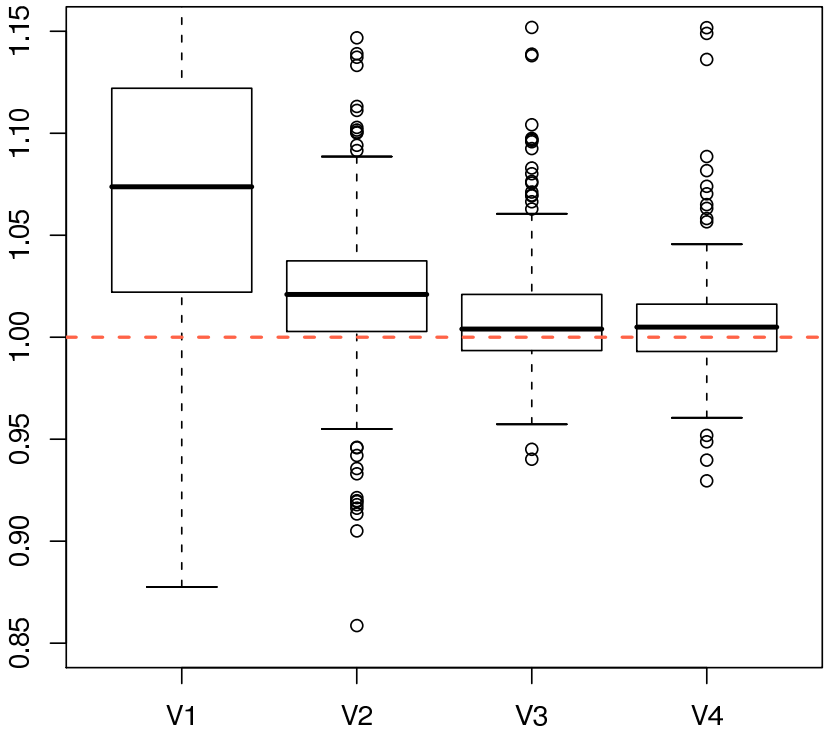


Nested sampling sequence with $M = 1000$ starting points.

Comparison

Monte Carlo and MCMC (=Gibbs) outputs based on $T = 10^4$ simulations and numerical integration based on a 850×950 grid in the (μ, σ) parameter space.
Nested sampling approximation based on a starting sample of $M = 1000$ points followed by at least 103 further simulations from the constr'd prior and a stopping rule at 95% of the observed maximum likelihood.
Constr'd prior simulation based on 50 values simulated by random walk accepting only steps leading to a lik'hood higher than the bound

Comparison (cont'd)



Graph based on a sample of 10 observations for $\mu = 2$ and $\sigma = 3/2$ (150 replicas).

Comparison (cont'd)

Nested sampling gets less reliable as sample size increases
Most reliable approach is mixture $\widehat{\mathfrak{E}}_3$ although harmonic solution $\widehat{\mathfrak{E}}_1$ close to Chib's solution [taken as golden standard]
Monte Carlo method $\widehat{\mathfrak{E}}_2$ also producing poor approximations to $\mathfrak{E}$
(Kernel ϕ used in $\widehat{\mathfrak{E}}_2$ is a t non-parametric kernel estimate with standard bandwidth estimation.)

Notions on Markov Chains

Basics

Definition (Markov chain)

A sequence of random variables whose distribution evolves over **time** as a function of past realizations

Chain defined through its **transition kernel**, a function K defined on $\mathscr{X} \times \mathscr{B}(\mathscr{X})$ such that

- $\forall x \in \mathscr{X}$, $K(x, \cdot)$ is a probability measure;
- $\forall A \in \mathscr{B}(\mathscr{X})$, $K(\cdot, A)$ is measurable.

no discrete

- When $\mathscr{X}$ is a **discrete** (finite or denumerable) set, the transition kernel simply is a (transition) matrix $\mathbb{K}$ with elements

$$P_{xy} = \mathsf{Pr}(X_n = y | X_{n-1} = x) \,, \qquad x, y \in \mathscr{X}$$

Since, for all $x \in \mathscr{X}$, $K(x, \cdot)$ is a probability, we must have

$$P_{xy} \geq 0 \quad \text{and} \quad K(x, \mathscr{X}) = \sum_{y \in \mathscr{X}} P_{xy} = 1$$

The matrix $\mathbb{K}$ is referred to as a **Markov transition matrix** or a **stochastic matrix**

- In the **continuous** case, the *kernel* also denotes the conditional density $\mathfrak{K}(x, x')$ of the transition $K(x, \cdot)$

$$\Pr(X \in A|x) = \int_A \mathfrak{K}(x, x')dx'.$$

Then, for any bounded ϕ, we may define

$$K\phi(x) = K(x, \phi) = \int_{\mathscr{X}} \mathfrak{K}(x, dy)\phi(y).$$

Note that

$$|K\phi(x)| \leq \int_{\mathscr{X}} \mathfrak{K}(x, dy)|\phi(y)| \leq |\phi|_\infty = \sup_{x \in \mathscr{X}} |\phi(x)|.$$

We may also associate to a probability measure μ the measure μK, defined as

$$\mu K(A) = \int_{\mathscr{X}} \mu(dx)K(x, A).$$

Markov chains

skip definition

Given a transition kernel K, a sequence $X_0, X_1, \ldots, X_n, \ldots$ of random variables is a **Markov chain** denoted by (X_n), if, for any t, the conditional distribution of X_t given $x_{t-1}, x_{t-2}, \ldots, x_0$ is the same as the distribution of X_t given x_{t-1}. That is,

$$\begin{aligned} \Pr(X_{k+1} \in A | x_0, x_1, x_2, \ldots, x_k) &= \Pr(X_{k+1} \in A | x_k) \\ &= \int_A \mathfrak{K}(x_k, dx) \end{aligned}$$

Note that the entire structure of the chain only depends on

- The transition function K
- The initial state x_0 or initial distribution $X_0 \sim \mu$

Example (Random walk)

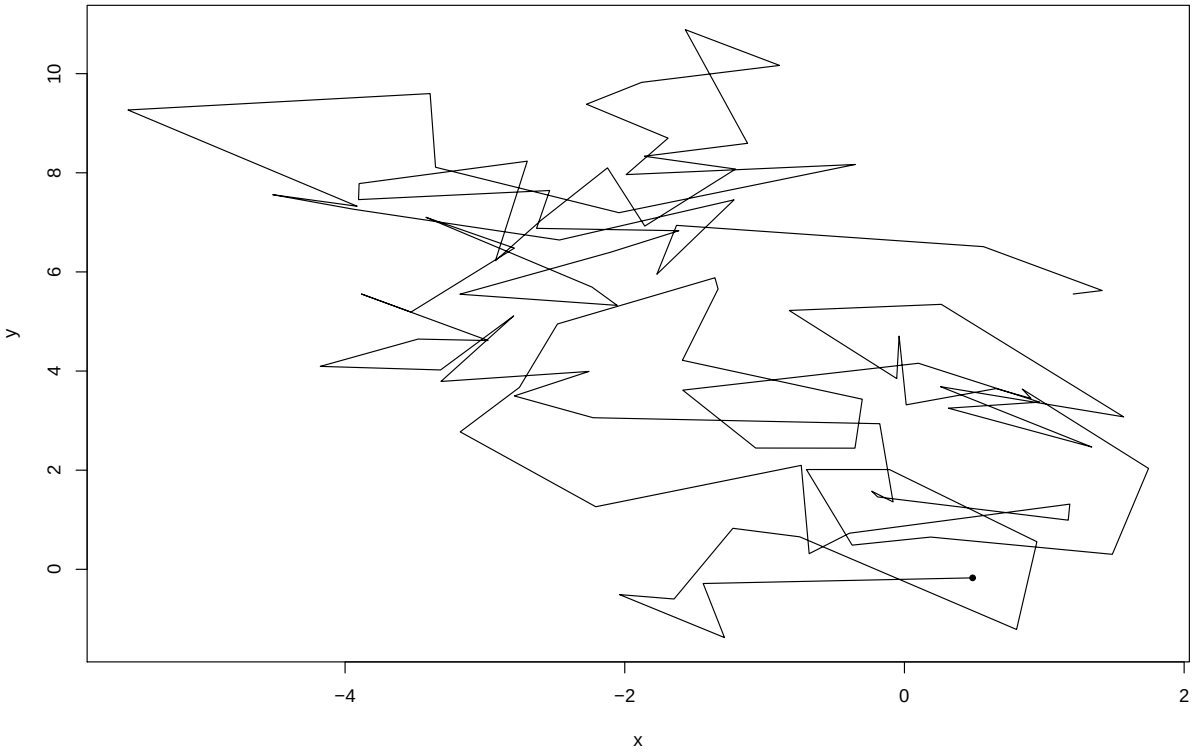
The normal random walk is the kernel $K(x, \cdot)$ associated with the distribution

$$\mathcal{N}_p(x, \tau^2 I_p)$$

which means

$$X_{t+1} = X_t + \tau \epsilon_t$$

ϵ_t being an iid additional noise



100 consecutive realisations of the random walk in $\mathbb{R}^2$ with $\tau = 1$

bypass remarks

On a **discrete state-space** $\mathscr{X} = \{x_0, x_1, \ldots\}$,

- A function ϕ on a discrete state space is uniquely defined by the (column) vector $\phi = (\phi(x_0), \phi(x_1), \ldots,)^{\mathrm{T}}$ and

$$K\phi(x) = \sum_{y \in \mathscr{X}} P_{xy}\phi(y)$$

  can be interpreted as the xth component of the product of the transition matrix $\mathbb{K}$ and of the vector ϕ.
- A probability distribution on $\mathcal{P}(\mathscr{X})$ is defined as a (row) vector $\mu = (\mu(x_0), \mu(x_1), \ldots)$ and the probability distribution μK is defined, for each $y \in \mathscr{X}$ as

$$\mu K(\{y\}) = \sum_{x \in \mathscr{X}} \mu(\{x\}) P_{xy}$$

  yth component of the product of the vector μ and of the transition matrix $\mathbb{K}$.

Composition of kernels

Let Q_1 and Q_2 be two probability kernels. Define, for any $x \in \mathscr{X}$ and any $A \in \mathcal{B}(\mathscr{X})$ the **product of kernels** Q_1Q_2 as

$$Q_1Q_2(x, A) = \int_{\mathscr{X}} \mathfrak{Q}_1(x, dy)\mathfrak{Q}_2(y, A)$$

When the state space $\mathscr{X}$ is discrete, the product of Markov kernels coincides with the product of matrices $\mathbb{Q}_1 \times \mathbb{Q}_2$.

Irreducibility

Irreducibility is one measure of the sensitivity of the Markov chain to initial conditions
It leads to a guarantee of convergence for MCMC algorithms

Definition (Irreducibility)

In the discrete case, the chain is *irreducible* if all states communicate, namely if

$$P_x(\tau_y < \infty) > 0 \,, \qquad \forall x, y \in \mathscr{X} \,,$$

τ_y being the first (positive) time y is visited

Irreducibility for a continuous chain

In the continuous case, the chain is φ-*irreducible* for some measure φ if for some n,

$$K^n(x, A) > 0$$

- for all $x \in \mathscr{X}$
- for every $A \in \mathscr{B}(\mathscr{X})$ with $\varphi(A) > 0$

Minoration condition

Assume there exist a probability measure ν and $\epsilon > 0$ such that, for all $x \in \mathscr{X}$ and all $A \in \mathscr{B}(\mathscr{X})$,

$$K(x, A) \geq \epsilon \nu(A)$$

This is called a **minoration condition**.
When K is a Markov chain on a discrete state space, this is equivalent to saying that $P_{xy} > 0$ for all $x, y \in \mathscr{X}$.

Small sets

Definition (Small set)

If there exist $C \in \mathscr{B}(\mathscr{X})$, $\varphi(C) > 0$, a probability measure ν and $\epsilon > 0$ such that, for all $x \in C$ and all $A \in \mathscr{B}(\mathscr{X})$,

$$K(x, A) \geq \epsilon \nu(A)$$

C is called a **small set**

For discrete state space, **atoms** are small sets.

Towards further stability

- Irreducibility: every set A has a chance to be visited by the Markov chain (X_n)
- This property is too weak to ensure that the trajectory of (X_n) will enter A often enough.
- A Markov chain must enjoy good *stability* properties to guarantee an acceptable approximation of the simulated model.
  - Formalizing this stability leads to different notions of *recurrence*
  - For discrete chains, the *recurrence of a state* equivalent to probability one of sure return.
  - Always satisfied for irreducible chains on finite spaces

Transience and Recurrence

In a finite state space $\mathscr{X}$, denote the average number of visits to a state ω by

$$\eta_\omega = \sum_{i=1}^{\infty} \mathbb{I}_\omega(X_i)$$

If $\mathbb{E}_\omega[\eta_\omega] = \infty$, the state is *recurrent*
If $\mathbb{E}_\omega[\eta_\omega] < \infty$, the state is *transient*
For irreducible chains, recurrence/transience is **property of the chain**, not of a particular state
Similar definitions for the continuous case.

Harris recurrence

Stronger form of recurrence:

Definition (Harris recurrence)

A set A is *Harris recurrent* if

$$P_x(\eta_A = \infty) = 1 \text{ for all } x \in A.$$

The chain (X_n) is Ψ*–Harris recurrent* if it is

- ψ–irreducible
- for every set A with $\psi(A) > 0$, A is Harris recurrent.

Note that

$$P_x(\eta_A = \infty) = 1 \text{ implies } \mathbb{E}_x[\eta_A] = \infty$$

Invariant measures

Stability increases for the chain (X_n) if marginal distribution of X_n independent of n
Requires the existence of a probability distribution π such that

$$X_{n+1} \sim \pi \quad \text{if} \quad X_n \sim \pi$$

Definition (Invariant measure)

A measure π is **invariant** for the transition kernel $K(\cdot, \cdot)$ if

$$\pi(B) = \int_{\mathscr{X}} K(x, B)\, \pi(dx)\,, \qquad \forall B \in \mathscr{B}(\mathscr{X})\,.$$

Stability properties and invariance

- The chain is **positive recurrent** if π is a probability measure.
- Otherwise it is **null recurrent** or **transient**

- If π probability measure, π also called *stationary distribution* since

$$X_0 \sim \pi \text{ implies that } X_n \sim \pi \text{ for every } n$$

- The stationary distribution is unique

Insights

no time for that!

Invariant probability measures are important not merely because they define stationary processes, but also because they turn out to be the measures which define the long-term or ergodic behavior of the chain.

To understand why, consider $P_\mu(X_n \in \cdot)$ for a starting distribution μ. If a limiting measure γ_μ exists such as

$$P_\mu(X_n \in A) \to \gamma_\mu(A)$$

for all $A \in \mathscr{B}(\mathscr{X})$, then

$$\begin{aligned}
\gamma_\mu(A) &= \lim_{n\to\infty} \int \mu(dx) P^n(x, A) \\
&= \lim_{n\to\infty} \int_{\mathscr{X}} \int P^{n-1}(x, dw) K(w, A) \\
&= \int_{\mathscr{X}} \gamma_\mu(dw) K(w, A)
\end{aligned}$$

since setwise convergence of $\int \mu P^n(x, \cdot)$ implies convergence of integrals of bounded measurable functions. Hence, if a limiting distribution exists, it is an invariant probability measure; and obviously, if there is a unique invariant probability measure, the limit γ_μ will be independent of μ whenever it exists.

Ergodicity and convergence

We finally consider: **to what is the chain converging?**
The invariant distribution π is a natural candidate for the *limiting distribution*
A fundamental property is **ergodicity**, or independence of initial conditions. In the discrete case, a state ω is *ergodic* if

$$\lim_{n\to\infty} |K^n(\omega,\omega) - \pi(\omega)| = 0 \; .$$

Norm and convergence

In general , we establish convergence using the *total variation norm*

$$\|\mu_1 - \mu_2\|_{\mathrm{TV}} = \sup_A \ |\mu_1(A) - \mu_2(A)|$$

and we want

$$\left\| \int \ K^n(x, \cdot)\mu(dx) - \pi \ \right\|_{\mathrm{TV}}$$

$$= \quad \sup_A \left| \int \ K^n(x, A)\mu(dx) - \pi(A) \ \right|$$

to be small.

skip minoration TV

Total variation distance and minoration

Lemma

Let μ and μ' be two probability measures. Then,

$$1 - \inf \left\{ \sum_i \mu(A_i) \wedge \mu'(A_i) \right\} = \|\mu - \mu'\|_{\mathrm{TV}}.$$

where the infimum is taken over all finite partitions $(A_i)_i$ of $\mathscr{X}$.

Total variation distance and minoration (2)

Assume that there exist a probability ν and $\epsilon > 0$ such that, for all $A \in \mathcal{B}(\mathscr{X})$ we have

$$\mu(A) \wedge \mu'(A) \geq \epsilon\nu(A).$$

Then, for all I and all partitions A_1, A_2, ..., A_I,

$$\sum_{i=1} \mu(A_i) \wedge \mu'(A_i) \geq \epsilon$$

and the previous result thus implies that

$$\|\mu - \mu'\|_{\mathrm{TV}} \leq (1 - \epsilon).$$

Harris recurrence and ergodicity

Theorem

If (X_n) Harris positive recurrent and aperiodic, then

$$\lim_{n\to\infty} \left\| \int K^n(x,\cdot)\mu(dx) - \pi \right\|_{TV} = 0$$

for every initial distribution μ.

We thus take "*Harris positive recurrent and aperiodic*" as equivalent to "*ergodic*"

[Meyn & Tweedie, 1993]

Convergence in total variation implies

$$\lim_{n\to\infty} |\mathbb{E}_\mu[h(X_n)] - \mathbb{E}^\pi[h(X)]| = 0$$

for every *bounded function* h.

▸ no detail of convergence

Convergences

There are difference speeds of convergence

- ergodic (fast enough)
- *geometrically* ergodic (faster)
- *uniformly* ergodic (fastest)

Geometric ergodicity

A ϕ-irreducible aperiodic Markov kernel P with invariant distribution π is **geometrically ergodic** if there exist $V \geq 1$, and constants $\rho < 1$, $R < \infty$ such that $(n \geq 1)$

$$\|P^n(x, .) - \pi(.)\|_V \leq RV(x)\rho^n \,,$$

on $\{V < \infty\}$ which is full and absorbing.

Geometric ergodicity implies a lot of important results

- CLT for additive functionals $n^{-1/2}\sum g(X_k)$ and functions $|g| < V$
- Rosenthal's type inequalities

$$\mathbb{E}_x \left| \sum_{k=1}^{n} g(X_k) \right|^p \leq C(p) n^{p/2}, \qquad |g|^p \leq 2$$

- exponential inequalities (for bounded functions and α small enough)

$$\mathbb{E}_x \left\{ \exp\left(\alpha \sum_{k=1}^{n} g(X_k) \right) \right\} < \infty$$

Minoration condition and uniform ergodicity

Under the minoration condition, the kernel K is thus contractant and standard results in functional analysis shows the existence and the unicity of a fixed point π. The previous relation implies that, for all $x \in \mathscr{X}$.

$$\|P^n(x, \cdot) - \pi\|_{\mathrm{TV}} \leq (1 - \epsilon)^n$$

Such Markov chains are called **uniformly ergodic**.

Uniform ergodicity

Theorem (S&n ergodicity)

The following conditions are equivalent:

- $(X_n)_n$ **is uniformly ergodic,**
- **there exist** $\rho < 1$ **and** $R < \infty$ **such that, for all** $x \in \mathscr{X}$ **,**

$$\|P^n(x,\cdot) - \pi\|_{\mathrm{TV}} \leq R\rho^n\,,$$

- **for some** $n > 0$**,**

$$\sup_{x\in\mathscr{X}} \|P^n(x,\cdot) - \pi(\cdot)\|_{\mathrm{TV}} < 1.$$

[Meyn and Tweedie, 1993]

Limit theorems

Ergodicity determines the probabilistic properties of **average** behavior of the chain.
But also need of *statistical inference*, made by induction from the observed sample.
If $\|P_x^n - \pi\|$ close to 0, no direct information about

$$X_n \sim P_x^n$$

© **We need LLN's and CLT's!!!**
Classical LLN's and CLT's not directly applicable due to:

- *Markovian dependence structure between the observations X_i*
- *Non-stationarity of the sequence*

The Theorem

Theorem (Ergodic Theorem)

If the Markov chain (X_n) is Harris recurrent, then for any function h with $\mathrm{E}|h| < \infty$,

$$\lim_{n\to\infty} \frac{1}{n} \sum_i h(X_i) = \int h(x) d\pi(x),$$

Central Limit Theorem

To get a CLT, we need more assumptions.

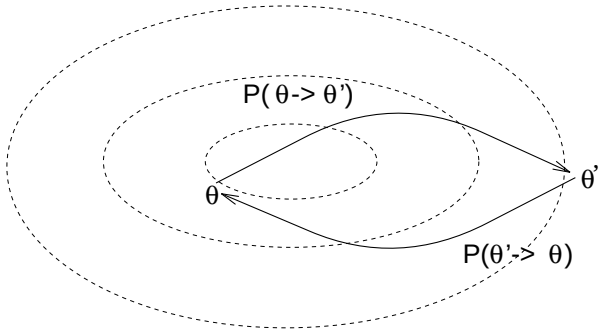
skip conditions and results

For MCMC, the easiest is

Definition (reversibility)

A Markov chain (X_n) is *reversible* if for all n

$$X_{n+1}|X_{n+2} = x \sim X_{n+1}|X_n = x$$



The direction of time does not matter

The CLT

Theorem

If the Markov chain (X_n) is Harris recurrent and reversible,

$$\frac{1}{\sqrt{N}} \left(\sum_{n=1}^{N} (h(X_n) - \mathbb{E}^{\pi}[h]) \right) \xrightarrow{\mathcal{L}} \mathcal{N}(0, \gamma_h^2) \; .$$

where

$$\begin{aligned} 0 < \gamma_h^2 &= \mathbb{E}_{\pi}[\overline{h}^2(X_0)] \\ &\quad + 2 \sum_{k=1}^{\infty} \mathbb{E}_{\pi}[\overline{h}(X_0)\overline{h}(X_k)] < +\infty. \end{aligned}$$

[Kipnis & Varadhan, 1986]

Quantitative convergence rates

skip detailed results

Let P a Markov transition kernel on $(\mathscr{X}, \mathscr{B}(\mathscr{X}))$, with P positive recurrent and π its stationary distribution

Convergence rate Determine, from the kernel, a sequence $B(\nu, n)$, such that

$$\|\nu P^n - \pi\|_V \leq B(\nu, n)$$

where $V : \mathscr{X} \to [1, \infty)$ and for any signed measure μ,

$$\|\mu\|_V = \sup_{|\phi| \leq V} |\mu(\phi)|$$

Practical purposes?

In the 90's, a wealth of contributions on quantitative bounds triggered by MCMC algorithms to answer questions like: what is the appropriate *burn in*? or how long should the sampling continue after burn in?

[Douc, Moulines and Rosenthal, 2001]

[Jones and Hobert, 2001]

Tools at hand

For MCMC algorithms, kernels are "explicitly" known.
Type of quantities (more or less directly) available:

- Minoration constants

$$K^s(x, A) \geq \epsilon\nu(A), \quad \text{for all} \quad x \in C,$$

- Foster-Lyapunov Drift conditions,

$$KV \leq \lambda V + b\mathbb{I}_C$$

and goal is to obtain a bound depending explicitly upon ϵ, λ, b, &tc...

Coupling

skip coupling

If $X \sim \mu$ and $X' \sim \mu'$ and $\mu \wedge \mu' \geq \epsilon\nu$, one can construct two random variables $\tilde{X}$ and $\tilde{X}'$ such that

$$\tilde{X} \sim \mu, \tilde{X}' \sim \mu' \quad \text{and} \quad \tilde{X} = \tilde{X}' \quad \text{with probability } \epsilon$$

The **basic coupling construction**

- with probability ϵ, draw Z according to ν and set $\tilde{X} = \tilde{X}' = Z$.
- with probability $1 - \epsilon$, draw $\tilde{X}$ and $\tilde{X}'$ under distributions

$$(\mu - \epsilon\nu)/(1 - \epsilon) \quad \text{and} \quad (\mu' - \epsilon\nu)/(1 - \epsilon),$$

respectively.

[Thorisson, 2000]

Coupling inequality

X, X' r.v.'s with probability distribution $K(x, .)$ and $K(x', .)$, respectively, can be coupled with probability ϵ if:

$$K(x, \cdot) \wedge K(x', \cdot) \geq \epsilon \nu_{x,x'}(.)$$

where $\nu_{x,x'}$ is a probability measure, or, equivalently,

$$\|K(x, \cdot) - K(x', \cdot)\|_{\mathrm{TV}} \leq (1 - \epsilon)$$

Define an ϵ-**coupling set** as a set $\bar{C} \subset \mathscr{X} \times \mathscr{X}$ satisfying :

$$\forall (x, x') \in \bar{C},\ \forall A \in \mathscr{B}(\mathscr{X}), \quad K(x, A) \wedge K(x', A) \geq \epsilon \nu_{x,x'}(A)$$

Small set and coupling sets

$C \subseteq \mathscr{X}$ **small set** if there exist $\epsilon > 0$ and a probability measure ν such that, for all $A \in \mathscr{B}(\mathscr{X})$

$$K(x, A) \geq \epsilon \nu(A), \qquad \forall x \in C. \tag{3}$$

Small sets always exist when the MC is φ-irreducible

[Jain and Jamieson, 1967]

For MCMC kernels, small sets in general easy to find.
If C is a small set, then $\bar{C} = C \times C$ is a coupling set:

$$\forall (x, x') \in \bar{C}, \forall A \in \mathscr{B}(\mathscr{X}), \quad K(x, A) \wedge K(x', A) \geq \epsilon \nu(A).$$

Coupling for Markov chains

$\bar{P}$ Markov transition kernel on $\mathscr{X} \times \mathscr{X}$ such that, for all $(x, x') \notin \bar{C}$ (where $\bar{C}$ is an ϵ-coupling set) and all $A \in \mathscr{B}(\mathscr{X})$:

$$\bar{P}(x, x'; A \times \mathscr{X}) = K(x, A) \quad \text{and} \quad \bar{P}(x, x'; \mathscr{X} \times A) = K(x', A)$$

For example,

- for $(x, x') \notin \bar{C}$, $\bar{P}(x, x'; A \times A') = K(x, A)K(x', A')$.
- For all $(x, x') \in \bar{C}$ and all $A, A' \in \mathscr{B}(\mathscr{X})$, define the **residual kernel**

$$\bar{R}(x, x'; A \times \mathscr{X}) = (1 - \epsilon)^{-1}(K(x, A) - \epsilon\nu_{x,x'}(A))$$
$$\bar{R}(x, x'; \mathscr{X} \times A') = (1 - \epsilon)^{-1}(K(x', A) - \epsilon\nu_{x,x'}(A')).$$

Coupling algorithm

- Initialisation Let $X_0 \sim \xi$ and $X'_0 \sim \xi'$ and set $d_0 = 0$.
- After coupling If $d_n = 1$, then draw $X_{n+1} \sim K(X_n, \cdot)$, and set $X'_{n+1} = X_{n+1}$.
- Before coupling If $d_n = 0$ and $(X_n, X'_n) \in \bar{C}$,
  - with probability ϵ, draw $X_{n+1} = X'_{n+1} \sim \nu_{X_n, X'_n}$ and set $d_{n+1} = 1$.
  - with probability $1 - \epsilon$, draw $(X_{n+1}, X'_{n+1}) \sim \bar{R}(X_n, X'_n; \cdot)$ and set $d_{n+1} = 0$.
  - If $d_n = 0$ and $(X_n, X'_n) \notin \bar{C}$, then draw $(X_{n+1}, X'_{n+1}) \sim \bar{P}(X_n, X'_n; \cdot)$.

(X_n, X'_n, d_n) [where d_n is the **bell variable** which indicates whether the chains have coupled or not] **is a Markov chain on** $(\mathscr{X} \times \mathscr{X} \times \{0, 1\})$**.**

Coupling inequality (again!)

Define the coupling time T as

$$T = \inf\{k \geq 1, d_k = 1\}$$

Coupling inequality

$$\sup_A |\xi P^k(A) - \xi' P^k(A)| \leq \; P_{\xi,\xi',0}[T > k]$$

[Pitman, 1976; Lindvall, 1992]

Drift conditions

To exploit the coupling construction, we need to control the hitting time
Moments of the return time to a set C are most often controlled using **Foster-Lyapunov drift condition**:

$$PV \leq \lambda V + b\mathbb{I}_C, \quad V \geq 1$$

$M_k = \lambda^{-k} V(X_k)\mathbb{I}(\tau_C \geq k), k \geq 1$ is a supermartingale and thus

$$\mathbb{E}_x[\lambda^{-\tau_C}] \leq V(x) + b\lambda^{-1}\mathbb{I}_C(x).$$

Conversely, if there exists a set C such that $\mathbb{E}_x[\lambda^{-\tau_C}] < \infty$ for all x (in a full and absorbing set), then there exists a drift function verifying the Foster-Lyapunov conditions.

[Meyn and Tweedie, 1993]

If the drift condition is imposed directly on the joint transition kernel $\bar{P}$, there exist $V \geq 1$, $0 < \lambda < 1$ and a set $\bar{C}$ such that :

$$\bar{P}V(x, x') \leq \lambda V(x, x') \quad \forall (x, x') \notin \bar{C}$$

When $\bar{P}(x, x'; A \times A') = K(x, A)K(x', A')$, one may consider

$$\bar{V}(x, x') = (1/2)\left(V(x) + V(x')\right)$$

where V drift function for P (but not necessarily the best choice)

Explicit bound

Theorem

For any distributions ξ and ξ', and any $j \leq k$, then:

$$\|\xi P^k(\cdot) - \xi' P^k(\cdot)\|_{TV} \leq (1-\epsilon)^j + \lambda^k B^{j-1} \mathbb{E}_{\xi,\xi',0}[V(X_0, X_0')]$$

where

$$B = 1 \vee \lambda^{-1}(1-\epsilon) \sup_{\bar{C}} \overline{R}V.$$

[DMR,2001]

Renewal and CLT

Given a Markov chain $(X_n)_n$, how good an approximation of

$$\mathfrak{I} = \int g(x)\pi(x)dx$$

is

$$\overline{g}_n := \frac{1}{n}\sum_{i=0}^{n-1} g(X_i) \ ?$$

Standard MC if CLT

$$\sqrt{n}\left(\overline{g}_n - \mathbb{E}_\pi[g(X)]\right) \xrightarrow{d} \mathcal{N}(0, \gamma_g^2)$$

and there exists an easy-to-compute, consistent estimate of γ_g^2...

Minoration

skip construction

Assume that the kernel density $\mathfrak{K}$ satisfies, for some density $\mathfrak{q}(\cdot)$, $\varepsilon \in (0,1)$ and a small set $C \subseteq \mathcal{X}$,

$$\mathfrak{K}(y|x) \geq \varepsilon\, \mathfrak{q}(y) \quad \text{for all } y \in \mathcal{X} \text{ and } x \in C$$

Then split $\mathfrak{K}$ into a **mixture**

$$\mathfrak{K}(y|x) = \varepsilon\, \mathfrak{q}(y) + (1-\varepsilon)\, \mathfrak{R}(y|x)$$

where $\mathfrak{R}$ is **residual kernel**

Split chain

Let $\delta_0, \delta_1, \delta_2, \ldots$ be iid $\mathcal{B}(\varepsilon)$. Then the *split chain*

$$\{(X_0, \delta_0), (X_1, \delta_1), (X_2, \delta_2), \ldots\}$$

is such that, when $X_i \in C$, δ_i determines X_{i+1}:

$$X_{i+1} \sim \begin{cases} \mathfrak{q}(x) & \text{if } \delta_i = 1, \\ \mathfrak{R}(x|X_i) & \text{otherwise} \end{cases}$$

[Regeneration] **When** $(X_i, \delta_i) \in C \times \{1\}$, $X_{i+1} \sim \mathfrak{q}$

Renewals

For $X_0 \sim q$ and R successive renewals, define by $\tau_1 < \ldots < \tau_R$ the renewal times.
Then

$$\sqrt{R}\left(\overline{g}_{\tau_R} - \mathbb{E}_\pi[g(X)]\right) = \frac{\sqrt{R}}{\overline{N}}\left[\frac{1}{R}\sum_{t=1}^{R}(S_t - N_t\,\mathbb{E}_\pi[g(X)])\right]$$

where N_t length of the t th tour, and S_t sum of the $g(X_j)$'s over the t th tour.
Since (N_t, S_t) are iid and $\mathbb{E}_{\mathfrak{q}}[S_t - N_t\,\mathbb{E}_\pi[g(X)]] = 0$, if N_t and S_t have finite 2nd moments,

- $\sqrt{R}\left(\overline{g}_{\tau_R} - \mathbb{E}_\pi g\right) \xrightarrow{d} \mathcal{N}(0, \gamma_g^2)$
- there is a simple, consistent estimator of γ_g^2

[Mykland & al., 1995; Robert, 1995]

Moment conditions

We need to show that, for the minoration condition, $\mathbb{E}_q[N_1^2]$ and $\mathbb{E}_q[S_1^2]$ are finite.

If

1. **the chain is geometrically ergodic, and**
2. $\mathbb{E}_\pi[|g|^{2+\alpha}] < \infty$ **for some** $\alpha > 0$**,**

then $\mathbb{E}_q[N_1^2] < \infty$ **and** $\mathbb{E}_q[S_1^2] < \infty$**.**

[Hobert & al., 2002]

Note that drift + minoration ensures geometric ergodicity

[Rosenthal, 1995; Roberts & Tweedie, 1999]

The Metropolis-Hastings Algorithm

Running Monte Carlo via Markov Chains

It is not necessary to use a sample from the distribution f to approximate the integral

$$\mathfrak{I} = \int h(x) f(x) dx \ ,$$

We can obtain $X_1, \ldots, X_n \sim f$ **(approx)** without directly simulating from f, **using an ergodic Markov chain with stationary distribution** f

Running Monte Carlo via Markov Chains (2)

Idea

For an arbitrary starting value $x^{(0)}$, an ergodic chain $(X^{(t)})$ is generated using a transition kernel with stationary distribution f

- Insures the convergence in distribution of $(X^{(t)})$ to a random variable from f.
- For a "large enough" T_0, $X^{(T_0)}$ can be considered as distributed from f
- Produce a *dependent* sample $X^{(T_0)}, X^{(T_0+1)}, \ldots$, which is generated from f, sufficient for most approximation purposes.

Problem: How can one build a Markov chain with a given stationary distribution?

The Metropolis–Hastings algorithm

Basics

The algorithm uses the **objective (target) density**

$$f$$

and a conditional density

$$q(y|x)$$

called the **instrumental (or proposal) distribution**

The MH algorithm

Algorithm (Metropolis–Hastings)

Given $x^{(t)}$,

1. Generate $Y_t \sim q(y|x^{(t)})$.
2. Take

$$X^{(t+1)} = \begin{cases} Y_t & \text{with prob. } \rho(x^{(t)}, Y_t), \\ x^{(t)} & \text{with prob. } 1 - \rho(x^{(t)}, Y_t), \end{cases}$$

where

$$\rho(x, y) = \min \left\{ \frac{f(y)}{f(x)} \, \frac{q(x|y)}{q(y|x)} \, , 1 \right\} .$$

Features

- Independent of normalizing constants for both f and $q(\cdot|x)$ (ie, those constants independent of x)
- Never move to values with $f(y) = 0$
- The chain $(x^{(t)})_t$ may take the same value several times in a row, even though f is a density wrt Lebesgue measure
- The sequence $(y_t)_t$ is usually **not** a Markov chain

Convergence properties

1. The M-H Markov chain is **reversible**, with invariant/stationary density f since it satisfies the **detailed balance condition**

$$\boxed{f(y)\,K(y,x) = f(x)\,K(x,y)}$$

2. As f is a probability measure, the chain is **positive recurrent**
3. If

$$\Pr\left[\frac{f(Y_t)\;q(X^{(t)}|Y_t)}{f(X^{(t)})\;q(Y_t|X^{(t)})} \geq 1\right] < 1. \qquad (1)$$

that is, the event $\{X^{(t+1)} = X^{(t)}\}$ is possible, then the chain is **aperiodic**

Convergence properties (2)

4. If
$$q(y|x) > 0 \text{ for every } (x, y), \tag{2}$$
the chain is **irreducible**
5. For M-H, f-irreducibility implies **Harris recurrence**
6. Thus, for M-H satisfying (1) and (2)
   (i) For h, with $\mathbb{E}_f|h(X)| < \infty$,
$$\lim_{T\to\infty} \frac{1}{T}\sum_{t=1}^{T} h(X^{(t)}) = \int h(x)df(x) \qquad \text{a.e. } f.$$
   (ii) and
$$\lim_{n\to\infty} \left\| \int K^n(x,\cdot)\mu(dx) - f \right\|_{TV} = 0$$
for every initial distribution μ, where $K^n(x,\cdot)$ denotes the kernel for n transitions.

The Independent Case

The instrumental distribution q is independent of $X^{(t)}$, and is denoted g by analogy with Accept-Reject.

Algorithm (Independent Metropolis-Hastings)

Given $x^{(t)}$,

a Generate $Y_t \sim g(y)$

b Take

$$X^{(t+1)} = \begin{cases} Y_t & \text{with prob. } \min\left\{ \dfrac{f(Y_t)\, g(x^{(t)})}{f(x^{(t)})\, g(Y_t)}\, , 1 \right\}, \\ x^{(t)} & \text{otherwise.} \end{cases}$$

Properties

The resulting sample is **not** iid but there exist strong convergence properties:

Theorem (Ergodicity)

The algorithm produces a uniformly ergodic chain if there exists a constant M such that

$$f(x) \leq Mg(x)\ , \quad x \in \text{supp}\ f.$$

In this case,

$$\|K^n(x,\cdot) - f\|_{TV} \leq \left(1 - \frac{1}{M}\right)^n\ .$$

[Mengersen & Tweedie, 1996]

Example (Noisy AR(1))

Hidden Markov chain from a regular AR(1) model,

$$x_{t+1} = \varphi x_t + \epsilon_{t+1} \qquad \epsilon_t \sim \mathcal{N}(0, \tau^2)$$

and observables

$$y_t | x_t \sim \mathcal{N}(x_t^2, \sigma^2)$$

The distribution of x_t given x_{t-1}, x_{t+1} and y_t is

$$\exp \frac{-1}{2\tau^2} \left\{ (x_t - \varphi x_{t-1})^2 + (x_{t+1} - \varphi x_t)^2 + \frac{\tau^2}{\sigma^2} (y_t - x_t^2)^2 \right\} .$$

Example (Noisy AR(1) too)

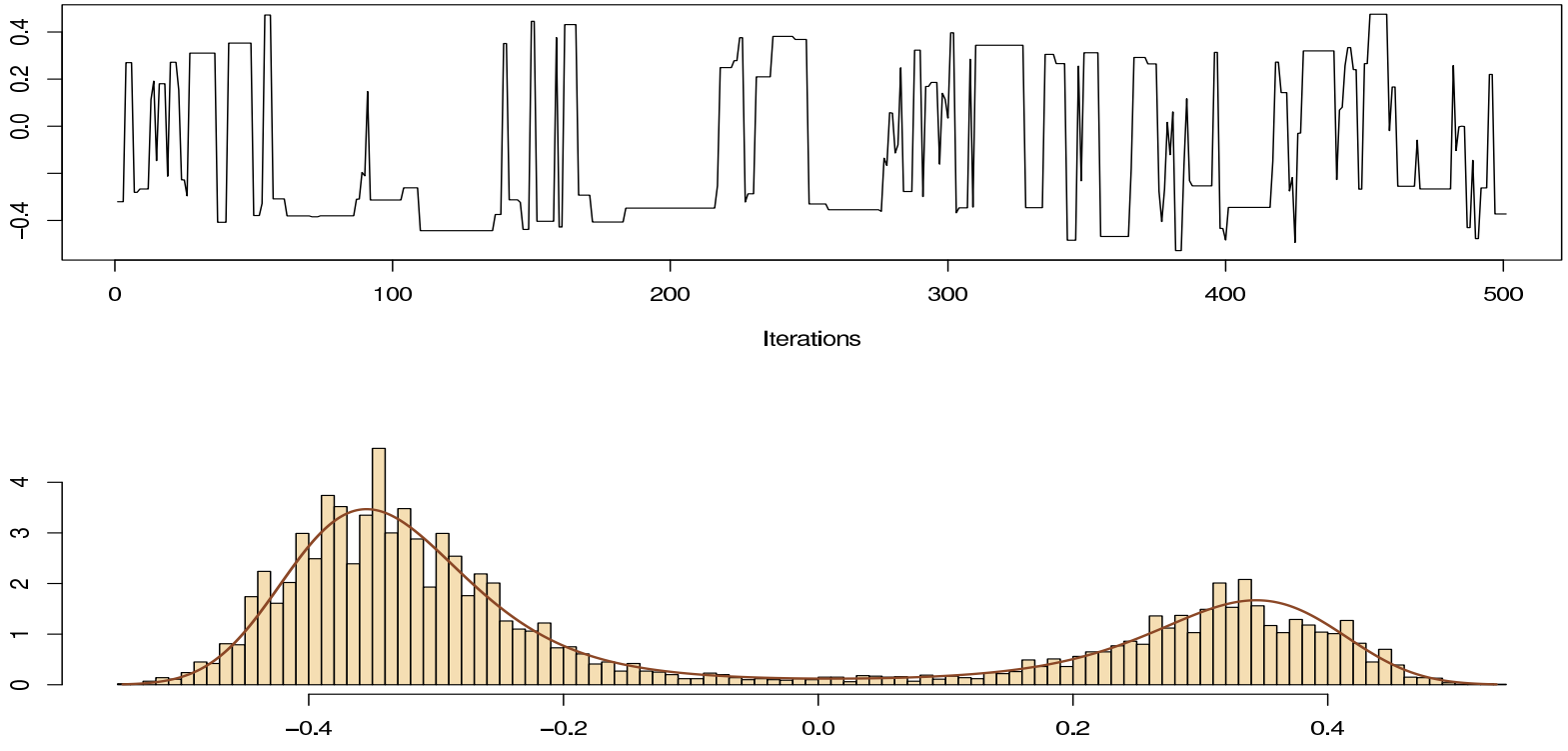
Use for proposal the $\mathcal{N}(\mu_t, \omega_t^2)$ distribution, with

$$\mu_t = \varphi \frac{x_{t-1} + x_{t+1}}{1+\varphi^2} \quad \text{and} \quad \omega_t^2 = \frac{\tau^2}{1+\varphi^2}\,.$$

Ratio

$$\pi(x)/q_{\text{ind}}(x) = \exp -(y_t - x_t^2)^2/2\sigma^2$$

is bounded



(top) Last 500 realisations of the chain $\{X_k\}_k$ out of $10,000$ iterations; (bottom) histogram of the chain, compared with the target distribution.

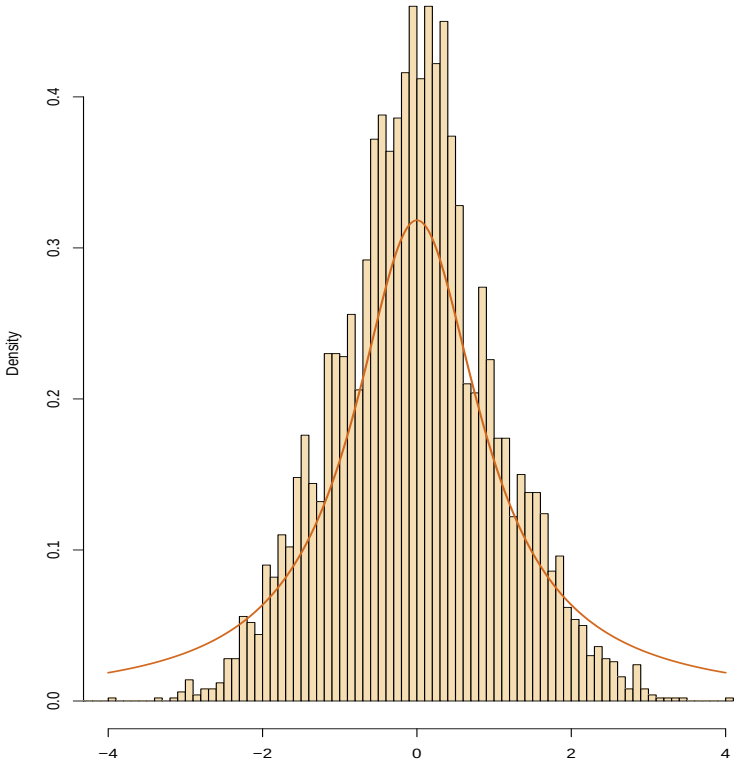
Example (Cauchy by normal)

▸ go random W Given a Cauchy $\mathscr{C}(0,1)$ distribution, consider a normal $\mathscr{N}(0,1)$ proposal
The Metropolis–Hastings acceptance ratio is

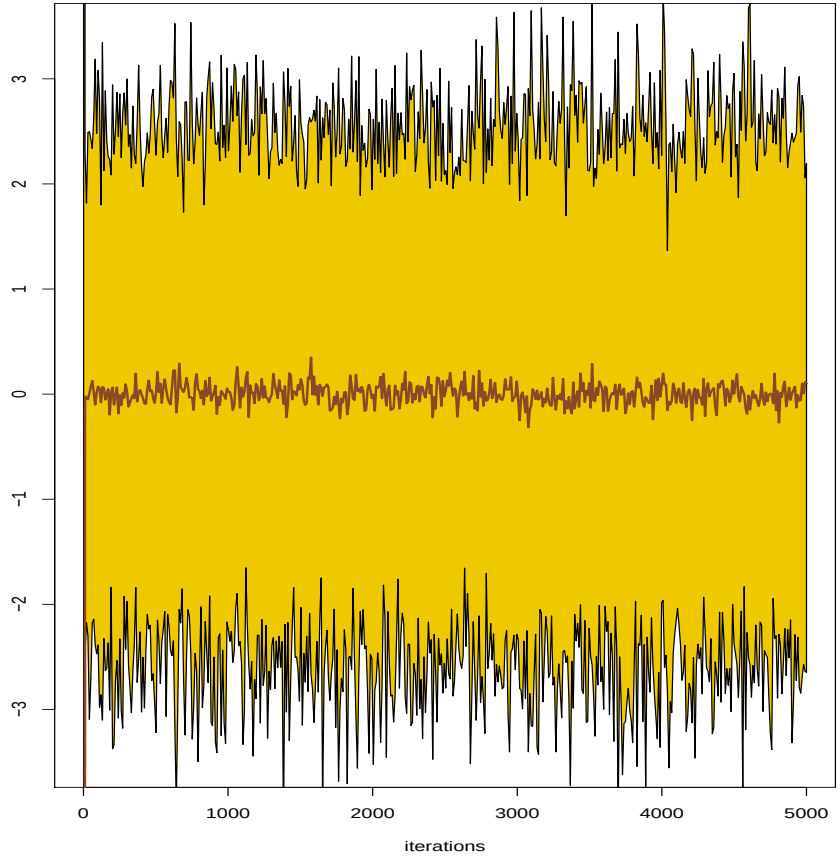
$$\frac{\pi(\xi')/\nu(\xi')}{\pi(\xi)/\nu(\xi))} = \exp\left[\left\{\xi^2 - (\xi')^2\right\}/2\right] \frac{1+(\xi')^2}{(1+\xi^2)}\,.$$

Poor perfomances: the proposal distribution has lighter tails than the target Cauchy and convergence to the stationary distribution is not even geometric!

[Mengersen & Tweedie, 1996]



Histogram of Markov chain $(\xi_t)_{1\leq t\leq 5000}$ against target $\mathscr{C}(0,1)$ distribution.



Range and average of 1000 parallel runs when initialized with a normal $\mathscr{N}(0,100^2)$ distribution.

Random walk Metropolis–Hastings

Use of a local perturbation as proposal

$$Y_t = X^{(t)} + \varepsilon_t,$$

where $\varepsilon_t \sim g$, independent of $X^{(t)}$.
The instrumental density is now of the form $g(y - x)$ and the Markov chain is a random walk if we take g to be *symmetric* $g(x) = g(-x)$

Algorithm (Random walk Metropolis)

Given $x^{(t)}$

1. Generate $Y_t \sim g(y - x^{(t)})$
2. Take

$$X^{(t+1)} = \begin{cases} Y_t & \text{with prob. } \min\left\{1, \dfrac{f(Y_t)}{f(x^{(t)})}\right\}, \\ x^{(t)} & \text{otherwise.} \end{cases}$$

Example (Random walk and normal target)

▸ forget History! Generate $\mathcal{N}(0,1)$ based on the uniform proposal $[-\delta,\delta]$ [Hastings (1970)]

The probability of acceptance is then

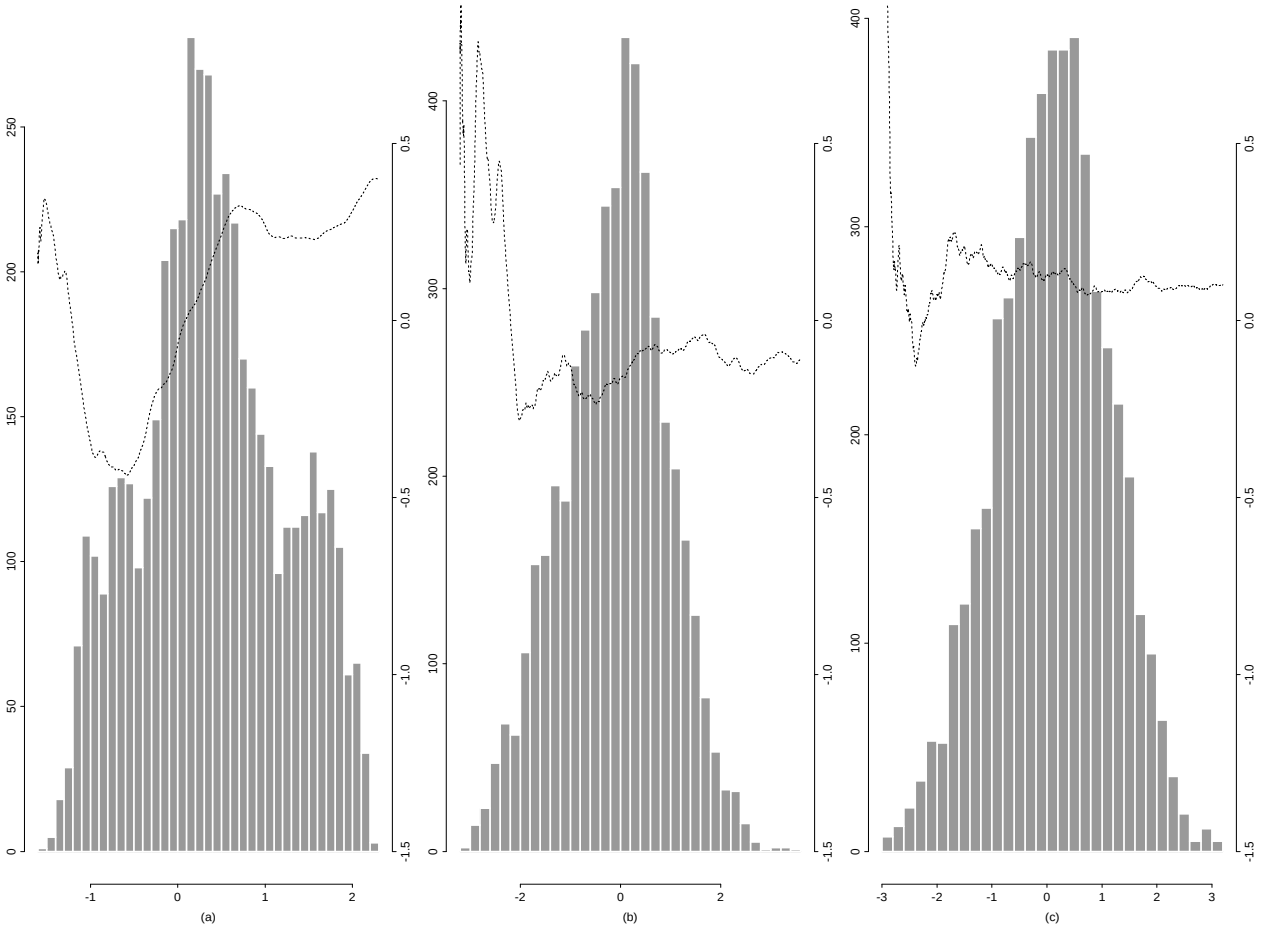
$$\rho(x^{(t)},y_t)=\exp\{(x^{(t)^2}-y_t^2)/2\}\wedge 1.$$

Example (Random walk & normal (2))

Sample statistics

δ	0.1	0.5	1.0
mean	0.399	-0.111	0.10
variance	0.698	1.11	1.06

© As $\delta \uparrow$, we get better histograms and a faster exploration of the support of f.



Three samples based on $\mathcal{U}[-\delta, \delta]$ with (a) $\delta = 0.1$, (b) $\delta = 0.5$ and (c) $\delta = 1.0$, superimposed with the convergence of the means ($15,000$ simulations).

Example (Mixture models (again!))

$$\pi(\theta|x) \propto \prod_{j=1}^{n} \left(\sum_{\ell=1}^{k} p_\ell f(x_j|\mu_\ell, \sigma_\ell) \right) \pi(\theta)$$

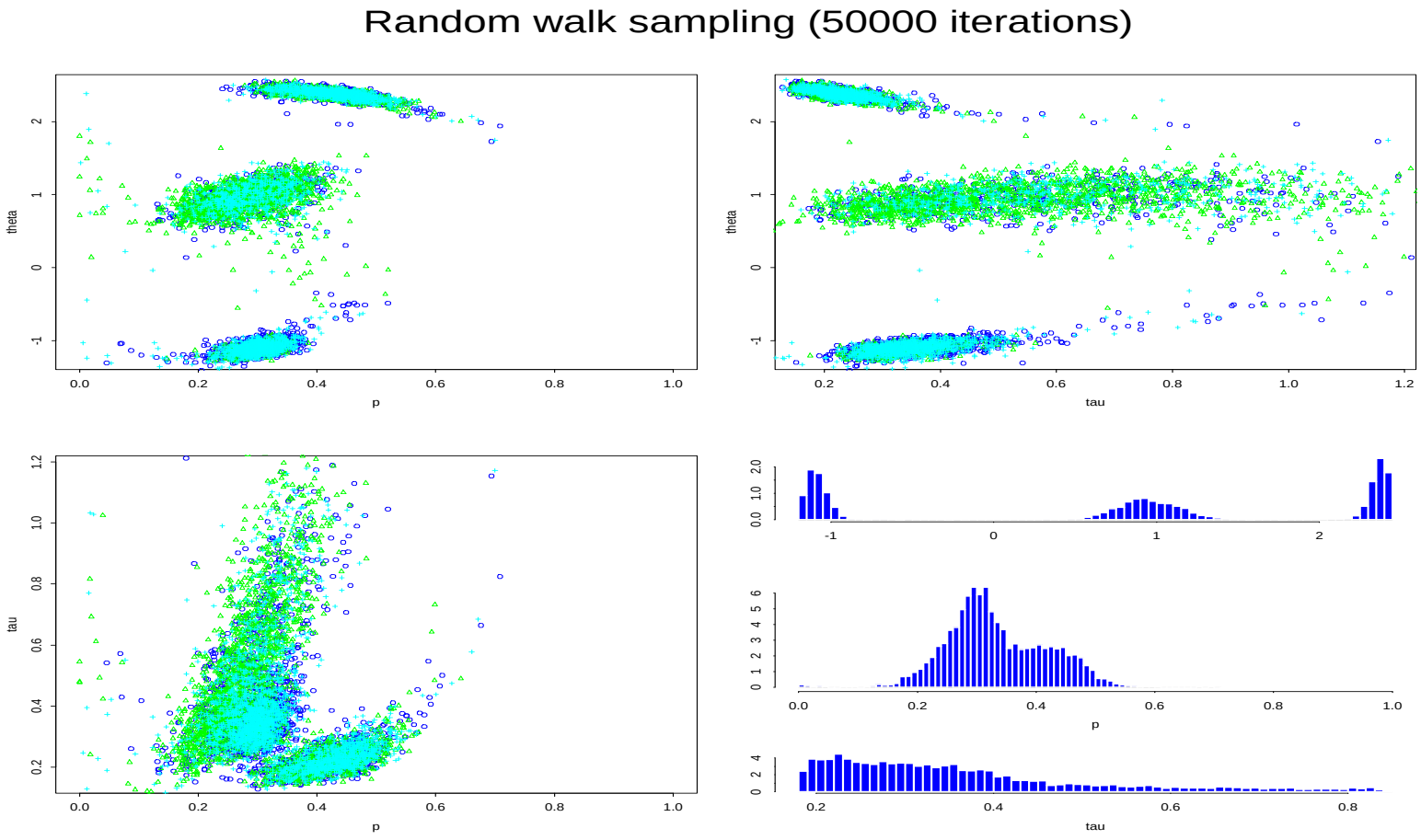
Metropolis-Hastings proposal:

$$\theta^{(t+1)} = \begin{cases} \theta^{(t)} + \omega\varepsilon^{(t)} & \text{if } u^{(t)} < \rho^{(t)} \\ \theta^{(t)} & \text{otherwise} \end{cases}$$

where

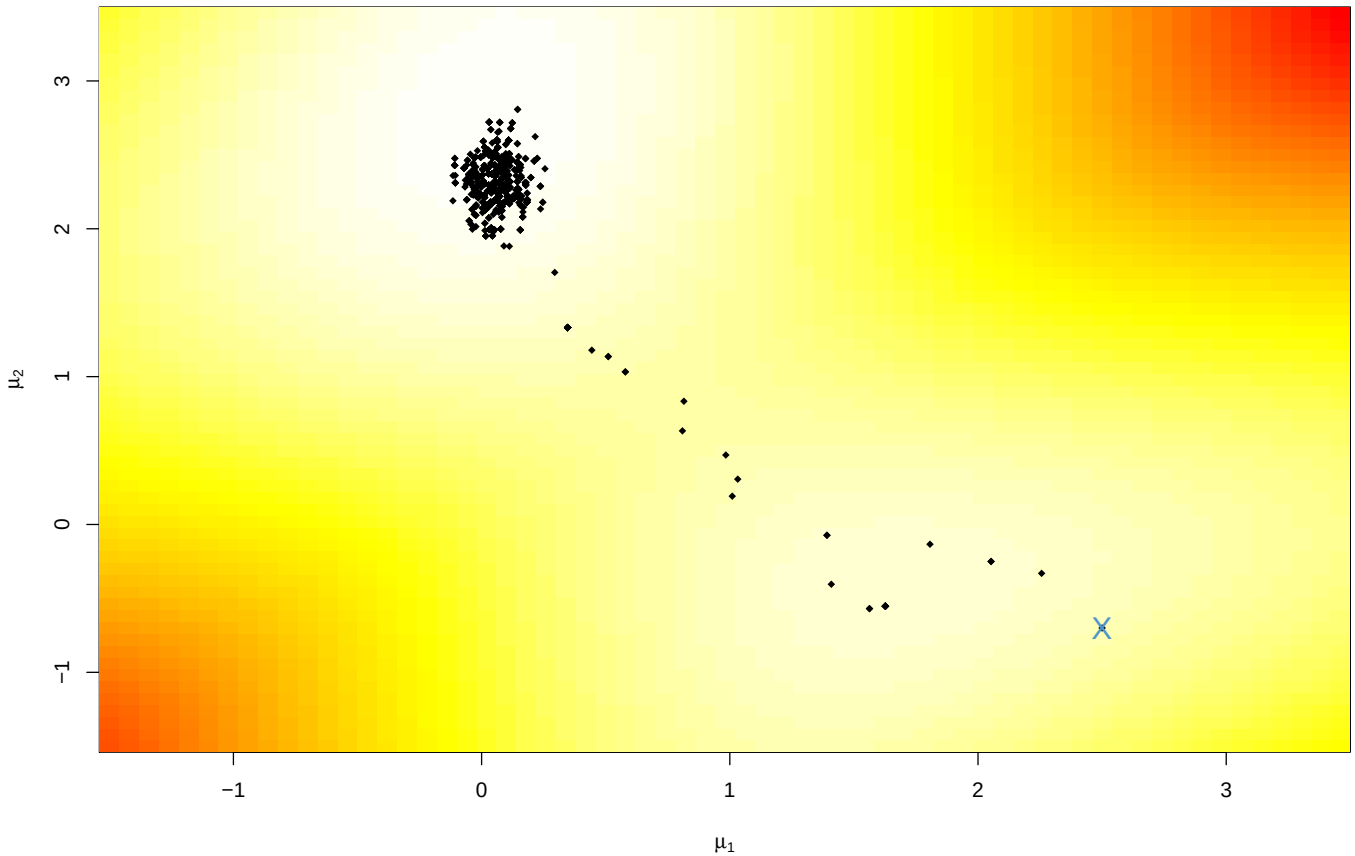
$$\rho^{(t)} = \frac{\pi(\theta^{(t)} + \omega\varepsilon^{(t)}|x)}{\pi(\theta^{(t)}|x)} \wedge 1$$

and ω scaled for good acceptance rate



General case of a 3 component normal mixture

[Celeux & al., 2000]



Random walk MCMC output for $.7\mathcal{N}(\mu_1, 1) + .3\mathcal{N}(\mu_2, 1)$

Example (probit model)

▸ skip probit

Likelihood of the **probit model**

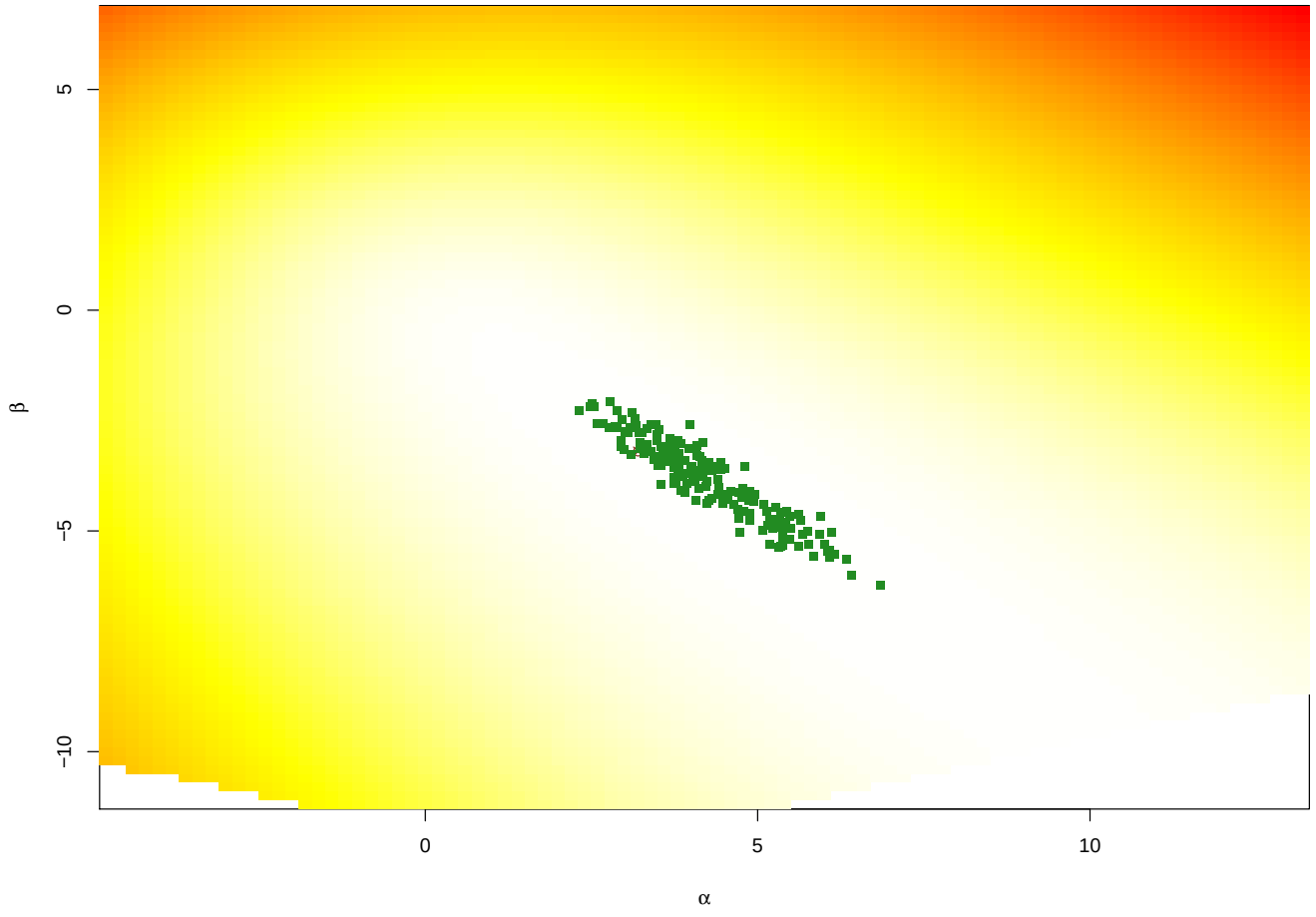
$$\prod_{i=1}^{n} \Phi(y_i^{\mathsf{T}}\beta)^{x_i}\, \Phi(-y_i^{\mathsf{T}}\beta)^{1-x_i}$$

Random walk proposal

$$\beta^{(t+1)} = \beta^{(t)} + \varepsilon_t \qquad \varepsilon_t \sim \mathcal{N}_p(0, \Sigma)$$

where, for instance,

$$\Sigma = \alpha(YY^{\mathsf{T}})^{-1}$$



Likelihood surface and random walk Metropolis-Hastings steps

Convergence properties

Uniform ergodicity prohibited by random walk structure
At best, geometric ergodicity:

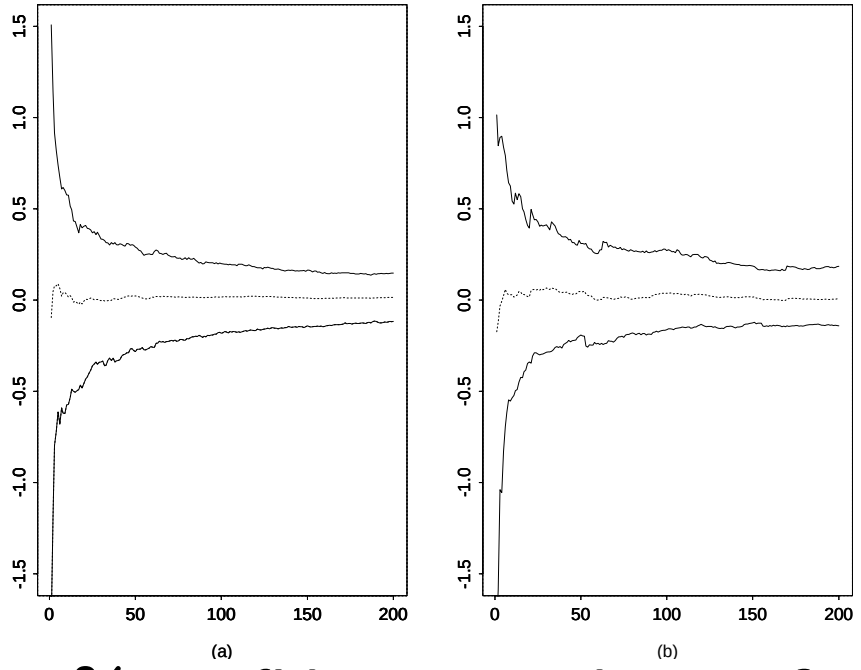
Theorem (Sufficient ergodicity)

For a symmetric density f, log-concave in the tails, and a positive and symmetric density g, the chain $(X^{(t)})$ is geometrically ergodic.
[Mengersen & Tweedie, 1996]

▸ no tail effect

Example (Comparison of tail effects)

Random-walk Metropolis–Hastings algorithms based on a $\mathcal{N}(0,1)$ instrumental for the generation of (a) a $\mathcal{N}(0,1)$ distribution and (b) a distribution with density $\psi(x) \propto (1+|x|)^{-3}$



90% confidence envelopes of the means, derived from 500 parallel independent chains

Example (Cauchy by normal continued)

Again, Cauchy $\mathscr{C}(0,1)$ target and Gaussian random walk proposal, $\xi' \sim \mathscr{N}(\xi, \sigma^2)$, with acceptance probability

$$\frac{1+\xi^2}{1+(\xi')^2} \wedge 1\,,$$

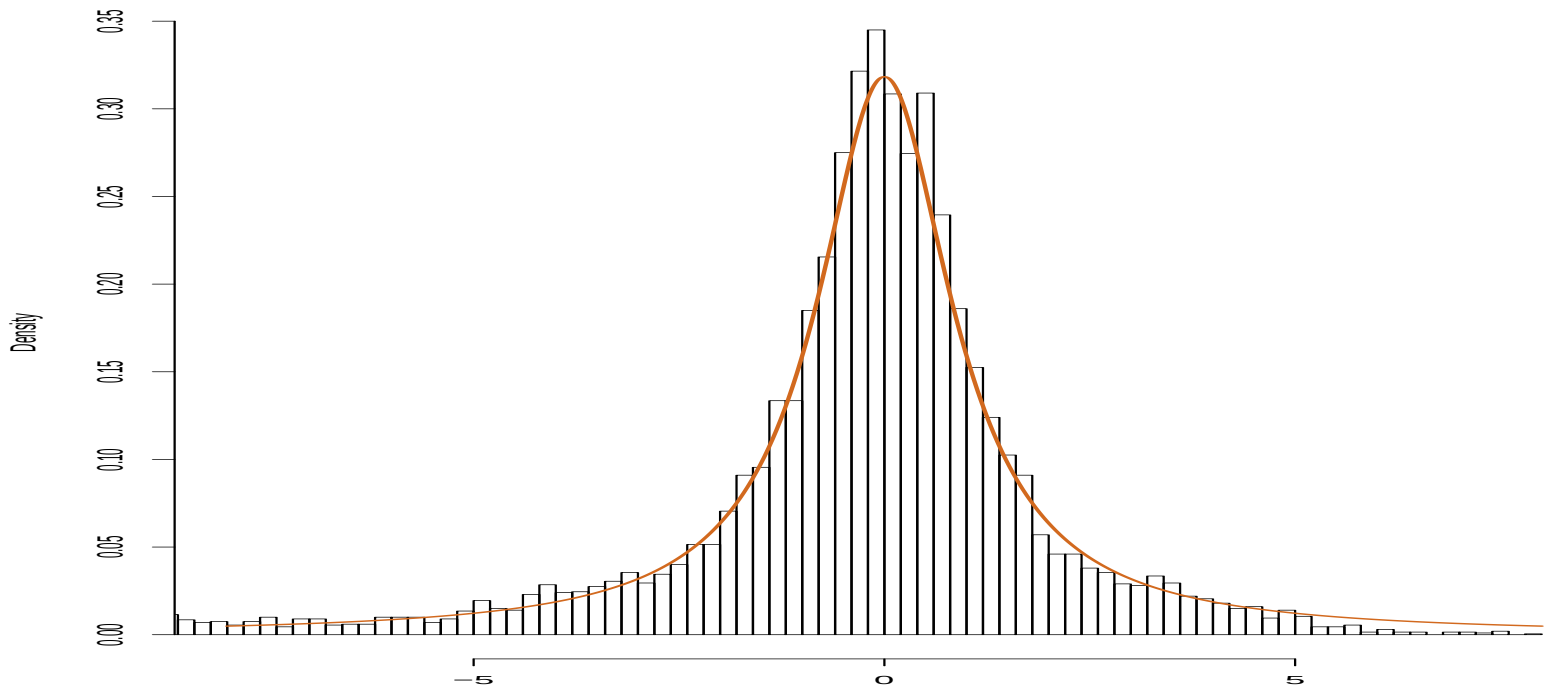
Overall fit of the Cauchy density by the histogram satisfactory, but poor exploration of the tails: 99% quantile of $\mathscr{C}(0,1)$ equal to 3, but no simulation exceeds 14 out of $10,000$!

[Roberts & Tweedie, 2004]

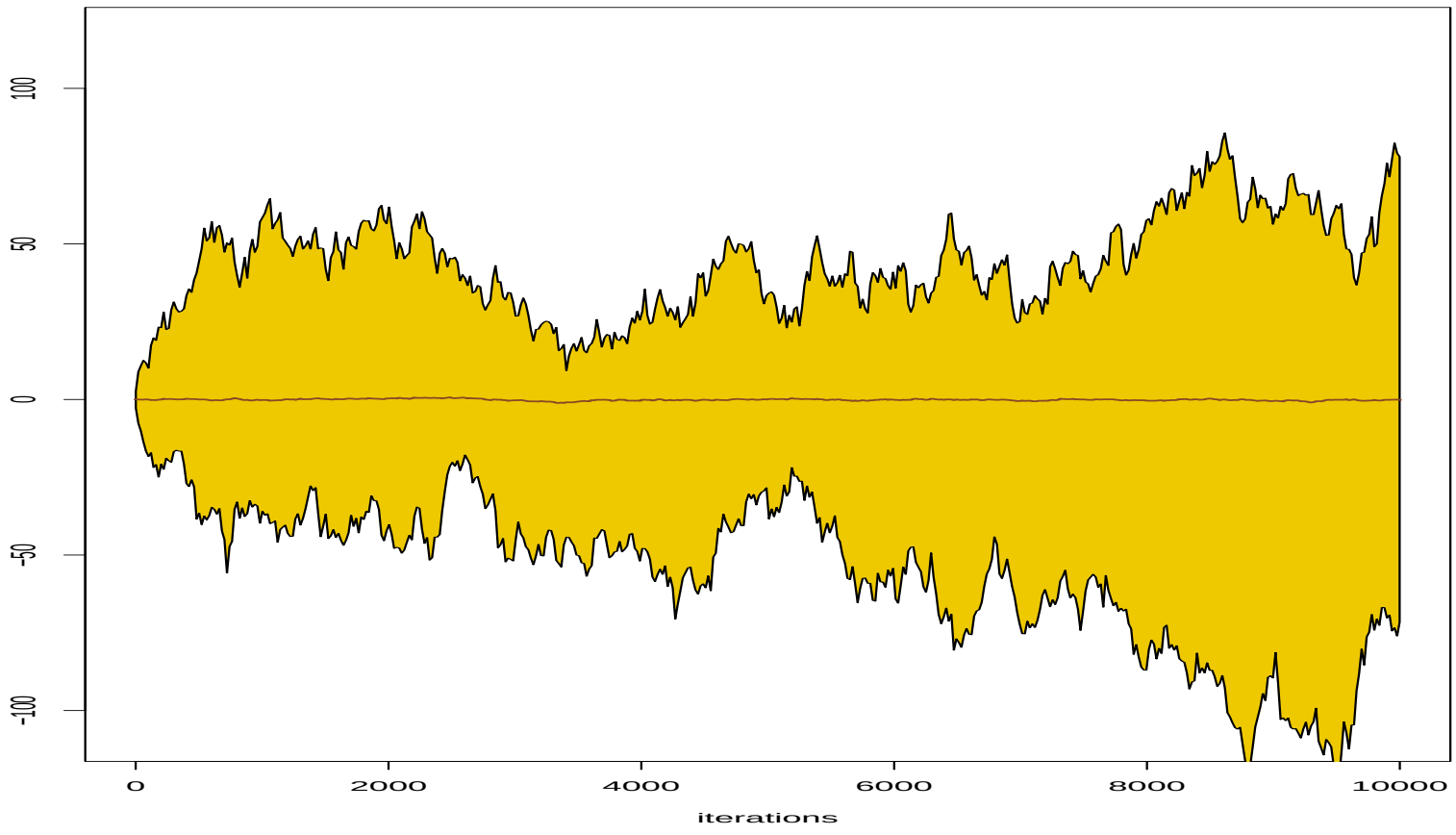
Again, lack of geometric ergodicity!

[Mengersen & Tweedie, 1996]

Slow convergence shown by the non-stable range after $10,000$ iterations.



Histogram of the $10,000$ first steps of a random walk Metropolis–Hastings algorithm using a $\mathcal{N}(\xi, 1)$ proposal



Range of 500 parallel runs for the same setup

Further convergence properties

Under assumptions

skip detailed convergence

- **(A1)** f is super-exponential, *i.e.* it is positive with positive continuous first derivative such that $\lim_{|x|\to\infty} n(x)'\nabla \log f(x) = -\infty$ where $n(x) := x/|x|$.
  In words : exponential decay of f in every direction with rate tending to ∞
- **(A2)** $\limsup_{|x|\to\infty} n(x)'m(x) < 0$, where $m(x) = \nabla f(x)/|\nabla f(x)|$.
  In words: non degeneracy of the countour manifold $\mathcal{C}_{f(y)} = \{y : f(y) = f(x)\}$

Q is geometrically ergodic, and
$V(x) \propto f(x)^{-1/2}$ verifies the drift condition

[Jarner & Hansen, 2000]

Further [further] convergence properties

skip hyperdetailed convergence

If P ψ-irreducible and aperiodic, for $r = (r(n))_{n\in\mathbb{N}}$ real-valued non decreasing sequence, such that, for all $n, m \in \mathbb{N}$,

$$r(n+m) \leq r(n)r(m),$$

and $r(0) = 1$, for C a small set, $\tau_C = \inf\{n \geq 1, X_n \in C\}$, and $h \geq 1$, assume

$$\sup_{x\in C} \mathbb{E}_x \left[\sum_{k=0}^{\tau_C - 1} r(k)h(X_k) \right] < \infty,$$

then,

$$S(f, C, r) := \left\{ x \in X, \mathbb{E}_x \left\{ \sum_{k=0}^{\tau_C - 1} r(k) h(X_k) \right\} < \infty \right\}$$

is full and absorbing and for $x \in S(f, C, r)$,

$$\lim_{n \to \infty} r(n) \| P^n(x, .) - f \|_h = 0.$$

[Tuominen & Tweedie, 1994]

Comments

- **[CLT, Rosenthal's inequality...]** h-ergodicity implies CLT for additive (possibly unbounded) functionals of the chain, Rosenthal's inequality and so on...
- **[Control of the moments of the return-time]** The condition implies (because $h \geq 1$) that

$$\sup_{x \in C} \mathbb{E}_x[r_0(\tau_C)] \leq \sup_{x \in C} \mathbb{E}_x \left\{ \sum_{k=0}^{\tau_C - 1} r(k) h(X_k) \right\} < \infty,$$

where $r_0(n) = \sum_{l=0}^{n} r(l)$ Can be used to derive bounds for the coupling time, an essential step to determine computable bounds, using coupling inequalities

[Roberts & Tweedie, 1998; Fort & Moulines, 2000]

Alternative conditions

The condition is not really easy to work with...

[Possible alternative conditions]

(a) **[Tuominen, Tweedie, 1994]** There exists a sequence $(V_n)_{n\in\mathbb{N}}$, $V_n \geq r(n)h$, such that

- (i) $\sup_C V_0 < \infty$,
- **(ii)** $\{V_0 = \infty\} \subset \{V_1 = \infty\}$ and
- **(iii)** $PV_{n+1} \leq V_n - r(n)h + br(n)\mathbb{I}_C$.

(b) **[Fort 2000]** $\exists V \geq f \geq 1$ and $b < \infty$, such that $\sup_C V < \infty$ and

$$PV(x) + \mathbb{E}_x \left\{ \sum_{k=0}^{\sigma_C} \Delta r(k) f(X_k) \right\} \leq V(x) + b\mathbb{I}_C(x)$$

where σ_C is the hitting time on C and

$$\Delta r(k) = r(k) - r(k-1), k \geq 1 \text{ and } \Delta r(0) = r(0).$$

Result (a) $\Leftrightarrow$ (b) $\Leftrightarrow$ $\sup_{x \in C} \mathbb{E}_x \left\{ \sum_{k=0}^{\tau_C - 1} r(k) f(X_k) \right\} < \infty.$

Extensions

There are many other families of HM algorithms

- *Adaptive Rejection Metropolis Sampling*
- *Reversible Jump (later!)*
- *Langevin algorithms*

to name just a few...

Langevin Algorithms

Proposal based on the *Langevin diffusion* L_t is defined by the stochastic differential equation

$$dL_t = dB_t + \frac{1}{2}\nabla \log f(L_t)dt,$$

where B_t is the standard *Brownian motion*

Theorem

The Langevin diffusion is the only non-explosive diffusion which is reversible with respect to f.

Discretization

Instead, consider the sequence

$$x^{(t+1)} = x^{(t)} + \frac{\sigma^2}{2}\nabla \log f(x^{(t)}) + \sigma\varepsilon_t, \qquad \varepsilon_t \sim \mathcal{N}_p(0, I_p)$$

where σ^2 corresponds to the discretization step
Unfortunately, the discretized chain may be be transient, for instance when

$$\lim_{x\to\pm\infty} \left|\sigma^2 \nabla \log f(x)|x|^{-1}\right| > 1$$

MH correction

Accept the new value Y_t with probability

$$\frac{f(Y_t)}{f(x^{(t)})} \cdot \frac{\exp\left\{-\left\|Y_t - x^{(t)} - \frac{\sigma^2}{2}\nabla \log f(x^{(t)})\right\|^2 \Big/ 2\sigma^2\right\}}{\exp\left\{-\left\|x^{(t)} - Y_t - \frac{\sigma^2}{2}\nabla \log f(Y_t)\right\|^2 \Big/ 2\sigma^2\right\}} \wedge 1 \,.$$

Choice of the scaling factor σ

Should lead to an acceptance rate of 0.574 to achieve optimal convergence rates (when the components of x are uncorrelated)

[Roberts & Rosenthal, 1998]

Optimizing the Acceptance Rate

Problem of choice of the transition kernel from a practical point of view

Most common alternatives:

(a) a fully automated algorithm like ARMS;

(b) an instrumental density g which approximates f, such that f/g is bounded for uniform ergodicity to apply;

(c) a random walk

In both cases (b) and (c), the choice of g is critical,

Case of the independent Metropolis–Hastings algorithm

Choice of g that maximizes the average acceptance rate

$$\begin{aligned}\rho &= \mathbb{E}\left[\min\left\{\frac{f(Y)\,g(X)}{f(X)\,g(Y)}, 1\right\}\right] \\ &= 2P\left(\frac{f(Y)}{g(Y)} \geq \frac{f(X)}{g(X)}\right), \qquad X \sim f,\ Y \sim g,\end{aligned}$$

Related to the speed of convergence of

$$\frac{1}{T}\sum_{t=1}^{T} h(X^{(t)})$$

to $\mathbb{E}_f[h(X)]$ and to the ability of the algorithm to explore any complexity of f

Case of the independent Metropolis–Hastings algorithm (2)

Practical implementation

Choose a parameterized instrumental distribution $g(\cdot|\theta)$ and adjusting the corresponding parameters θ based on the evaluated acceptance rate

$$\hat{\rho}(\theta) = \frac{2}{m} \sum_{i=1}^{m} \mathbb{I}_{\{f(y_i)g(x_i) > f(x_i)g(y_i)\}} \ ,$$

where $x_1, \ldots, x_m$ sample from f and $y_1, \ldots, y_m$ iid sample from g.

Example (Inverse Gaussian distribution)

▸ no inverse

Simulation from

$$f(z|\theta_1,\theta_2) \propto z^{-3/2}\ \exp\left\{-\theta_1 z - \frac{\theta_2}{z} + 2\sqrt{\theta_1\theta_2} + \log\ \sqrt{2\theta_2}\right\}\ \mathbb{I}_{\mathbb{R}_+}(z)$$

based on the Gamma distribution $\mathcal{G}a(\alpha,\beta)$ with $\alpha = \beta\sqrt{\theta_2/\theta_1}$
Since

$$\frac{f(x)}{g(x)} \propto x^{-\alpha-1/2}\ \exp\left\{(\beta-\theta_1)x - \frac{\theta_2}{x}\right\}\ ,$$

the maximum is attained at

$$x^*_\beta = \frac{(\alpha+1/2) - \sqrt{(\alpha+1/2)^2 + 4\theta_2(\theta_1-\beta)}}{2(\beta-\theta_1)}\ .$$

Example (Inverse Gaussian distribution (2))

The analytical optimization (in β) of

$$M(\beta) = (x^*_\beta)^{-\alpha-1/2} \exp\left\{(\beta-\theta_1)x^*_\beta - \frac{\theta_2}{x^*_\beta}\right\}$$

is impossible

β	0.2	0.5	0.8	0.9	1	1.1	1.2	1.5
$\hat{\rho}(\beta)$	0.22	0.41	0.54	0.56	0.60	0.63	0.64	0.71
$\mathbb{E}[Z]$	1.137	1.158	1.164	1.154	1.133	1.148	1.181	1.148
$\mathbb{E}[1/Z]$	1.116	1.108	1.116	1.115	1.120	1.126	1.095	1.115

($\theta_1 = 1.5, \theta_2 = 2$, and $m = 5000$).

Case of the random walk

Different approach to acceptance rates
A high acceptance rate does not indicate that the algorithm is moving correctly since it indicates that the random walk is moving too slowly on the surface of f.
If $x^{(t)}$ and y_t are close, i.e. $f(x^{(t)}) \simeq f(y_t)$ y is accepted with probability

$$\min\left(\frac{f(y_t)}{f(x^{(t)})}, 1\right) \simeq 1\ .$$

For multimodal densities with well separated modes, the negative effect of limited moves on the surface of f clearly shows.

Case of the random walk (2)

If the average acceptance rate is low, the successive values of $f(y_t)$ tend to be small compared with $f(x^{(t)})$, which means that the random walk moves quickly on the surface of f since it often reaches the "borders" of the support of f

Rule of thumb

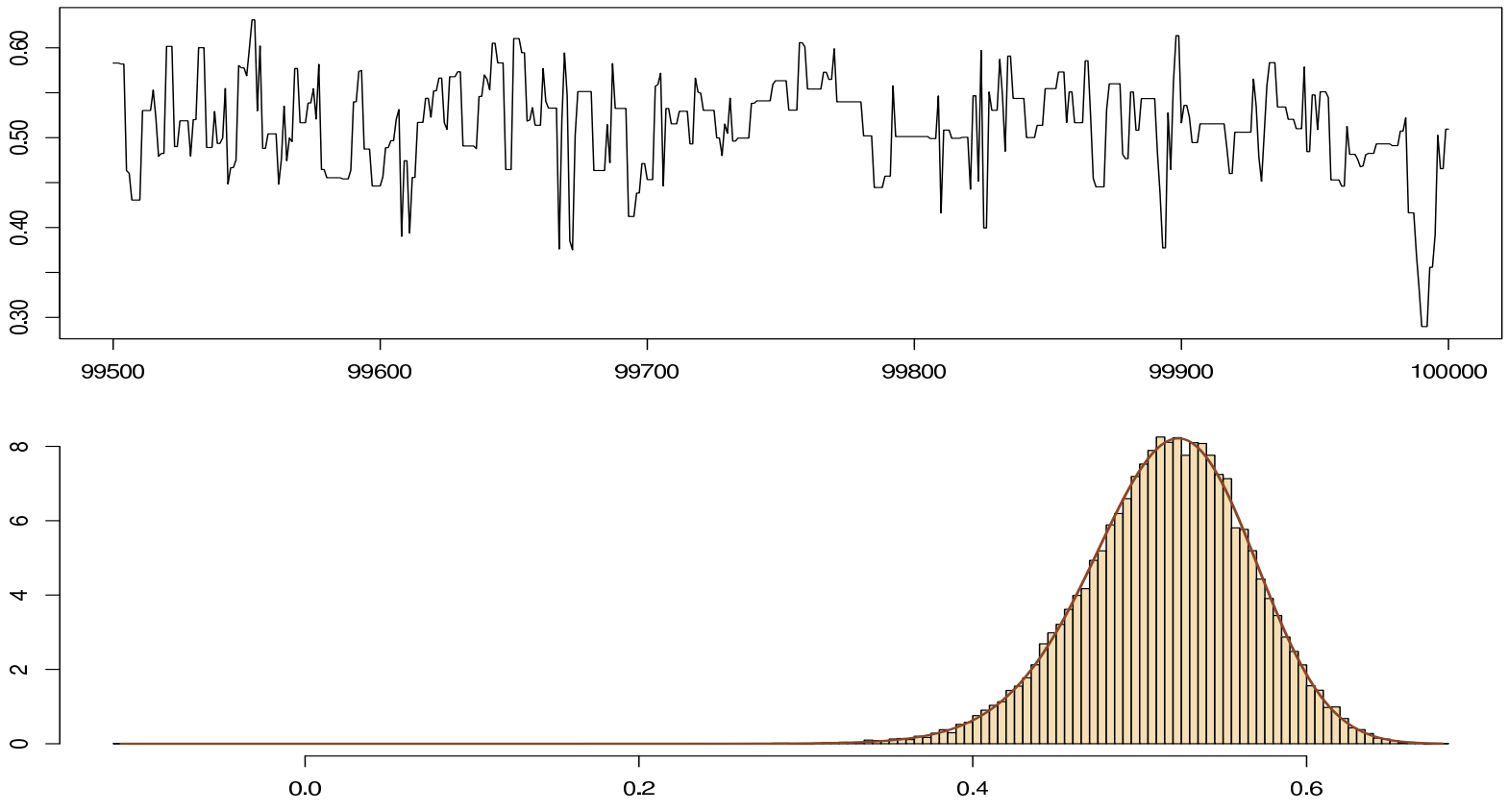
In small dimensions, aim at an average acceptance rate of 50%. In large dimensions, at an average acceptance rate of 25%.

[Gelman,Gilks and Roberts, 1995]

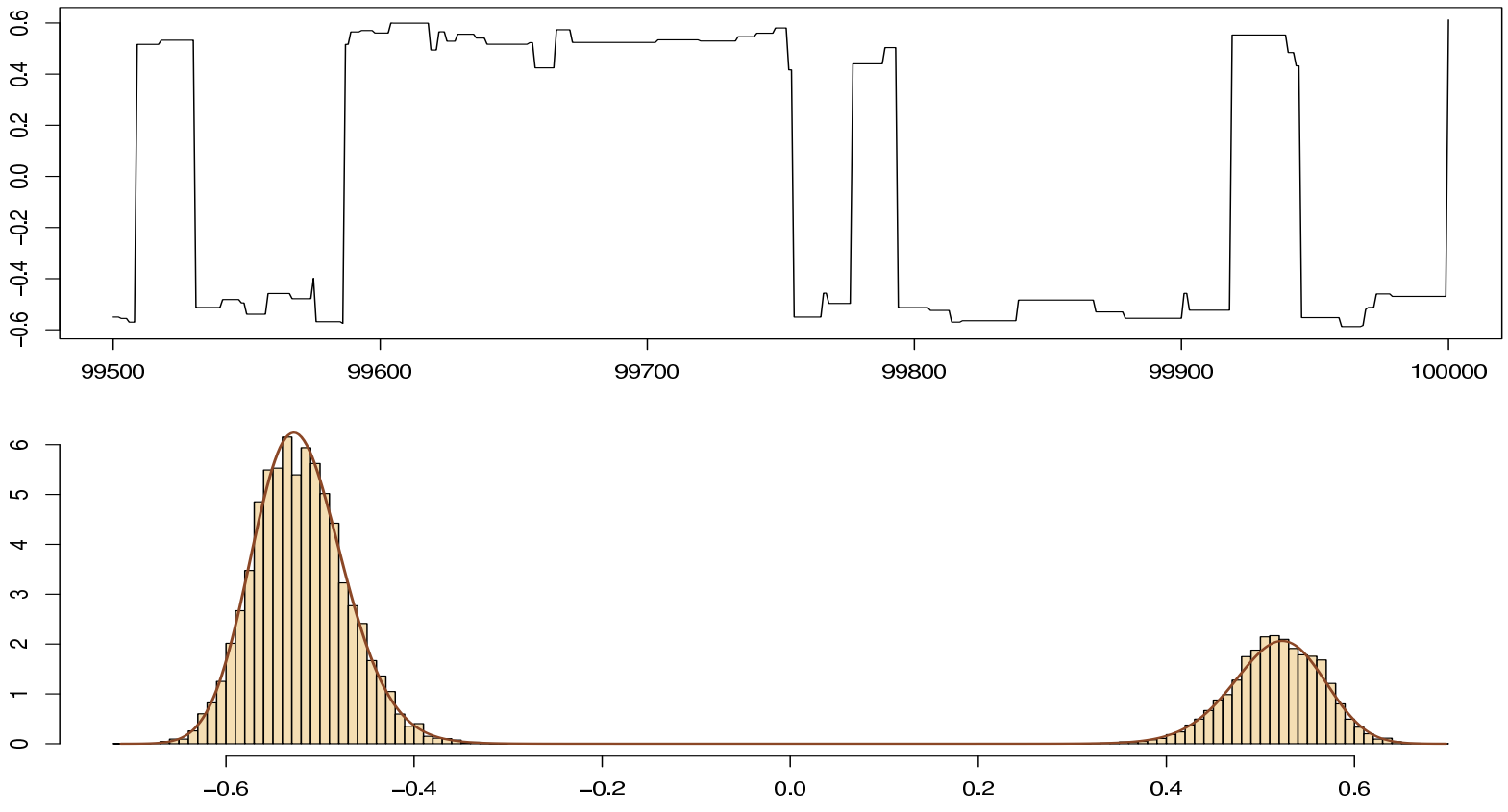
This rule is to be taken with a pinch of salt!

Example (Noisy AR(1) continued)

For a Gaussian random walk with scale ω small enough, the random walk never jumps to the other mode. But if the scale ω is sufficiently large, the Markov chain explores both modes and give a satisfactory approximation of the target distribution.



Markov chain based on a random walk with scale $\omega = .1$.



Markov chain based on a random walk with scale $\omega = .5$.

The Gibbs Sampler

General Principles

A very **specific** simulation algorithm based on the target distribution f:

1. Uses the conditional densities $f_1, \ldots, f_p$ from f
2. Start with the random variable $\mathbf{X} = (X_1, \ldots, X_p)$
3. Simulate from the conditional densities,

$$\begin{aligned} X_i | x_1, x_2, \ldots, x_{i-1}, x_{i+1}, \ldots, x_p \\ \sim f_i(x_i | x_1, x_2, \ldots, x_{i-1}, x_{i+1}, \ldots, x_p) \end{aligned}$$

for $i = 1, 2, \ldots, p$.

Algorithm (Gibbs sampler)

Given $\mathbf{x}^{(t)} = (x_1^{(t)}, \ldots, x_p^{(t)})$, generate

1. $X_1^{(t+1)} \sim f_1(x_1 | x_2^{(t)}, \ldots, x_p^{(t)})$;
2. $X_2^{(t+1)} \sim f_2(x_2 | x_1^{(t+1)}, x_3^{(t)}, \ldots, x_p^{(t)})$,

   $\ldots$

p. $X_p^{(t+1)} \sim f_p(x_p | x_1^{(t+1)}, \ldots, x_{p-1}^{(t+1)})$

$$\mathbf{X}^{(t+1)} \to \mathbf{X} \sim f$$

Properties

The full conditionals densities $f_1, \ldots, f_p$ are the only densities used for simulation. Thus, even in a high dimensional problem, all of the simulations may be univariate

The Gibbs sampler **is not reversible** with respect to f. However, each of its p components is. Besides, it can be turned into a reversible sampler, either using the *Random Scan Gibbs sampler* see section or running instead the (double) sequence

$$f_1 \cdots f_{p-1} f_p f_{p-1} \cdots f_1$$

Example (Bivariate Gibbs sampler)

$$(X, Y) \sim f(x, y)$$

Generate a sequence of observations by

Set $X_0 = x_0$

For $t = 1, 2, \ldots,$ generate

$$\begin{aligned} Y_t &\sim f_{Y|X}(\cdot|x_{t-1}) \\ X_t &\sim f_{X|Y}(\cdot|y_t) \end{aligned}$$

where $f_{Y|X}$ and $f_{X|Y}$ are the conditional distributions

A Very Simple Example: Independent $\mathcal{N}(\mu, \sigma^2)$ Observations

When $Y_1, \ldots, Y_n \overset{\text{iid}}{\sim} \mathcal{N}(y|\mu, \sigma^2)$ with both μ and σ unknown, the posterior in (μ, σ^2) is conjugate outside a standard familly

But...

$$\mu|\boldsymbol{Y}_{0:n}, \sigma^2 \sim \mathcal{N}\left(\mu \left| \frac{1}{n}\sum_{i=1}^n Y_i, \frac{\sigma^2}{n}\right.\right)$$

$$\sigma^2|\boldsymbol{Y}_{1:n}, \mu \sim \mathcal{IG}\left(\sigma^2 \left| \frac{n}{2} - 1, \frac{1}{2}\sum_{i=1}^n (Y_i - \mu)^2\right.\right)$$

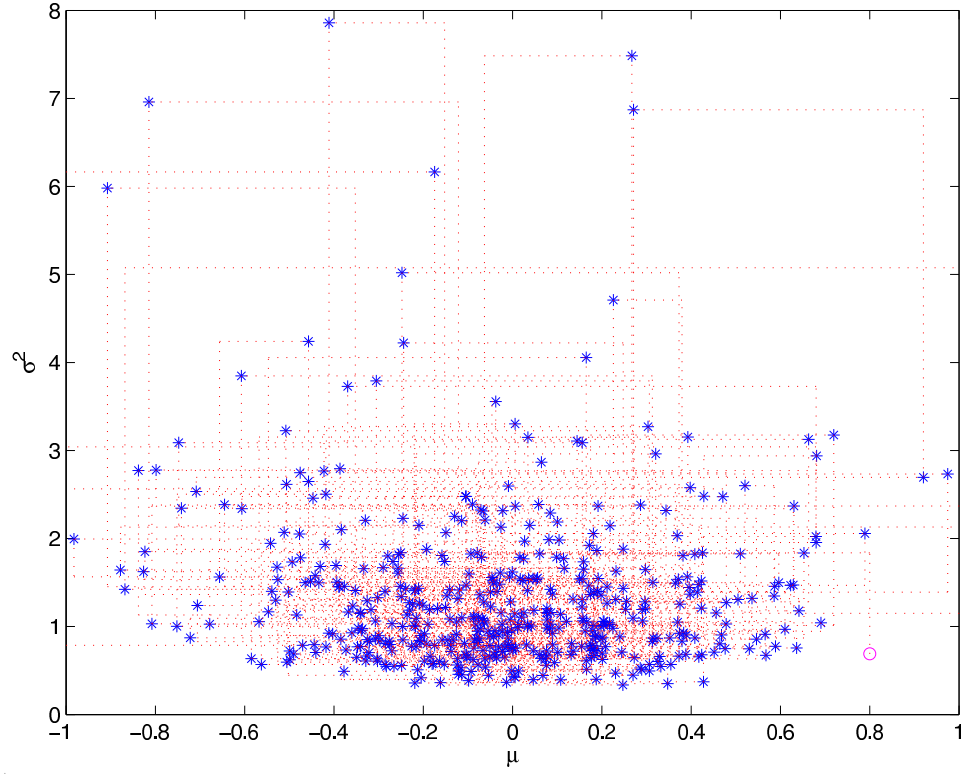
assuming constant (improper) priors on both μ and σ^2

- Hence we may use the Gibbs sampler for simulating from the posterior of (μ, σ^2)

R Gibbs Sampler for Gaussian posterior

```
n = length(Y);
S = sum(Y);
mu = S/n;
for (i in 1:500)
    S2 = sum((Y-mu)^2);
    sigma2 = 1/rgamma(1,n/2-1,S2/2);
    mu = S/n + sqrt(sigma2/n)*rnorm(1);
```

Example of results with $n = 10$ observations from the $\mathcal{N}(0, 1)$ distribution



Number of Iterations 1, 2, 3, 4, 5, 10, 25, 50, 100, 500

Limitations of the Gibbs sampler

Formally, a special case of a sequence of 1-D M-H kernels, all with acceptance rate uniformly equal to 1.
The Gibbs sampler

1. limits the choice of instrumental distributions
2. requires some knowledge of f
3. is, by construction, multidimensional
4. does not apply to problems where the number of parameters varies as the resulting chain is not irreducible.

Latent variables are back

The Gibbs sampler can be generalized in much wider generality
A density g is a completion of f if

$$\int_{\mathcal{Z}} g(x, z)\, dz = f(x)$$

Note

The variable z may be meaningless for the problem

Purpose

g should have full conditionals that are easy to simulate for a Gibbs sampler to be implemented with g rather than f

For $p > 1$, write $y = (x, z)$ and denote the conditional densities of $g(y) = g(y_1, \ldots, y_p)$ by

$$\begin{aligned} Y_1|y_2, \ldots, y_p &\sim g_1(y_1|y_2, \ldots, y_p), \\ Y_2|y_1, y_3, \ldots, y_p &\sim g_2(y_2|y_1, y_3, \ldots, y_p), \\ &\ldots, \\ Y_p|y_1, \ldots, y_{p-1} &\sim g_p(y_p|y_1, \ldots, y_{p-1}). \end{aligned}$$

The move from $Y^{(t)}$ to $Y^{(t+1)}$ is defined as follows:

Algorithm (Completion Gibbs sampler)

Given $(y_1^{(t)}, \ldots, y_p^{(t)})$, simulate

1. $Y_1^{(t+1)} \sim g_1(y_1 | y_2^{(t)}, \ldots, y_p^{(t)})$,
2. $Y_2^{(t+1)} \sim g_2(y_2 | y_1^{(t+1)}, y_3^{(t)}, \ldots, y_p^{(t)})$,

   $\ldots$

p. $Y_p^{(t+1)} \sim g_p(y_p | y_1^{(t+1)}, \ldots, y_{p-1}^{(t+1)})$.

Example (Mixtures all over again)

Hierarchical missing data structure:

If

$$X_1, \ldots, X_n \sim \sum_{i=1}^{k} p_i f(x|\theta_i),$$

then

$$X|Z \sim f(x|\theta_Z), \quad Z \sim p_1 \mathbb{I}(z = 1) + \ldots + p_k \mathbb{I}(z = k),$$

Z is the component indicator associated with observation x

Example (Mixtures (2))

Conditionally on $(Z_1, \ldots, Z_n) = (z_1, \ldots, z_n)$:

$$\begin{aligned}
&\pi(p_1, \ldots, p_k, \theta_1, \ldots, \theta_k | x_1, \ldots, x_n, z_1, \ldots, z_n) \\
&\propto p_1^{\alpha_1 + n_1 - 1} \ldots p_k^{\alpha_k + n_k - 1} \\
&\quad \times \pi(\theta_1 | y_1 + n_1 \bar{x}_1, \lambda_1 + n_1) \ldots \pi(\theta_k | y_k + n_k \bar{x}_k, \lambda_k + n_k),
\end{aligned}$$

with

$$n_i = \sum_j \mathbb{I}(z_j = i) \qquad \text{and} \qquad \bar{x}_i = \sum_{j;\, z_j = i} x_j / n_i.$$

Algorithm (Mixture Gibbs sampler)

1. Simulate

$$\theta_i \sim \pi(\theta_i | y_i + n_i \bar{x}_i, \lambda_i + n_i) \quad (i = 1, \ldots, k)$$
$$(p_1, \ldots, p_k) \sim D(\alpha_1 + n_1, \ldots, \alpha_k + n_k)$$

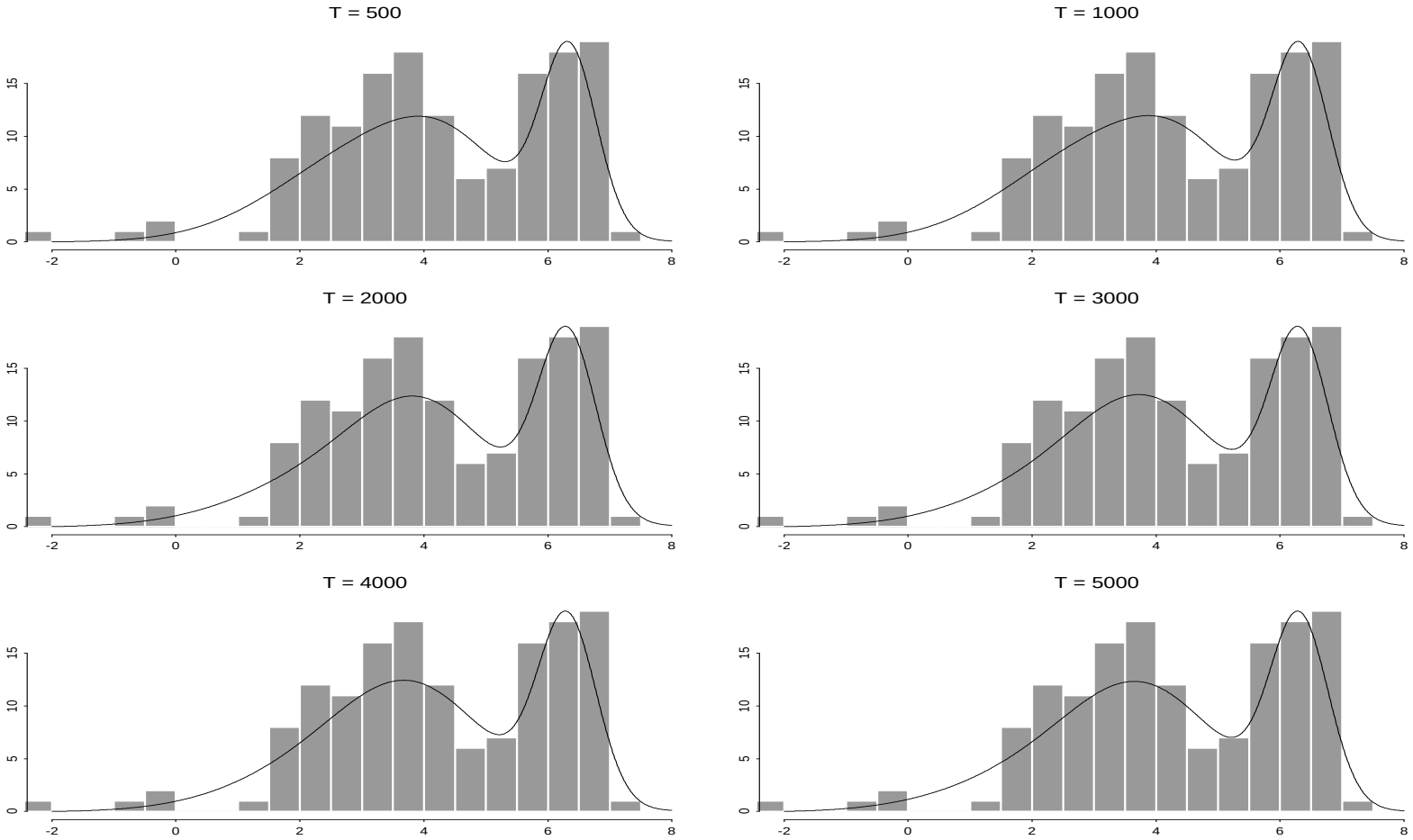
2. Simulate $(j = 1, \ldots, n)$

$$Z_j | x_j, p_1, \ldots, p_k, \theta_1, \ldots, \theta_k \sim \sum_{i=1}^{k} p_{ij} \mathbb{I}(z_j = i)$$

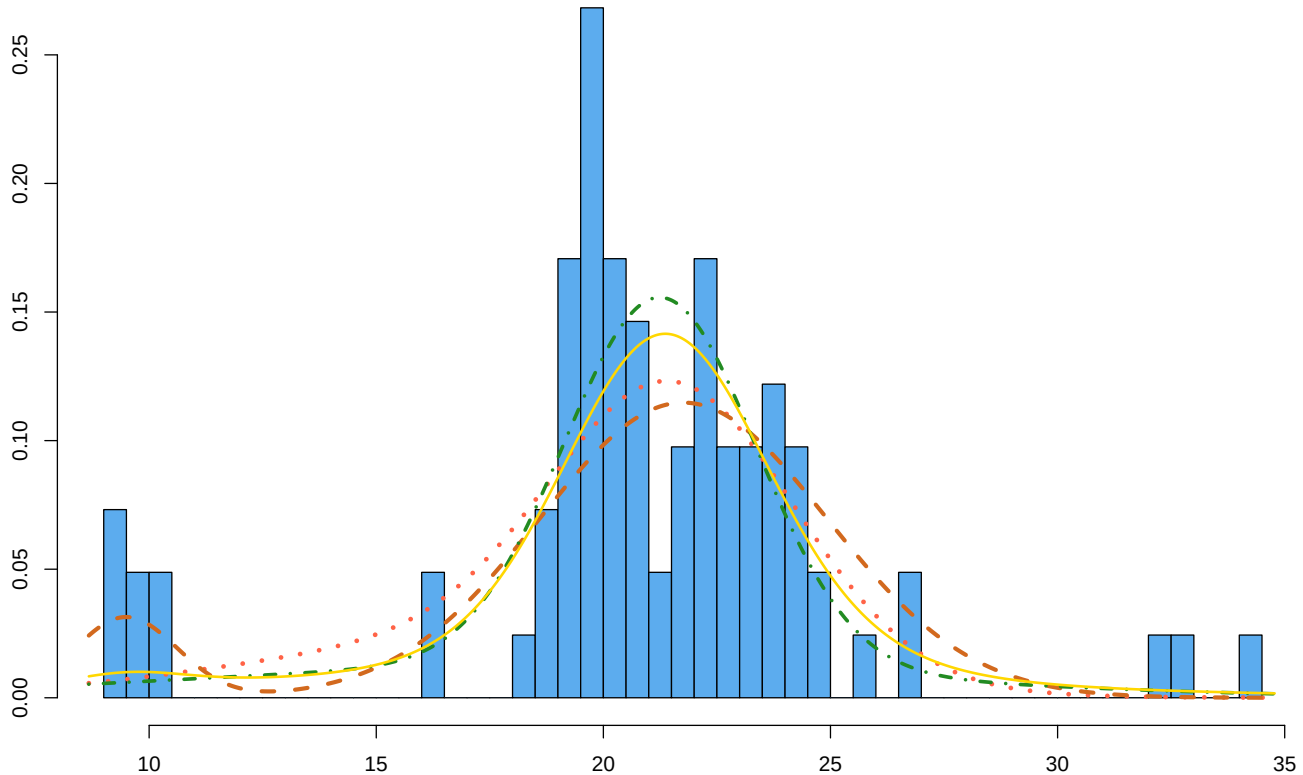
with $(i = 1, \ldots, k)$

$$p_{ij} \propto p_i f(x_j | \theta_i)$$

and update n_i and $\bar{x}_i$ $(i = 1, \ldots, k)$.

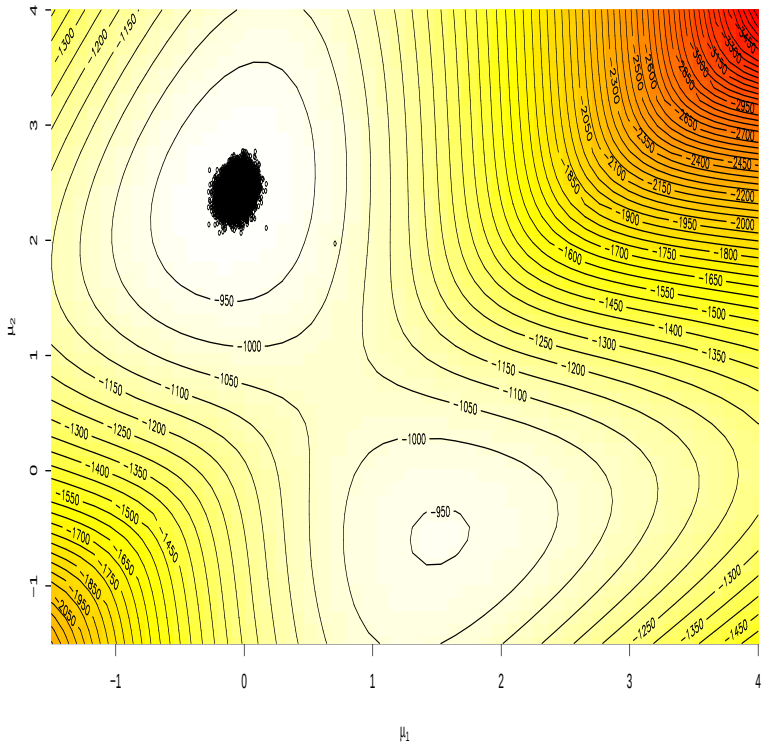


Estimation of the pluggin density for 3 components and T iterations for 149 observations of acidity levels in US lakes



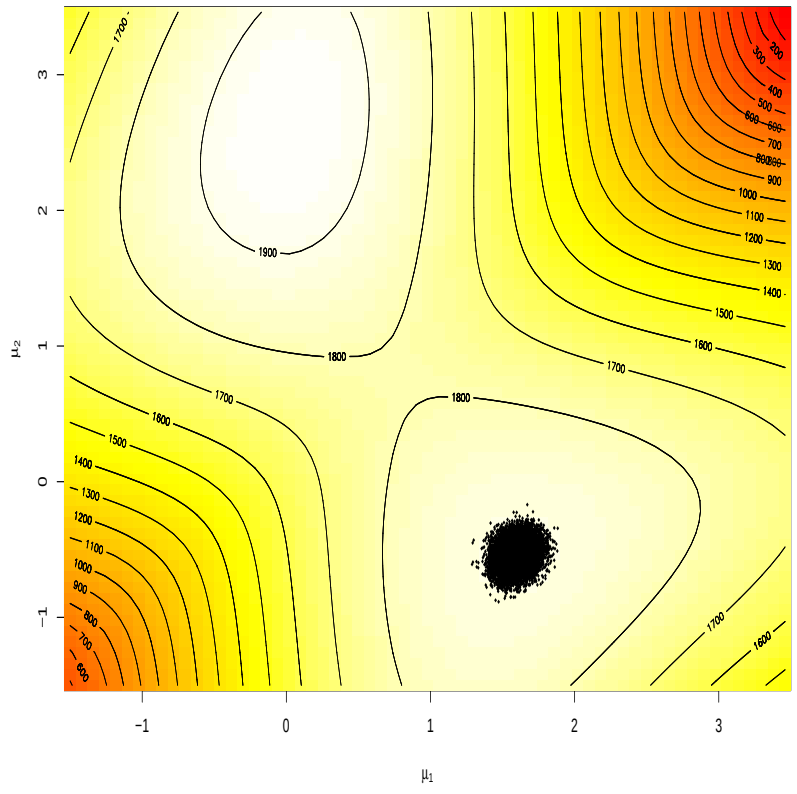
Galaxy dataset (82 observations) with $k = 2$ components
average density (yellow), and pluggins:
average (tomato), marginal MAP (green), MAP (marroon)

A wee problem



Gibbs started at random

Gibbs stuck at the wrong mode



Random Scan Gibbs sampler

back to basics

don't do random

Modification of the above Gibbs sampler where, with probability $1/p$, the i-th component is drawn from $f_i(x_i|X_{-i})$, ie when the components are chosen at random

Motivation

The Random Scan Gibbs sampler is reversible.

Slice sampler as generic Gibbs

If $f(\theta)$ can be written as a product

$$\prod_{i=1}^{k} f_i(\theta),$$

it can be completed as

$$\prod_{i=1}^{k} \mathbb{I}_{0 \le \omega_i \le f_i(\theta)},$$

leading to the following Gibbs algorithm:

Algorithm (Slice sampler)

Simulate

1. $\omega_1^{(t+1)} \sim \mathcal{U}_{[0,f_1(\theta^{(t)})]}$;

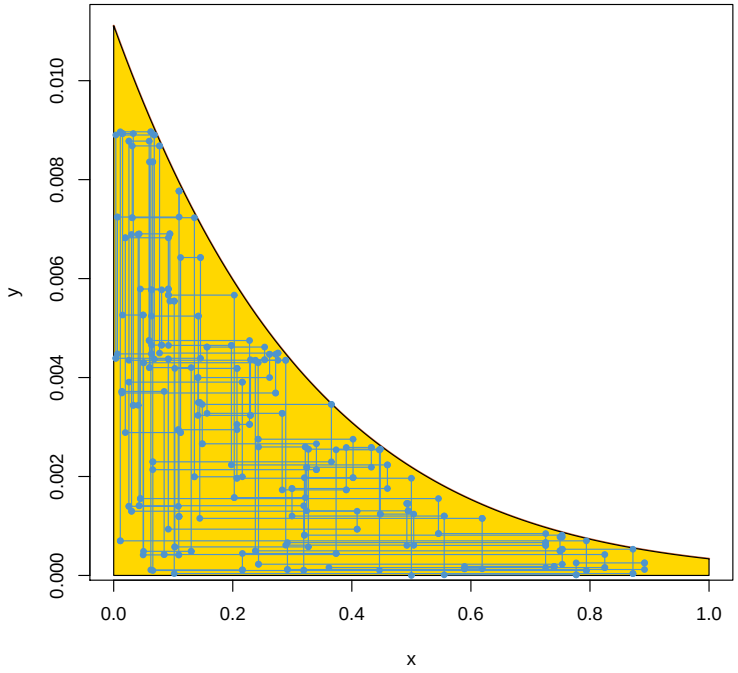
$\ldots$

k. $\omega_k^{(t+1)} \sim \mathcal{U}_{[0,f_k(\theta^{(t)})]}$;

k+1. $\theta^{(t+1)} \sim \mathcal{U}_{A^{(t+1)}}$, with

$$A^{(t+1)} = \{y;\ f_i(y) \geq \omega_i^{(t+1)},\ i = 1, \ldots, k\}.$$

Example of results with a truncated $\mathcal{N}(-3, 1)$ distribution



Number of Iterations 2, 3, 4, 5, 10, 50, 100

Good slices

The slice sampler usually enjoys good theoretical properties (like geometric ergodicity and even uniform ergodicity under bounded f and bounded $\mathscr{X}$).
As k increases, the determination of the set $A^{(t+1)}$ may get increasingly complex.

Example (Stochastic volatility core distribution)

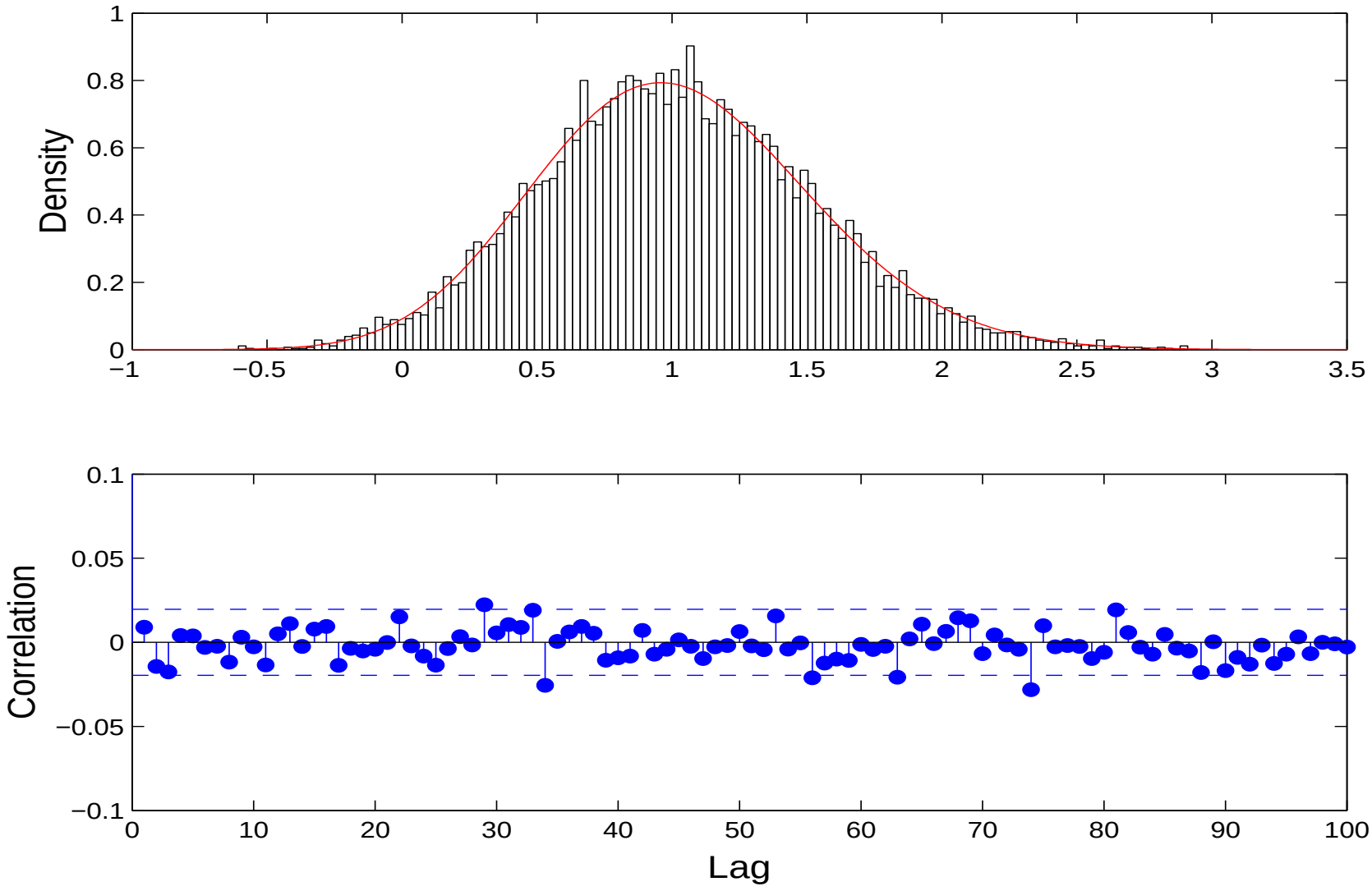
Difficult part of the stochastic volatility model

$$\pi(x) \propto \exp - \left\{\sigma^2(x-\mu)^2 + \beta^2 \exp(-x) y^2 + x\right\}/2\,,$$

simplified in $\exp - \left\{x^2 + \alpha \exp(-x)\right\}$
Slice sampling means simulation from a uniform distribution on

$$\begin{aligned} \mathfrak{A} &= \left\{x; \exp - \left\{x^2 + \alpha \exp(-x)\right\}/2 \geq u\right\} \\ &= \left\{x; x^2 + \alpha \exp(-x) \leq \omega\right\} \end{aligned}$$

if we set $\omega = -2 \log u$.
Note Inversion of $x^2 + \alpha \exp(-x) = \omega$ needs to be done by trial-and-error.



Histogram of a Markov chain produced by a slice sampler and target distribution in overlay.

Properties of the Gibbs sampler

Theorem (Convergence)

For

$$(Y_1, Y_2, \cdots, Y_p) \sim g(y_1, \ldots, y_p),$$

if either

[Positivity condition]

(*i*) $g^{(i)}(y_i) > 0$ *for every* $i = 1, \cdots, p$, *implies that* $g(y_1, \ldots, y_p) > 0$, *where* $g^{(i)}$ *denotes the marginal distribution of* Y_i, *or*

(*ii*) *the transition kernel is absolutely continuous with respect to* g,

then the chain is irreducible and positive Harris recurrent.

Properties of the Gibbs sampler (2)

Consequences

(i) If $\int h(y)g(y)dy < \infty$, then

$$\lim_{nT\to\infty} \frac{1}{T}\sum_{t=1}^{T} h_1(Y^{(t)}) = \int h(y)g(y)dy \text{ a.e. } g.$$

(ii) If, in addition, $(Y^{(t)})$ is aperiodic, then

$$\lim_{n\to\infty} \left\| \int K^n(y,\cdot)\mu(dx) - f \right\|_{TV} = 0$$

for every initial distribution μ.

Slice sampler

▸ fast on that slice

For convergence, the properties of X_t and of $f(X_t)$ are identical

Theorem (Uniform ergodicity)

If f is bounded and $\mathrm{supp} f$ is bounded, the simple slice sampler is uniformly ergodic.

[Mira & Tierney, 1997]

A small set for a slice sampler

no slice detail

For $\epsilon^\star > \epsilon_\star$,

$$C = \{x \in \mathcal{X};\ \epsilon_\star < f(x) < \epsilon^\star\}$$

is a **small set**:

$$\Pr(x, \cdot) \geq \frac{\epsilon_\star}{\epsilon^\star}\, \mu(\cdot)$$

where

$$\mu(A) = \frac{1}{\epsilon_\star} \int_0^{\epsilon_\star} \frac{\lambda(A \cap L(\epsilon))}{\lambda(L(\epsilon))} d\epsilon$$

if $L(\epsilon) = \{x \in \mathcal{X}; f(x) > \epsilon\}$‘

[Roberts & Rosenthal, 1998]

Slice sampler: drift

Under differentiability and monotonicity conditions, the slice sampler also verifies a drift condition with $V(x) = f(x)^{-\beta}$, is geometrically ergodic, and there even exist explicit bounds on the total variation distance

[Roberts & Rosenthal, 1998]

Example (Exponential $\mathcal{E}xp(1)$)

For $n > 23$,

$$||K^n(x, \cdot) - f(\cdot)||_{TV} \leq .054865\,(0.985015)^n\,(n - 15.7043)$$

Slice sampler: convergence

▸ no more slice detail

Theorem

For any density *such that*

$$\epsilon \frac{\partial}{\partial \epsilon} \lambda\left(\{x \in \mathcal{X};\, f(x) > \epsilon\}\right) \quad \textit{is non-increasing}$$

then

$$||K^{523}(x, \cdot) - f(\cdot)||_{TV} \leq .0095$$

[Roberts & Rosenthal, 1998]

A poor slice sampler

Example

Consider

$$f(x) = \exp\{-||x||\} \qquad x \in \mathbb{R}^d$$

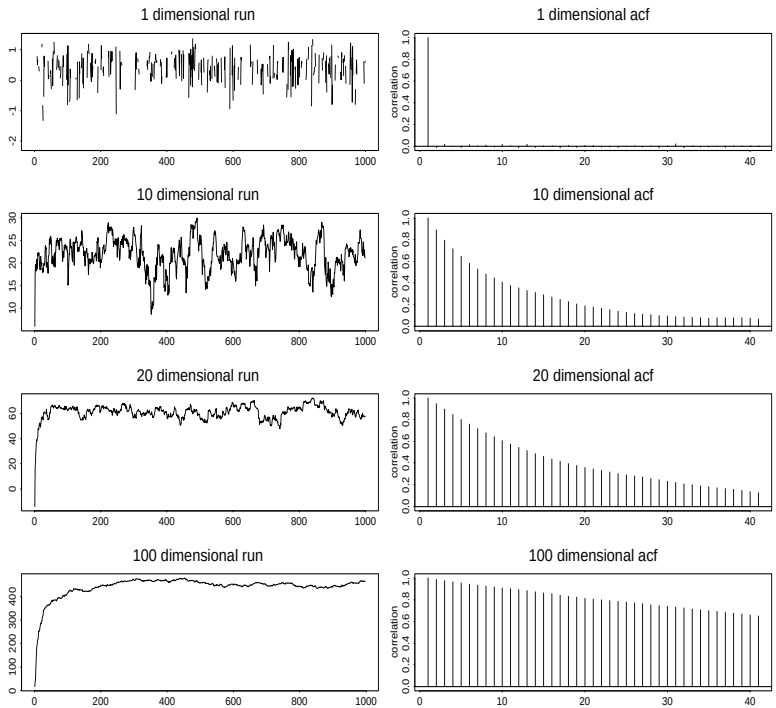
Slice sampler equivalent to one-dimensional slice sampler on

$$\pi(z) = z^{d-1}\, e^{-z} \qquad z > 0$$

or on

$$\pi(u) = e^{-u^{1/d}} \qquad u > 0$$

Poor performances when d large (heavy tails)



Sample runs of $\log(u)$ and ACFs for $\log(u)$ (Roberts & Rosenthal, 1999)

Hammersley-Clifford theorem

An illustration that conditionals determine the joint distribution

Theorem

If the joint density $g(y_1, y_2)$ *have conditional distributions* $g_1(y_1|y_2)$ *and* $g_2(y_2|y_1)$*, then*

$$g(y_1, y_2) = \frac{g_2(y_2|y_1)}{\int g_2(v|y_1)/g_1(y_1|v)\, dv}.$$

[Hammersley & Clifford, circa 1970]

General HC decomposition

Under the positivity condition, the joint distribution g satisfies

$$g(y_1, \ldots, y_p) \propto \prod_{j=1}^{p} \frac{g_{\ell_j}(y_{\ell_j} | y_{\ell_1}, \ldots, y_{\ell_{j-1}}, y'_{\ell_{j+1}}, \ldots, y'_{\ell_p})}{g_{\ell_j}(y'_{\ell_j} | y_{\ell_1}, \ldots, y_{\ell_{j-1}}, y'_{\ell_{j+1}}, \ldots, y'_{\ell_p})}$$

for every permutation ℓ on $\{1, 2, \ldots, p\}$ and every $y' \in \mathscr{Y}$.

Hierarchical models

▸ no hierarchy

The Gibbs sampler is particularly well suited to *hierarchical models*

Example (Animal epidemiology)

Counts of the number of cases of clinical mastitis in 127 dairy cattle herds over a one year period
Number of cases in herd i

$$X_i \sim \mathscr{P}(\lambda_i) \qquad i = 1, \cdots, m$$

where λ_i is the underlying rate of infection in herd i
Lack of independence might manifest itself as overdispersion.

Example (Animal epidemiology (2))

Modified model

$$\begin{aligned} X_i &\sim \mathscr{P}(\lambda_i) \\ \lambda_i &\sim \mathscr{G}a(\alpha, \beta_i) \\ \beta_i &\sim \mathscr{IG}(a, b), \end{aligned}$$

The Gibbs sampler corresponds to conditionals

$$\begin{aligned} \lambda_i &\sim \pi(\lambda_i|\mathbf{x}, \alpha, \beta_i) = \mathscr{G}a(x_i + \alpha, [1 + 1/\beta_i]^{-1}) \\ \beta_i &\sim \pi(\beta_i|\mathbf{x}, \alpha, a, b, \lambda_i) = \mathscr{IG}(\alpha + a, [\lambda_i + 1/b]^{-1}) \end{aligned}$$

▸ if you hate rats

Example (Rats)

Experiment where rats are intoxicated by a substance, then treated by either a placebo or a drug:

$$\begin{aligned} x_{ij} &\sim \mathcal{N}(\theta_i, \sigma_c^2), & 1 \leq j \leq J_i^c\,, & \quad \text{control} \\ y_{ij} &\sim \mathcal{N}(\theta_i + \delta_i, \sigma_a^2), & 1 \leq j \leq J_i^a\,, & \quad \text{intoxication} \\ z_{ij} &\sim \mathcal{N}(\theta_i + \delta_i + \xi_i, \sigma_t^2), & 1 \leq j \leq J_i^t\,, & \quad \text{treatment} \end{aligned}$$

Additional variable w_i, equal to 1 if the rat is treated with the drug, and 0 otherwise.

Example (Rats (2))

Prior distributions $(1 \leq i \leq I)$,

$$\theta_i \sim \mathcal{N}(\mu_\theta, \sigma_\theta^2), \qquad \delta_i \sim \mathcal{N}(\mu_\delta, \sigma_\delta^2),$$

and

$$\xi_i \sim \mathcal{N}(\mu_P, \sigma_P^2) \qquad \text{or} \qquad \xi_i \sim \mathcal{N}(\mu_D, \sigma_D^2),$$

if ith rat treated with a placebo (P) or a drug (D)
Hyperparameters of the model,

$$\mu_\theta, \mu_\delta, \mu_P, \mu_D, \sigma_c, \sigma_a, \sigma_t, \sigma_\theta, \sigma_\delta, \sigma_P, \sigma_D\ ,$$

associated with Jeffreys' noninformative priors.
Alternative prior with two possible levels of intoxication

$$\delta_i \sim p\mathcal{N}(\mu_{\delta 1}, \sigma_{\delta 1}^2) + (1-p)\mathcal{N}(\mu_{\delta 2}, \sigma_{\delta 2}^2),$$

Conditional decompositions

Easy decomposition of the posterior distribution
For instance, if

$$\theta|\theta_1 \sim \pi_1(\theta|\theta_1), \qquad \theta_1 \sim \pi_2(\theta_1),$$

then

$$\pi(\theta|x) = \int_{\Theta_1} \pi(\theta|\theta_1, x)\pi(\theta_1|x)\, d\theta_1,$$

Conditional decompositions (2)

where

$$\begin{aligned}
\pi(\theta|\theta_1, x) &= \frac{f(x|\theta)\pi_1(\theta|\theta_1)}{m_1(x|\theta_1)}, \\
m_1(x|\theta_1) &= \int_\Theta f(x|\theta)\pi_1(\theta|\theta_1)\, d\theta, \\
\pi(\theta_1|x) &= \frac{m_1(x|\theta_1)\pi_2(\theta_1)}{m(x)}, \\
m(x) &= \int_{\Theta_1} m_1(x|\theta_1)\pi_2(\theta_1)\, d\theta_1.
\end{aligned}$$

Conditional decompositions (3)

Moreover, this decomposition works for the posterior moments, that is, for every function h,

$$\mathbb{E}^{\pi}[h(\theta)|x] = \mathbb{E}^{\pi(\theta_1|x)}\left[\mathbb{E}^{\pi_1}\left[h(\theta)|\theta_1, x\right]\right],$$

where

$$\mathbb{E}^{\pi_1}[h(\theta)|\theta_1, x] = \int_{\Theta} h(\theta)\pi(\theta|\theta_1, x)\, d\theta.$$

Example (Rats inc., continued ▸ if you still hate rats)

Posterior complete distribution given by

$$\pi((\theta_i,\delta_i,\xi_i)_i,\mu_\theta,\ldots,\sigma_c,\ldots|\mathscr{D}) \propto$$
$$\prod_{i=1}^{I}\{\exp-\{(\theta_i-\mu_\theta)^2/2\sigma_\theta^2+(\delta_i-\mu_\delta)^2/2\sigma_\delta^2\}$$
$$\prod_{j=1}^{J_i^c}\exp-\{(x_{ij}-\theta_i)^2/2\sigma_c^2\}\prod_{j=1}^{J_i^a}\exp-\{(y_{ij}-\theta_i-\delta_i)^2/2\sigma_a^2\}$$
$$\prod_{j=1}^{J_i^t}\exp-\{(z_{ij}-\theta_i-\delta_i-\xi_i)^2/2\sigma_t^2\}\Big\}$$
$$\prod_{\ell_i=0}\exp-\{(\xi_i-\mu_P)^2/2\sigma_P^2\}\prod_{\ell_i=1}\exp-\{(\xi_i-\mu_D)^2/2\sigma_D^2\}$$
$$\sigma_c^{-\sum_i J_i^c-1}\sigma_a^{-\sum_i J_i^a-1}\sigma_t^{-\sum_i J_i^t-1}(\sigma_\theta\sigma_\delta)^{-I-1}\sigma_D^{-I_D-1}\sigma_P^{-I_P-1},$$

Local conditioning property

For the hierarchical model

$$\pi(\theta) = \int_{\Theta_1 \times \ldots \times \Theta_n} \pi_1(\theta|\theta_1)\pi_2(\theta_1|\theta_2) \cdots \pi_{n+1}(\theta_n)\, d\theta_1 \cdots d\theta_{n+1}.$$

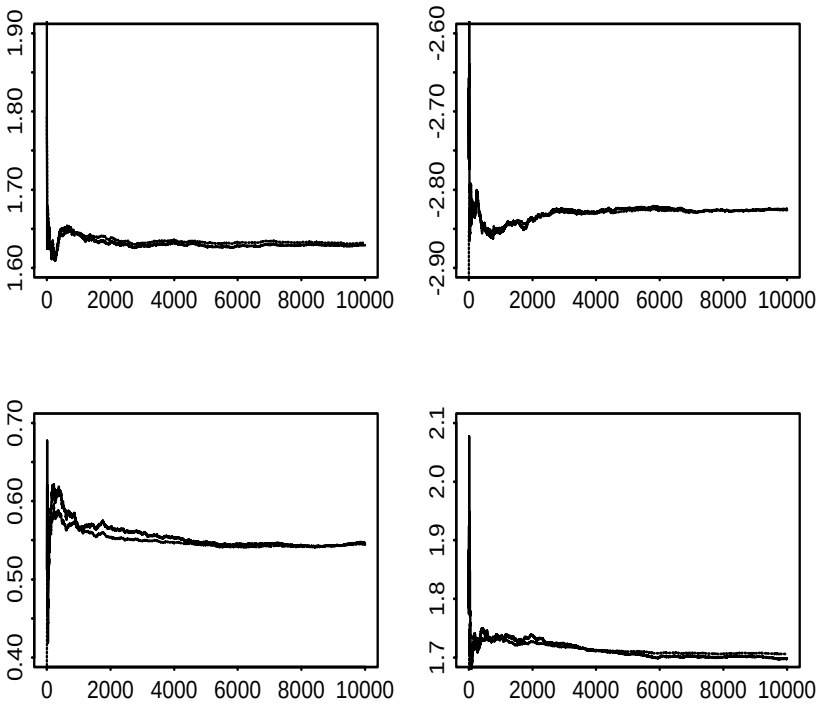
we have

$$\pi(\theta_i|x, \theta, \theta_1, \ldots, \theta_n) = \pi(\theta_i|\theta_{i-1}, \theta_{i+1})$$

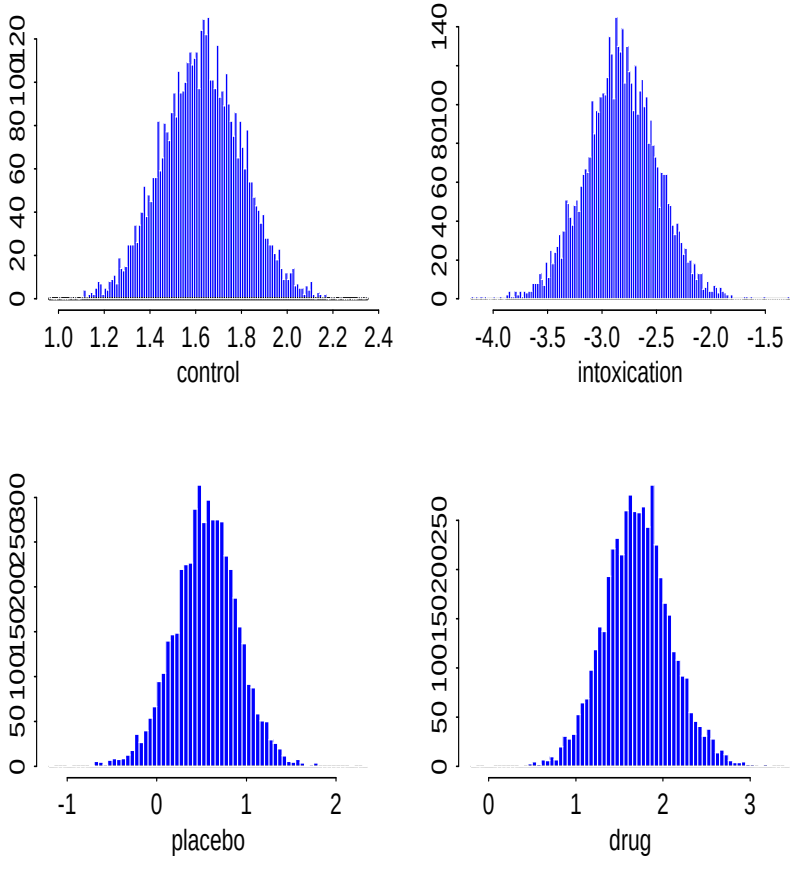
with the convention $\theta_0 = \theta$ and $\theta_{n+1} = 0$.

Example (Rats inc., terminated ▸ still this zemmiphobia?!)

The full conditional distributions correspond to standard distributions and Gibbs sampling applies.



Convergence of the posterior means



Posteriors of the effects

Posterior Gibbs inference

	μ_δ	μ_D	μ_P	$\mu_D - \mu_P$
Probability	1.00	0.9998	0.94	0.985
Confidence	[-3.48,-2.17]	[0.94,2.50]	[-0.17,1.24]	[0.14,2.20]

Posterior probabilities of significant effects

Data Augmentation

The Gibbs sampler with only two steps is particularly useful

Algorithm (Data Augmentation)

Given $y^{(t)}$,

1.. Simulate $Y_1^{(t+1)} \sim g_1(y_1|y_2^{(t)})$;

2.. Simulate $Y_2^{(t+1)} \sim g_2(y_2|y_1^{(t+1)})$.

Theorem (Markov property)

Both $(Y_1^{(t)})$ and $(Y_2^{(t)})$ are Markov chains, with transitions

$$\mathfrak{K}_i(x, x^*) = \int g_i(y|x) g_{3-i}(x^*|y)\, dy,$$

Example (Grouped counting data)

360 consecutive records of the number of passages per unit time

Number of passages	0	1	2	3	4 or more
Number of observations	139	128	55	25	13

Example (Grouped counting data (2))

Feature Observations with 4 passages and more are grouped
If observations are Poisson $\mathscr{P}(\lambda)$, the likelihood is

$$\ell(\lambda|x_1,\ldots,x_5) \propto e^{-347\lambda}\lambda^{128+55\times 2+25\times 3}\left(1-e^{-\lambda}\sum_{i=0}^{3}\frac{\lambda^i}{i!}\right)^{13},$$

which can be difficult to work with.
Idea With a prior $\pi(\lambda)=1/\lambda$, complete the vector $(y_1,\ldots,y_{13})$ of the 13 units larger than 4

Algorithm (Poisson-Gamma Gibbs)

a Simulate $Y_i^{(t)} \sim \mathscr{P}(\lambda^{(t-1)})\, \mathbb{I}_{y \geq 4} \quad i = 1, \ldots, 13$

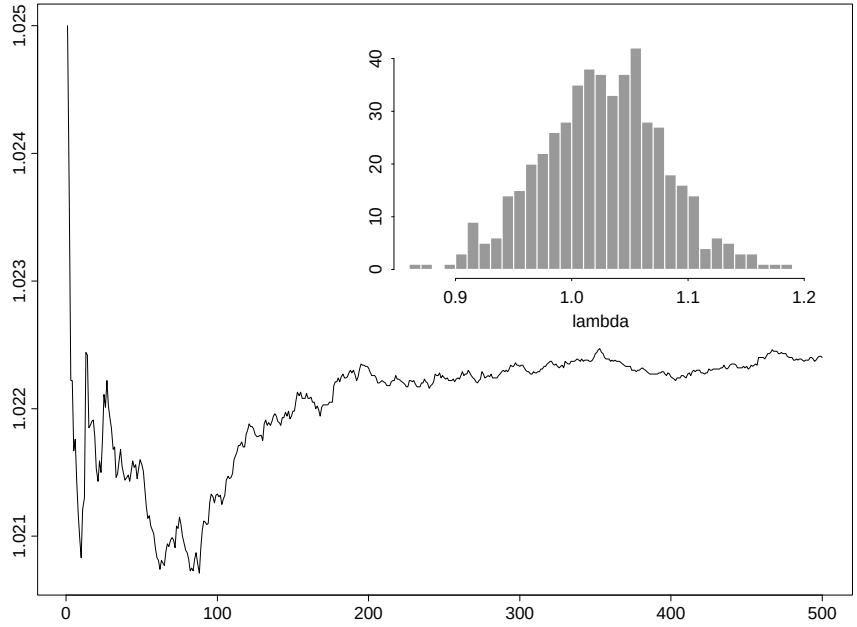
b Simulate

$$\lambda^{(t)} \sim \mathcal{G}a\left(313 + \sum_{i=1}^{13} y_i^{(t)},\ 360\right).$$

The Bayes estimator

$$\delta^{\pi} = \frac{1}{360T} \sum_{t=1}^{T} \left(313 + \sum_{i=1}^{13} y_i^{(t)}\right)$$

converges quite rapidly ▸ to R& B



Rao-Blackwellization

If $(y_1, y_2, \ldots, y_p)^{(t)}, t = 1, 2, \ldots T$ is the output from a Gibbs sampler

$$\delta_0 = \frac{1}{T} \sum_{t=1}^{T} h\left(y_1^{(t)}\right) \rightarrow \int h(y_1) g(y_1) dy_1$$

and is unbiased.
The Rao-Blackwellization replaces δ_0 with its conditional expectation

$$\delta_{rb} = \frac{1}{T} \sum_{t=1}^{T} \mathbb{E}\left[h(Y_1)|y_2^{(t)}, \ldots, y_p^{(t)}\right].$$

Rao-Blackwellization (2)

Then

- Both estimators converge to $\mathbb{E}[h(Y_1)]$
- Both are unbiased,
- and

$$\operatorname{var}\left(\mathbb{E}\left[h(Y_1)|Y_2^{(t)},\ldots,Y_p^{(t)}\right]\right) \leq \operatorname{var}(h(Y_1)),$$

so δ_{rb} is uniformly better (for Data Augmentation)

Examples of Rao-Blackwellization

Example

Bivariate normal Gibbs sampler

$$\begin{aligned} X \mid y &\sim \mathcal{N}(\rho y,\ 1-\rho^2) \\ Y \mid x &\sim \mathcal{N}(\rho x,\ 1-\rho^2). \end{aligned}$$

Then

$$\delta_0 = \frac{1}{T}\sum_{i=1}^{T} X^{(i)} \quad \text{and} \quad \delta_1 = \frac{1}{T}\sum_{i=1}^{T} \mathbb{E}[X^{(i)}|Y^{(i)}] = \frac{1}{T}\sum_{i=1}^{T} \varrho Y^{(i)},$$

estimate $\mathbb{E}[X]$ and $\sigma^2_{\delta_0}/\sigma^2_{\delta_1} = \frac{1}{\rho^2} > 1$.

Examples of Rao-Blackwellization (2)

Example (Poisson-Gamma Gibbs cont'd)

Naïve estimate

$$\delta_0 = \frac{1}{T}\sum_{t=1}^{T} \lambda^{(t)}$$

and Rao-Blackwellized version

$$\begin{aligned}\delta^\pi &= \frac{1}{T}\sum_{t=1}^{T} \mathbb{E}[\lambda^{(t)}|x_1, x_2, \ldots, x_5, y_1^{(i)}, y_2^{(i)}, \ldots, y_{13}^{(i)}] \\ &= \frac{1}{360T}\sum_{t=1}^{T}\left(313 + \sum_{i=1}^{13} y_i^{(t)}\right),\end{aligned}$$

◂ back to graph

NP Rao-Blackwellization & Rao-Blackwellized NP

Another substantial benefit of Rao-Blackwellization is in the approximation of densities of different components of y without nonparametric density estimation methods.

Lemma

The estimator

$$\frac{1}{T}\sum_{t=1}^{T} g_i(y_i|y_j^{(t)}, j \neq i) \longrightarrow g_i(y_i),$$

is unbiased.

The Duality Principle

skip dual part

Ties together the properties of the two Markov chains in Data Augmentation

Consider a Markov chain $(X^{(t)})$ and a sequence $(Y^{(t)})$ of random variables generated from the conditional distributions

$$\begin{aligned} X^{(t)}|y^{(t)} &\sim \pi(x|y^{(t)}) \\ Y^{(t+1)}|x^{(t)}, y^{(t)} &\sim f(y|x^{(t)}, y^{(t)}) \,. \end{aligned}$$

Theorem (Duality properties)

If the chain $(Y^{(t)})$ is ergodic then so is $(X^{(t)})$ and the duality also holds for geometric or uniform ergodicity.

Note

The chain $(Y^{(t)})$ can be discrete, and the chain $(X^{(t)})$ continuous.

Improper Priors

↯ Unsuspected danger resulting from careless use of MCMC algorithms:
It may happen that

- all conditional distributions are well defined,
- all conditional distributions may be simulated from, but...
- the system of conditional distributions may not correspond to any joint distribution

Warning The problem is due to careless use of the Gibbs sampler in a situation for which the underlying assumptions are violated

Example (Conditional exponential distributions)

For the model

$$X_1|x_2 \sim \mathscr{E}xp(x_2)\ , \quad X_2|x_1 \sim \mathscr{E}xp(x_1)$$

the only candidate $f(x_1, x_2)$ for the joint density is

$$f(x_1, x_2) \propto \exp(-x_1 x_2),$$

but

$$\int f(x_1, x_2) dx_1 dx_2 = \infty$$

© **These conditionals do not correspond to a joint probability distribution**

Example (Improper random effects)

Consider

$$Y_{ij} = \mu + \alpha_i + \varepsilon_{ij}, \quad i = 1, \ldots, I,\ j = 1, \ldots, J,$$

where

$$\alpha_i \sim \mathcal{N}(0, \sigma^2) \text{ and } \varepsilon_{ij} \sim \mathcal{N}(0, \tau^2),$$

the Jeffreys (improper) prior for the parameters μ, σ and τ is

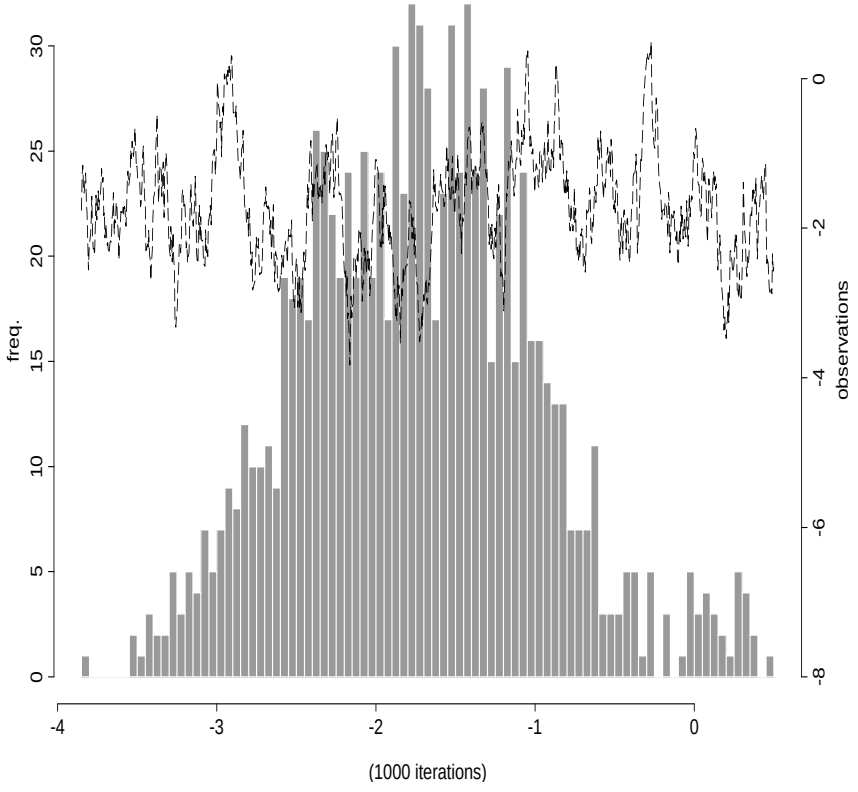
$$\pi(\mu, \sigma^2, \tau^2) = \frac{1}{\sigma^2 \tau^2}\ .$$

Example (Improper random effects 2)

The conditional distributions

$$\begin{aligned}
\alpha_i|y,\mu,\sigma^2,\tau^2 &\sim \mathscr{N}\left(\frac{J(\bar{y}_i-\mu)}{J+\tau^2\sigma^{-2}}, (J\tau^{-2}+\sigma^{-2})^{-1}\right) , \\
\mu|\alpha,y,\sigma^2,\tau^2 &\sim \mathscr{N}(\bar{y}-\bar{\alpha}, \tau^2/JI) , \\
\sigma^2|\alpha,\mu,y,\tau^2 &\sim \mathcal{IG}\left(I/2, (1/2)\sum_i \alpha_i^2\right) , \\
\tau^2|\alpha,\mu,y,\sigma^2 &\sim \mathcal{IG}\left(IJ/2, (1/2)\sum_{i,j}(y_{ij}-\alpha_i-\mu)^2\right) ,
\end{aligned}$$

are well-defined and a Gibbs sampler can be easily implemented in this setting.



Example (Improper random effects 2)

The figure shows the sequence of $\mu^{(t)}$'s and its histogram over $1,000$ iterations. They both **fail to** indicate that the corresponding "joint distribution" **does not exist**

Final notes on impropriety

The improper posterior Markov chain cannot be positive recurrent

The major task in such settings is to find indicators that flag that something is wrong. However, the output of an "improper" Gibbs sampler may not differ from a positive recurrent Markov chain.

Example

The random effects model was initially treated in Gelfand et al. (1990) as a legitimate model

MCMC tools for variable dimension problems

A new brand of problems

There exist setups where

> **One of the things we do not know is the number of things we do not know**

[Peter Green]

Bayesian Model Choice

Typical in model choice settings

- **model construction (nonparametrics)**
- **model checking (goodness of fit)**
- **model improvement (expansion)**
- **model prunning (contraction)**
- **model comparison**
- ***hypothesis* testing (Science)**
- **prediction (finance)**

Bayesian Model Choice II

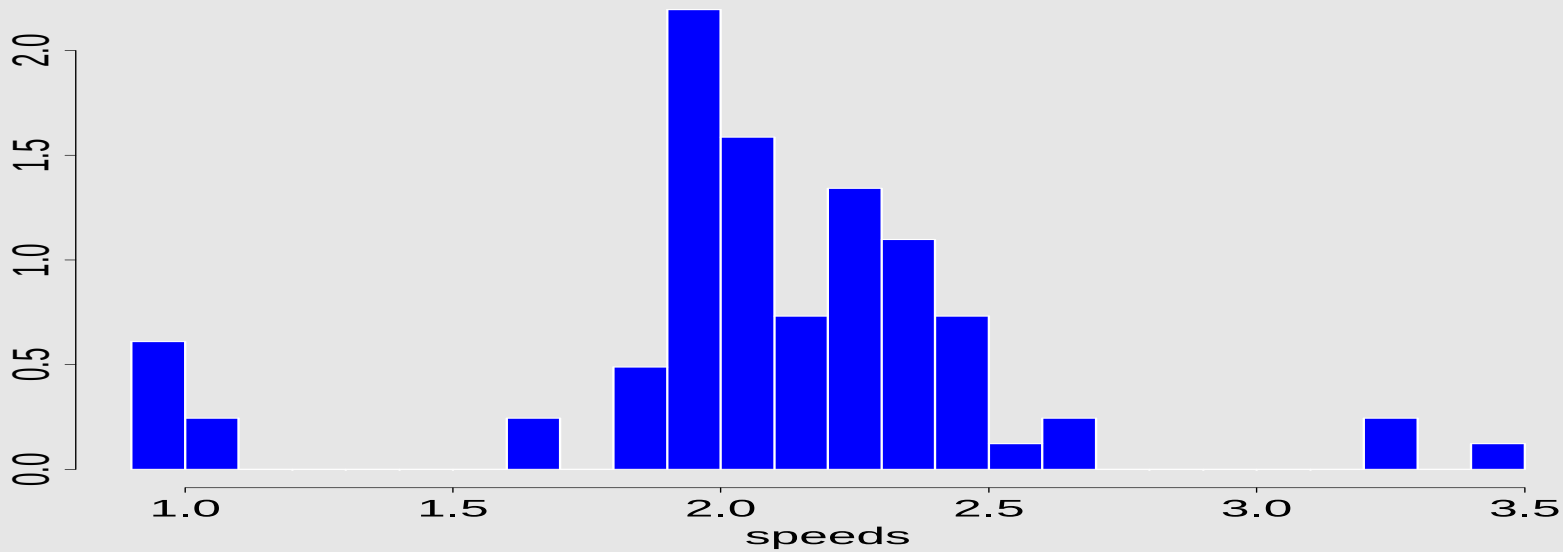
Many areas of application

- *variable* **selection**
- **change point(s) determination**
- **image analysis**
- **graphical models and expert systems**
- *variable* **dimension models**
- **causal inference**

Example (Mixture again, yes!)

Benchmark dataset: Speed of galaxies

[Roeder, 1990; Richardson & Green, 1997]



Example (Mixture again (2))

Modelling by a mixture model

$$\mathfrak{M}_i : x_j \sim \sum_{\ell=1}^{i} p_{\ell i} \mathcal{N}(\mu_{\ell i}, \sigma_{\ell i}^2) \qquad (j = 1, \ldots, 82)$$

i?

Bayesian variable dimension model

Definition

A variable dimension model is defined as a collection of models $(k = 1 \ldots, K)$,

$$\mathfrak{M}_k = \{f(\cdot|\theta_k);\ \theta_k \in \Theta_k\}\ ,$$

associated with a collection of priors on the parameters of these models,

$$\pi_k(\theta_k)\,,$$

and a prior distribution on the indices of these models,

$$\{\varrho(k)\,, k = 1, \ldots, K\}\ .$$

Alternative notation:

$$\pi(\mathfrak{M}_k, \theta_k) = \varrho(k)\,\pi_k(\theta_k)$$

Bayesian solution

Formally over:

1. Compute

$$p(\mathfrak{M}_i|x) = \frac{p_i \int_{\Theta_i} f_i(x|\theta_i)\pi_i(\theta_i)d\theta_i}{\sum_j p_j \int_{\Theta_j} f_j(x|\theta_j)\pi_j(\theta_j)d\theta_j}$$

2. Take largest $p(\mathfrak{M}_i|x)$ to determine model, or use

$$\sum_j p_j \int_{\Theta_j} f_j(x|\theta_j)\pi_j(\theta_j)d\theta_j$$

as predictive

[Different decision theoretic perspectives]

Difficulties

Not at

- (formal) inference level ◂ [see above]
- parameter space representation

$$\Theta = \bigoplus_k \Theta_k \,,$$

[even if there are parameters common to several models]

Rather at

- (practical) inference level:
  model separation, interpretation, overfitting, prior modelling, prior coherence
- computational level:
  infinity of models, moves between models, predictive computation

Green's resolution

Setting up a proper measure–theoretic framework for designing moves *between* models $\mathfrak{M}_k$

[Green, 1995]

Create a **reversible kernel** $\mathfrak{K}$ on $\mathfrak{H} = \bigcup_k \{k\} \times \Theta_k$ such that

$$\int_A \int_B \mathfrak{K}(x, dy)\pi(x)dx = \int_B \int_A \mathfrak{K}(y, dx)\pi(y)dy$$

for the invariant density π [x is of the form $(k, \theta^{(k)})$]

Green's resolution (2)

Write $\mathfrak{K}$ as

$$\mathfrak{K}(x, B) = \sum_{m=1}^{\infty} \int \rho_m(x, y) \mathfrak{q}_m(x, dy) + \omega(x) \mathbb{I}_B(x)$$

where $\mathfrak{q}_m(x, dy)$ is a transition measure to model $\mathfrak{M}_m$ and $\rho_m(x, y)$ the corresponding acceptance probability.

Introduce a **symmetric** measure $\xi_m(dx, dy)$ on $\mathfrak{H}^2$ and impose on $\pi(dx)\mathfrak{q}_m(x, dy)$ to be absolutely continuous wrt ξ_m,

$$\frac{\pi(dx)\mathfrak{q}_m(x, dy)}{\xi_m(dx, dy)} = g_m(x, y)$$

Then

$$\rho_m(x, y) = \min \left\{ 1, \frac{g_m(y, x)}{g_m(x, y)} \right\}$$

ensures reversibility

Special case

When contemplating a move between two models, $\mathfrak{M}_1$ and $\mathfrak{M}_2$, the Markov chain being in state $\theta_1 \in \mathfrak{M}_1$, denote by $\mathfrak{K}_{1\to 2}(\theta_1, d\theta)$ and $\mathfrak{K}_{2\to 1}(\theta_2, d\theta)$ the corresponding kernels, under the *detailed balance condition*

$$\pi(d\theta_1)\, \mathfrak{K}_{1\to 2}(\theta_1, d\theta) = \pi(d\theta_2)\, \mathfrak{K}_{2\to 1}(\theta_2, d\theta)\,,$$

and take, wlog, $\dim(\mathfrak{M}_2) > \dim(\mathfrak{M}_1)$.
Proposal expressed as

$$\theta_2 = \Psi_{1\to 2}(\theta_1, v_{1\to 2})$$

where $v_{1\to 2}$ is a random variable of dimension $\dim(\mathfrak{M}_2) - \dim(\mathfrak{M}_1)$, generated as

$$v_{1\to 2} \sim \varphi_{1\to 2}(v_{1\to 2})\,.$$

Special case (2)

In this case, $\mathfrak{q}_{1\to 2}(\theta_1, d\theta_2)$ has density

$$\varphi_{1\to 2}(v_{1\to 2}) \left| \frac{\partial \Psi_{1\to 2}(\theta_1, v_{1\to 2})}{\partial(\theta_1, v_{1\to 2})} \right|^{-1},$$

by the Jacobian rule.
If probability $\varpi_{1\to 2}$ of choosing move to $\mathfrak{M}_2$ while in $\mathfrak{M}_1$, acceptance probability reduces to

$$\alpha(\theta_1, v_{1\to 2}) = 1 \wedge \frac{\pi(\mathfrak{M}_2, \theta_2)\, \varpi_{2\to 1}}{\pi(\mathfrak{M}_1, \theta_1)\, \varpi_{1\to 2}\, \varphi_{1\to 2}(v_{1\to 2})} \left| \frac{\partial \Psi_{1\to 2}(\theta_1, v_{1\to 2})}{\partial(\theta_1, v_{1\to 2})} \right| .$$

Interpretation (1)

The representation puts us back in a fixed dimension setting:

- $\mathfrak{M}_1 \times \mathfrak{V}_{1\to 2}$ and $\mathfrak{M}_2$ are in one-to-one relation
- *regular* Metropolis–Hastings move from the couple $(\theta_1, v_{1\to 2})$ to θ_2 when stationary distributions are

$$\pi(\mathfrak{M}_1, \theta_1) \times \varphi_{1\to 2}(v_{1\to 2})$$

and $\pi(\mathfrak{M}_2, \theta_2)$, and when proposal distribution is *deterministic* (??)

Interpretation (2)

Consider, instead, the proposals

$$\theta_2 \sim \mathcal{N}(\Psi_{1\to 2}(\theta_1, v_{1\to 2}), \varepsilon) \qquad \text{and} \qquad \Psi_{1\to 2}(\theta_1, v_{1\to 2}) \sim \mathcal{N}(\theta_2, \varepsilon)$$

Reciprocal proposal has density

$$\frac{\exp\left\{-(\theta_2 - \Psi_{1\to 2}(\theta_1, v_{1\to 2}))^2/2\varepsilon\right\}}{\sqrt{2\pi\varepsilon}} \times \left|\frac{\partial \Psi_{1\to 2}(\theta_1, v_{1\to 2})}{\partial(\theta_1, v_{1\to 2})}\right|$$

by the Jacobian rule.
Thus Metropolis–Hastings acceptance probability is

$$1 \wedge \frac{\pi(\mathfrak{M}_2, \theta_2)}{\pi(\mathfrak{M}_1, \theta_1)\, \varphi_{1\to 2}(v_{1\to 2})} \left|\frac{\partial \Psi_{1\to 2}(\theta_1, v_{1\to 2})}{\partial(\theta_1, v_{1\to 2})}\right|$$

Does not depend on ε: **Let ε go to 0**

Saturation

[Brooks, Giudici, Roberts, 2003]

Consider series of models $\mathfrak{M}_i$ $(i = 1, \ldots, k)$ such that

$$\max_i \dim(\mathfrak{M}_i) = n_{\max} < \infty$$

Parameter of model $\mathfrak{M}_i$ then completed with an auxiliary variable U_i such that

$$\dim(\theta_i, u_i) = n_{\max} \quad \text{and} \quad U_i \sim q_i(u_i)$$

Posit the following joint distribution for [augmented] model $\mathfrak{M}_i$

$$\pi(\mathfrak{M}_i, \theta_i)\, q_i(u_i)$$

Back to fixed dimension

Saturation: no varying dimension anymore since (θ_i, u_i) of fixed dimension.

Algorithm (Three stage MCMC update)

1. Update the current value of the parameter, θ_i;
2. Update u_i conditional on θ_i;
3. Update the current model from $\mathfrak{M}_i$ to $\mathfrak{M}_j$ using the bijection

$$(\theta_j, u_j) = \Psi_{i \to j}(\theta_i, u_i)$$

Example (Mixture of normal distributions)

$$\mathfrak{M}_k : \sum_{j=1}^{k} p_{jk} \mathcal{N}(\mu_{jk}, \sigma_{jk}^2)$$

[Richardson & Green, 1997]

Moves:

(i) Split

$$\begin{cases} p_{jk} & = & p_{j(k+1)} + p_{(j+1)(k+1)} \\ p_{jk}\mu_{jk} & = & p_{j(k+1)}\mu_{j(k+1)} + p_{(j+1)(k+1)}\mu_{(j+1)(k+1)} \\ p_{jk}\sigma_{jk}^2 & = & p_{j(k+1)}\sigma_{j(k+1)}^2 + p_{(j+1)(k+1)}\sigma_{(j+1)(k+1)}^2 \end{cases}$$

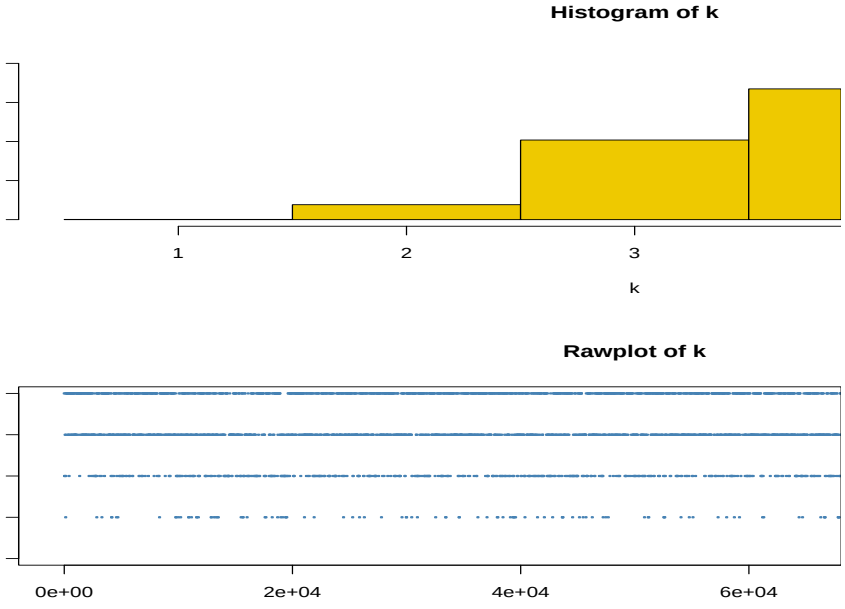
(ii) Merge (*reverse*)

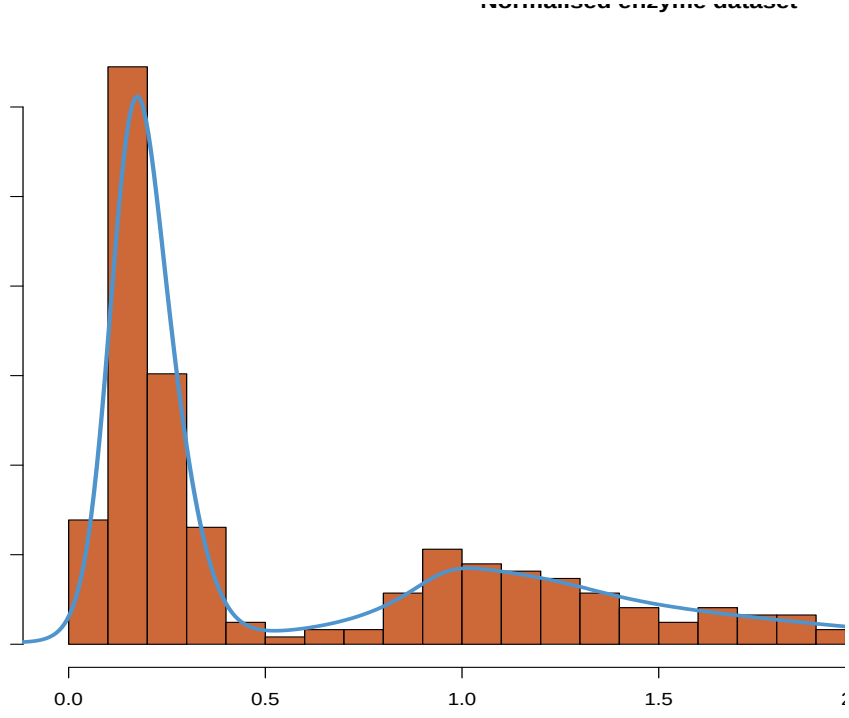
Example (Mixture (2))

Additional **Birth and Death** moves for empty components (created from the prior distribution)
Equivalent

(i). Split

$$(T) \begin{cases} u_1, u_2, u_3 & \sim & \mathcal{U}(0,1) \\ p_{j(k+1)} & = & u_1 p_{jk} \\ \mu_{j(k+1)} & = & u_2 \mu_{jk} \\ \sigma^2_{j(k+1)} & = & u_3 \sigma^2_{jk} \end{cases}$$



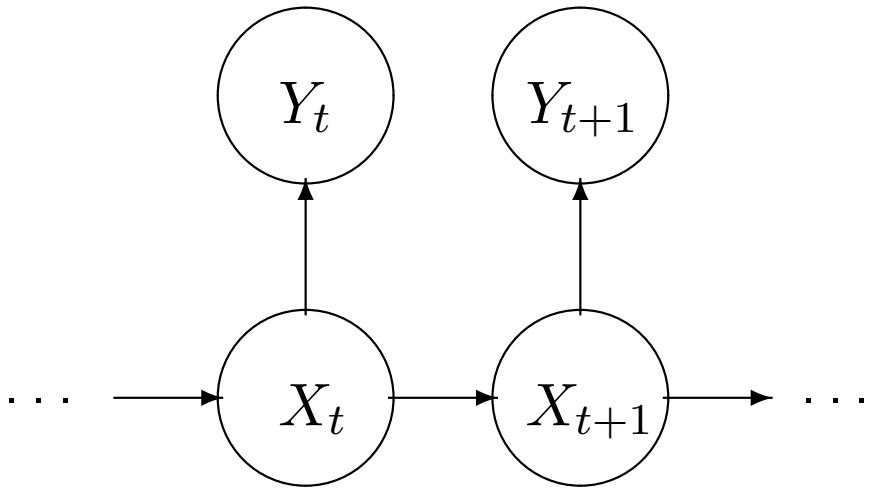


Histogram and rawplot of $100,000$ k's under the constraint $k \leq 5$.

Example (Hidden Markov model)

move to birth Extension of the mixture model

$$\begin{aligned} P(X_t + 1 = j | X_t = i) &= w_{ij}, \\ w_{ij} &= \omega_{ij} / \sum_{\ell} \omega_{i\ell}, \\ Y_t | X_t = i &\sim \mathcal{N}(\mu_i, \sigma_i^2). \end{aligned}$$


Y_t
Y_{t+1}
X_t
X_{t+1}

Example (Hidden Markov model (2))

Move to split component $j_\star$ into j_1 and j_2:

$$\omega_{ij_1} = \omega_{ij_\star}\varepsilon_i, \quad \omega_{ij_2} = \omega_{ij_\star}(1-\varepsilon_i), \quad \varepsilon_i \sim \mathcal{U}(0,1);$$

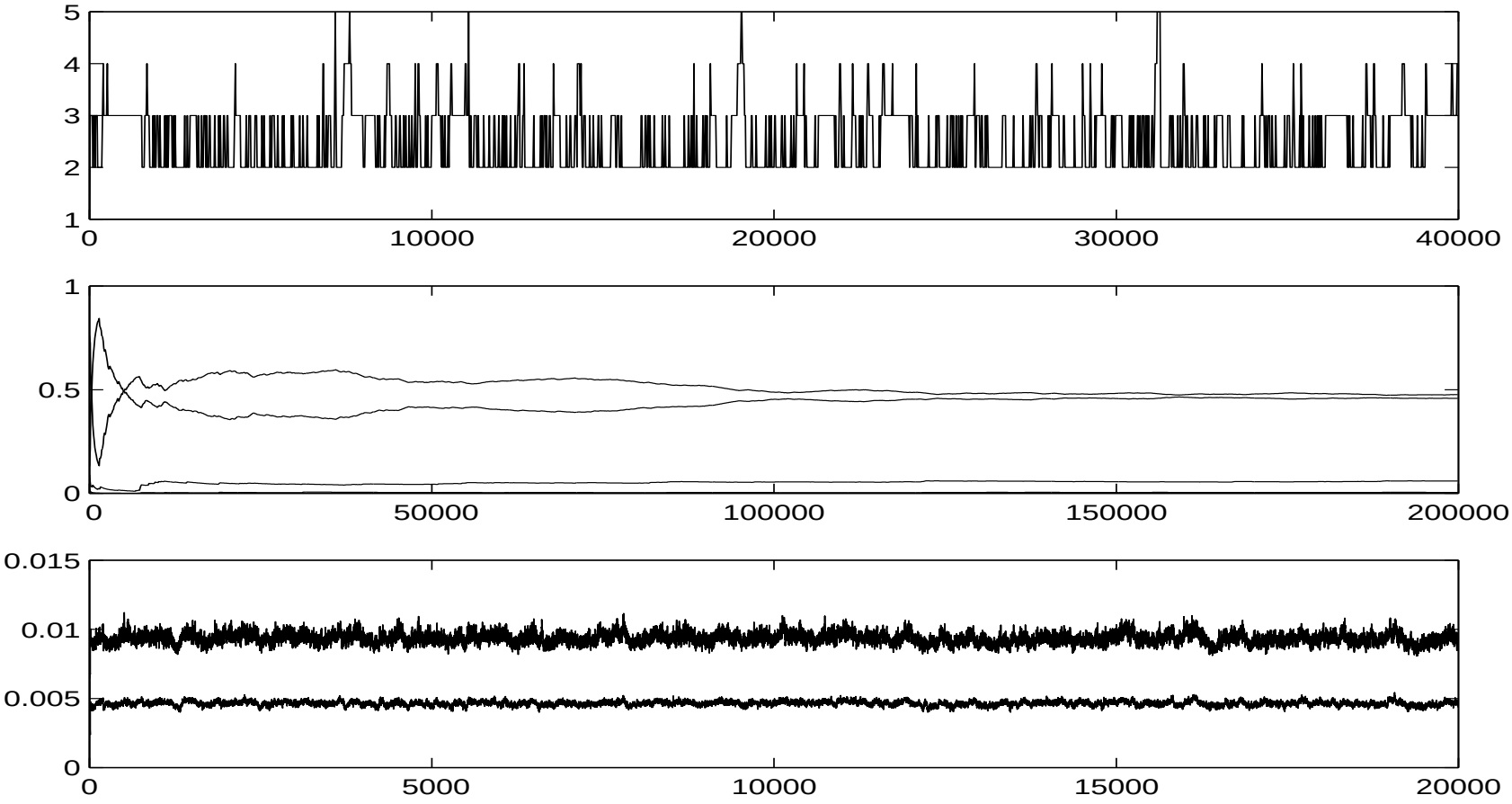
$$\omega_{j_1 j} = \omega_{j_\star j}\xi_j, \quad \omega_{j_2 j} = \omega_{j_\star j}/\xi_j, \quad \xi_j \sim \log\mathcal{N}(0,1);$$

similar ideas give $\omega_{j_1 j_2}$ etc.;

$$\mu_{j_1} = \mu_{j_\star} - 3\sigma_{j_\star}\varepsilon_\mu, \quad \mu_{j_2} = \mu_{j_\star} + 3\sigma_{j_\star}\varepsilon_\mu, \quad \varepsilon_\mu \sim \mathcal{N}(0,1);$$

$$\sigma^2_{j_1} = \sigma^2_{j_*}\xi_\sigma, \quad \sigma^2_{j_2} = \sigma^2_{j_*}/\xi_\sigma, \quad \xi_\sigma \sim \log\mathcal{N}(0,1).$$

[Robert & al., 2000]



Upper panel: First 40,000 values of k for S&P 500 data, plotted every 20th sweep. Middle panel: estimated posterior distribution of k for S&P 500 data as a function of number of sweeps. Lower panel: σ_1 and σ_2 in first 20,000 sweeps with $k = 2$ for S&P 500 data.

Example (Autoregressive model)

move to birth

Typical setting for model choice: determine order p of $AR(p)$ model

Consider the (less standard) representation

$$\prod_{i=1}^{p} (1 - \lambda_i B)\, X_t = \epsilon_t\,, \quad \epsilon_t \sim \mathcal{N}(0, \sigma^2)$$

where the λ_i's are within the unit circle if complex and within $[-1, 1]$ if real.

[Huerta and West, 1998]

$AR(p)$ reversible jump algorithm

Example (Autoregressive (2))

Uniform priors for the real and complex roots λ_j,

$$\frac{1}{\lfloor k/2 \rfloor + 1} \prod_{\lambda_i \in \mathbb{R}} \frac{1}{2} \mathbb{I}_{|\lambda_i|<1} \prod_{\lambda_i \notin \mathbb{R}} \frac{1}{\pi} \mathbb{I}_{|\lambda_i|<1}$$

and (purely birth-and-death) proposals based on these priors

- k $\to$ k+1 [Creation of real root]
- k $\to$ k+2 [Creation of complex root]
- k $\to$ k-1 [Deletion of real root]
- k $\to$ k-2 [Deletion of complex root]

Birth and Death processes

▸ instant death!

Use of an alternative methodology based on a Birth–&-Death (point) process
[Preston, 1976; Ripley, 1977; Geyer & Møller, 1994; Stevens, 1999]

Idea: Create a Markov chain in *continuous time*, i.e. a *Markov jump process*, moving between models $\mathfrak{M}_k$, by births (to increase the dimension), deaths (to decrease the dimension), and other moves.

Birth and Death processes

Time till next modification **(jump)** is exponentially distributed with rate depending on current state
Remember: if $\xi_1, \ldots, \xi_v$ are exponentially distributed, $\xi_i \sim \mathcal{E}(\lambda_i)$,

$$\min \xi_i \sim \mathcal{E}\left(\sum_i \lambda_i\right)$$

Difference with MH-MCMC: Whenever a jump occurs, the corresponding move *is always accepted*. Acceptance probabilities replaced with holding times.
Implausible configurations

$$L(\boldsymbol{\theta})\pi(\boldsymbol{\theta}) \ll 1$$

die quickly.

Balance condition

Sufficient to have **detailed balance**

$$L(\boldsymbol{\theta})\pi(\boldsymbol{\theta})q(\boldsymbol{\theta},\boldsymbol{\theta}') = L(\boldsymbol{\theta}')\pi(\boldsymbol{\theta}')q(\boldsymbol{\theta}',\boldsymbol{\theta}) \quad \textbf{for all } \boldsymbol{\theta},\boldsymbol{\theta}'$$

for $\tilde{\pi}(\boldsymbol{\theta}) \propto L(\boldsymbol{\theta})\pi(\boldsymbol{\theta})$ to be stationary.
Here $q(\boldsymbol{\theta},\boldsymbol{\theta}')$ rate of moving from state $\boldsymbol{\theta}$ to $\boldsymbol{\theta}'$.
Possibility to add split/merge and fixed-k processes if balance condition satisfied.

Example (Mixture cont'd)

Stephen's original modelling:

- Representation as a (marked) point process

$$\Phi = \left\{ \{p_j, (\mu_j, \sigma_j)\} \right\}_j$$

- Birth rate λ_0 (constant)
- Birth proposal from the prior
- Death rate $\delta_j(\Phi)$ for removal of point j
- Death proposal removes component and modifies weights

Example (Mixture cont'd (2))

- Overall death rate

$$\sum_{j=1}^{k} \delta_j(\Phi) = \delta(\Phi)$$

- Balance condition

$$(k+1)\, d(\Phi \cup \{p, (\mu, \sigma)\})\, L(\Phi \cup \{p, (\mu, \sigma)\}) = \lambda_0 L(\Phi) \frac{\pi(k)}{\pi(k+1)}$$

with

$$d(\Phi \setminus \{p_j, (\mu_j, \sigma_j)\}) = \delta_j(\Phi)$$

- Case of Poisson prior $k \sim \mathcal{P}oi(\lambda_1)$

$$\delta_j(\Phi) = \frac{\lambda_0}{\lambda_1} \frac{L(\Phi \setminus \{p_j, (\mu_j, \sigma_j)\})}{L(\Phi)}$$

Stephen's original algorithm

Algorithm (Mixture Birth& Death)

For $v = 0, 1, \cdots, V$

$t \leftarrow v$

Run till $t > v + 1$

1. Compute $\delta_j(\Phi) = \dfrac{L(\Phi|\Phi_j)}{L(\Phi)} \dfrac{\lambda_0}{\lambda_1}$
2. $\delta(\Phi) \leftarrow \sum_{j=1}^{k} \delta_j(\Phi_j)$, $\xi \leftarrow \lambda_0 + \delta(\Phi)$, $u \sim \mathcal{U}([0, 1])$
3. $t \leftarrow t - u \log(u)$

Algorithm (Mixture Birth& Death (cont'd))

4. With probability $\delta(\Phi)/\xi$

   Remove component j with probability $\delta_j(\Phi)/\delta(\Phi)$

   $k \leftarrow k-1$

   $p_\ell \leftarrow p_\ell/(1-p_j) \;\; (\ell \neq j)$

   Otherwise,

   Add component j from the prior $\pi(\mu_j, \sigma_j)$ $p_j \sim \mathcal{B}e(\gamma, k\gamma)$

   $p_\ell \leftarrow p_\ell(1-p_j) \;\; (\ell \neq j)$

   $k \leftarrow k+1$

5. Run I MCMC(k, β, p)

Rescaling time

move to HMM In discrete-time RJMCMC, let the time unit be $1/N$, put

$$\beta_k = \lambda_k/N \quad \text{and} \quad \delta_k = 1 - \lambda_k/N$$

As $N \to \infty$, each birth proposal will be accepted, and having k components births occur according to a Poisson process with rate λ_k while component (w, ϕ) dies with rate

$$\begin{aligned} &\lim_{N\to\infty} N\delta_{k+1} \times \frac{1}{k+1} \times \min(A^{-1}, 1) \\ &\qquad = \lim_{N\to\infty} N\frac{1}{k+1} \times \text{likelihood ratio}^{-1} \times \frac{\beta_k}{\delta_{k+1}} \times \frac{b(w,\phi)}{(1-w)^{k-1}} \\ &\qquad = \text{likelihood ratio}^{-1} \times \frac{\lambda_k}{k+1} \times \frac{b(w,\phi)}{(1-w)^{k-1}}. \end{aligned}$$

Hence **"RJMCMC→BDMCMC"**. This holds more generally.

Example (HMM models (cont'd))

Implementation of the split-and-combine rule of Richardson and Green (1997) in continuous time
Move to split component j_* into j_1 and j_2:

$$\omega_{ij_1} = \omega_{ij_*}\epsilon_i, \quad \omega_{ij_2} = \omega_{ij_*}(1-\epsilon_i), \quad \epsilon_i \sim \mathcal{U}(0,1);$$

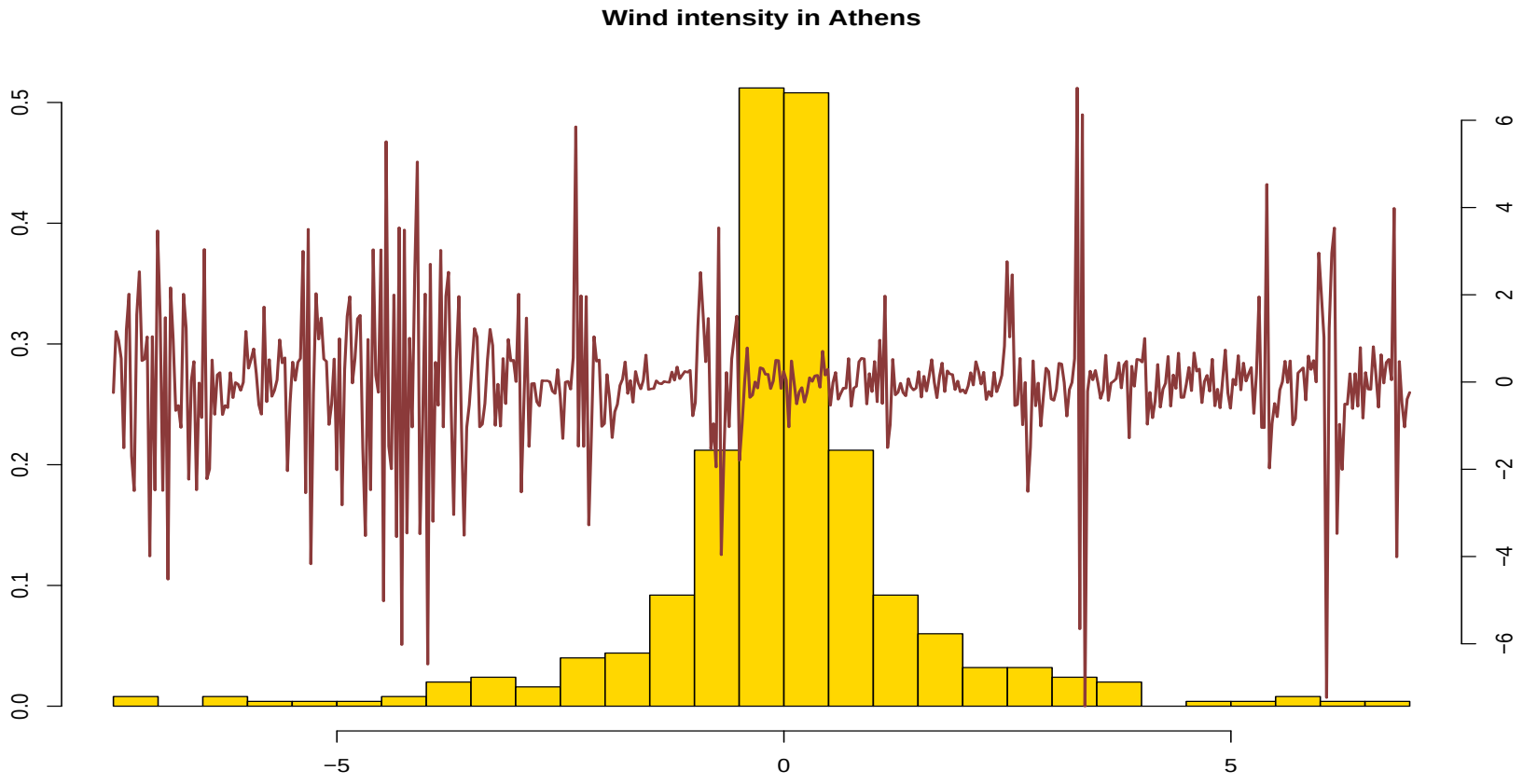
$$\omega_{j_1 j} = \omega_{j_* j}\xi_j, \quad \omega_{j_2 j} = \omega_{j_* j}/\xi_j, \quad \xi_j \sim \log\mathcal{N}(0,1);$$

similar ideas give $\omega_{j_1 j_2}$ etc.;

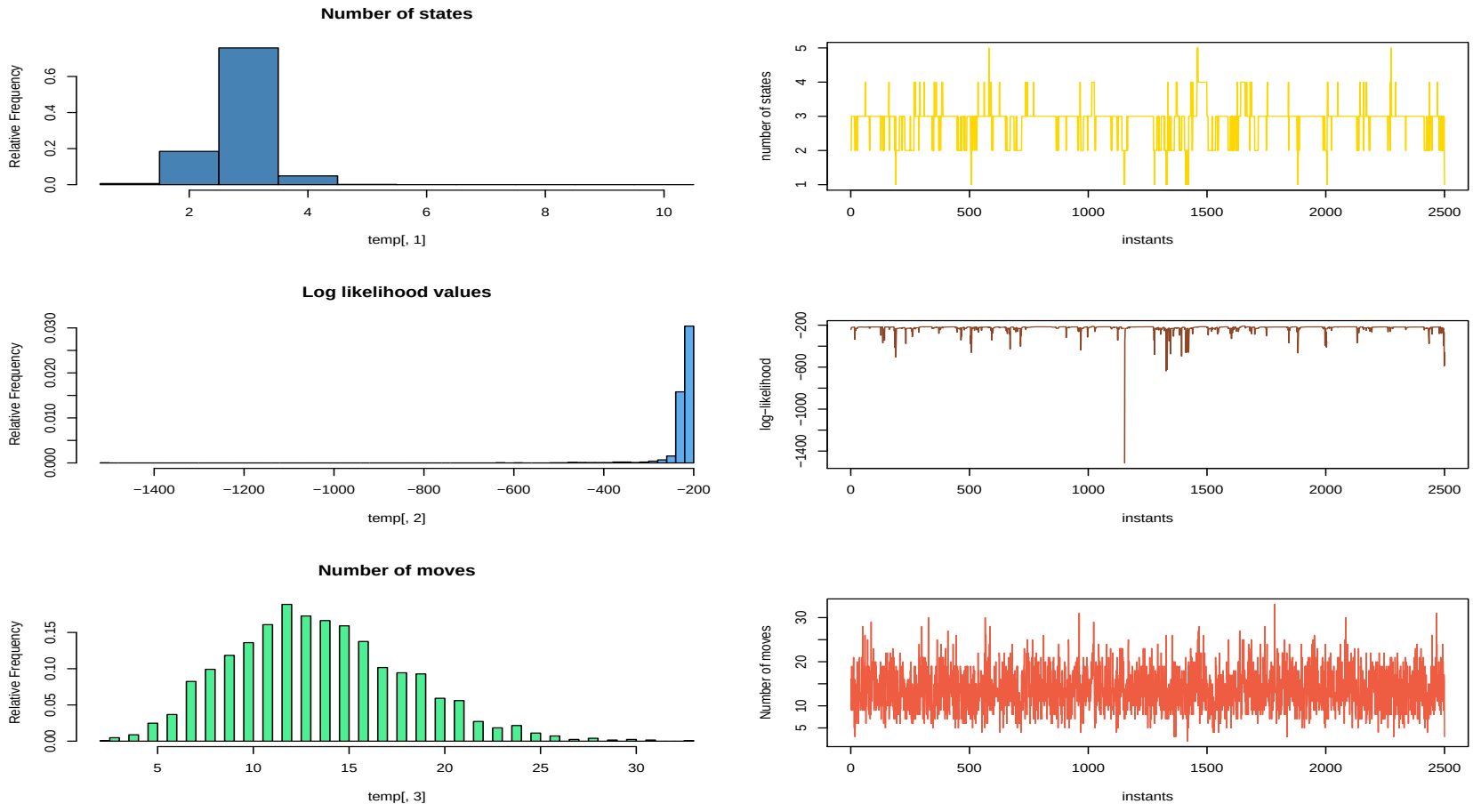
$$\mu_{j_1} = \mu_{j_*} - 3\sigma_{j_*}\epsilon_\mu, \quad \mu_{j_2} = \mu_{j_*} + 3\sigma_{j_*}\epsilon_\mu, \quad \epsilon_\mu \sim \mathcal{N}(0,1);$$

$$\sigma^2_{j_1} = \sigma^2_{j_*}\xi_\sigma, \quad \sigma^2_{j_2} = \sigma^2_{j_*}/\xi_\sigma, \quad \xi_\sigma \sim \log\mathcal{N}(0,1).$$

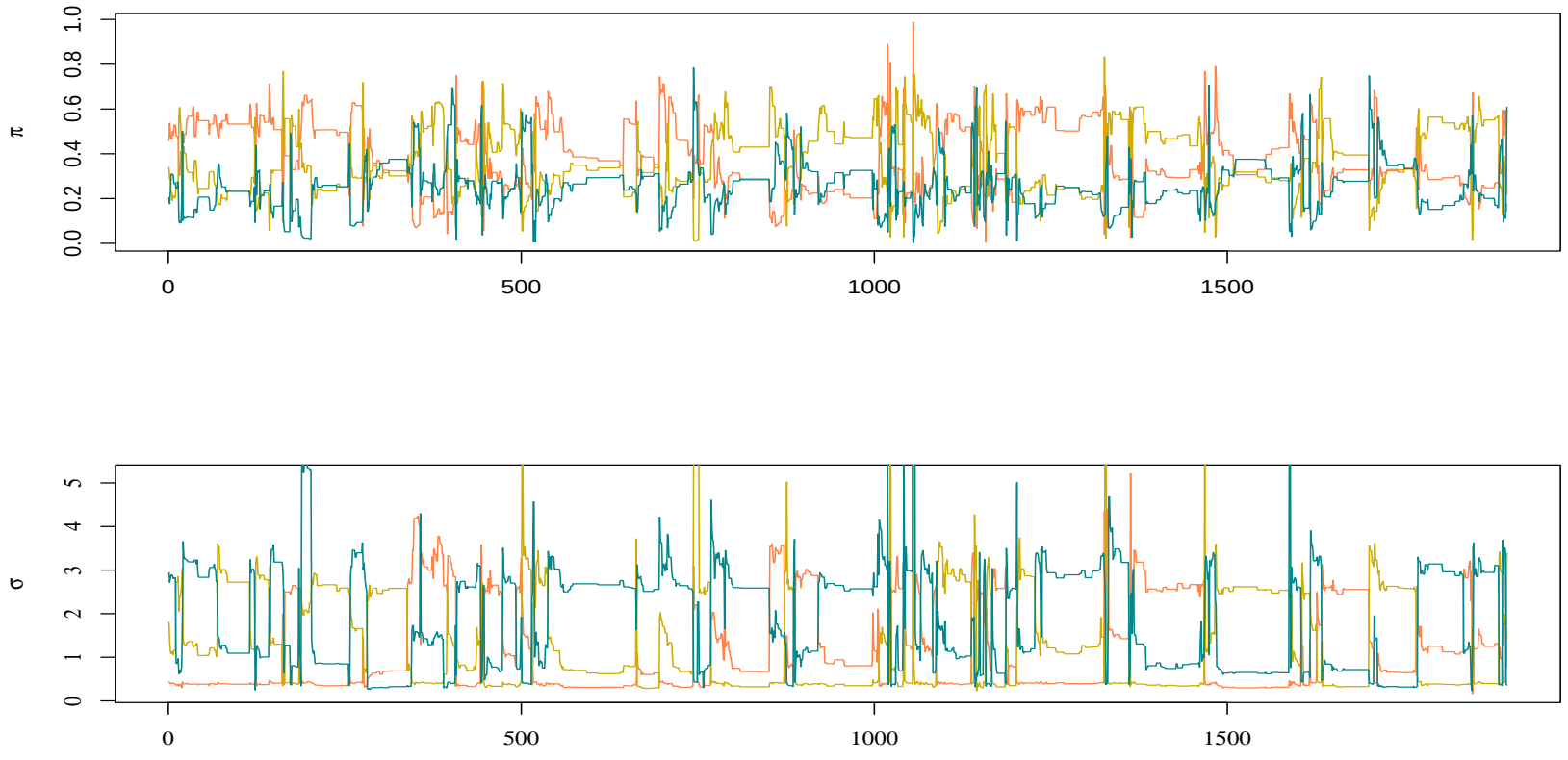
[Cappé & al, 2001]



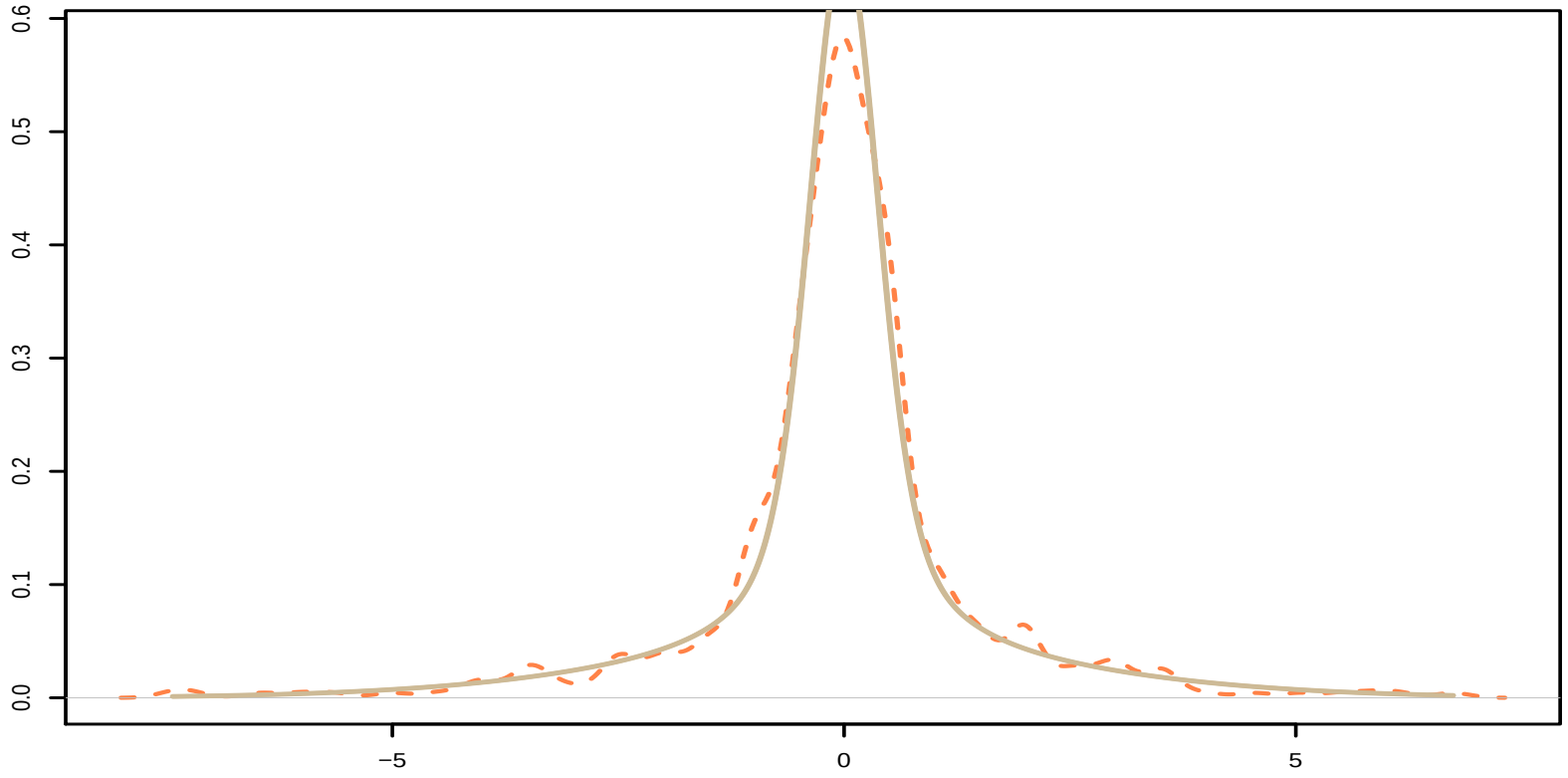
Histogram and rawplot of 500 wind intensities in Athens



MCMC output on k (histogram and rawplot), corresponding loglikelihood values (histogram and rawplot), and number of moves (histogram and rawplot)



MCMC sequence of the probabilities π_j of the stationary distribution (top) and the parameters σ (bottom) of the three components when conditioning on $k = 3$



MCMC evaluation of the marginal density of the dataset (dashes), compared with R nonparametric density estimate (solid lines).

Sequential importance sampling

◂ basic importance

Adaptive MCMC is not possible

↯ **Algorithms trained on-line usually invalid:**
using the whole past of the "chain" implies that this is not a Markov chain any longer!

Example (Poly t distribution)

Consider a t-distribution $\mathcal{T}(3, \theta, 1)$ sample $(x_1, \ldots, x_n)$ with a flat prior $\pi(\theta) = 1$
If we try fit a normal proposal from empirical mean and variance of the chain so far,

$$\mu_t = \frac{1}{t}\sum_{i=1}^{t}\theta^{(i)} \quad \text{and} \quad \sigma_t^2 = \frac{1}{t}\sum_{i=1}^{t}(\theta^{(i)} - \mu_t)^2\,,$$

Metropolis–Hastings algorithm with acceptance probability

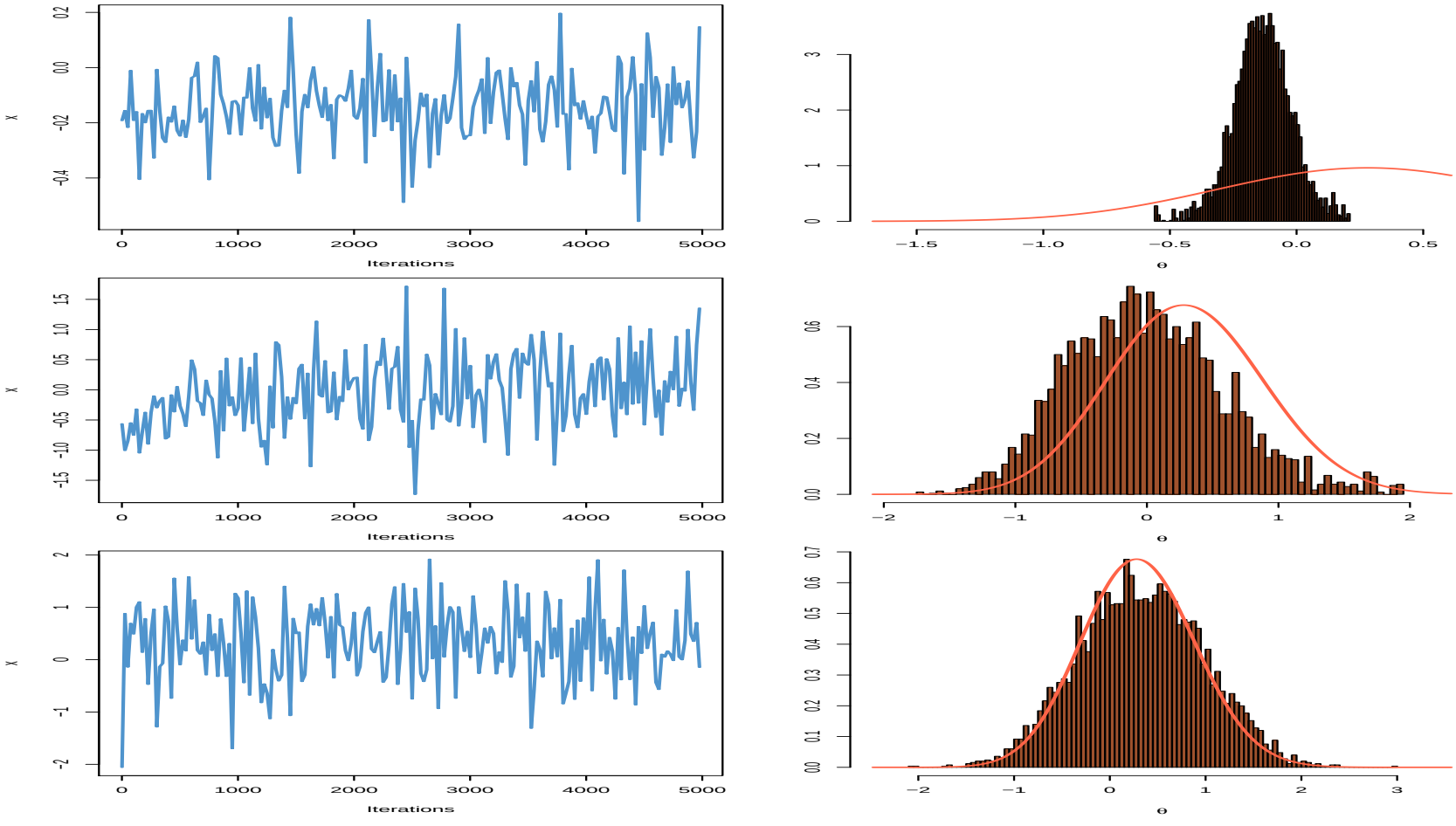
$$\prod_{j=2}^{n}\left[\frac{\nu + (x_j - \theta^{(t)})^2}{\nu + (x_j - \xi)^2}\right]^{-(\nu+1)/2} \frac{\exp -(\mu_t - \theta^{(t)})^2/2\sigma_t^2}{\exp -(\mu_t - \xi)^2/2\sigma_t^2}\,,$$

where $\xi \sim \mathcal{N}(\mu_t, \sigma_t^2)$.

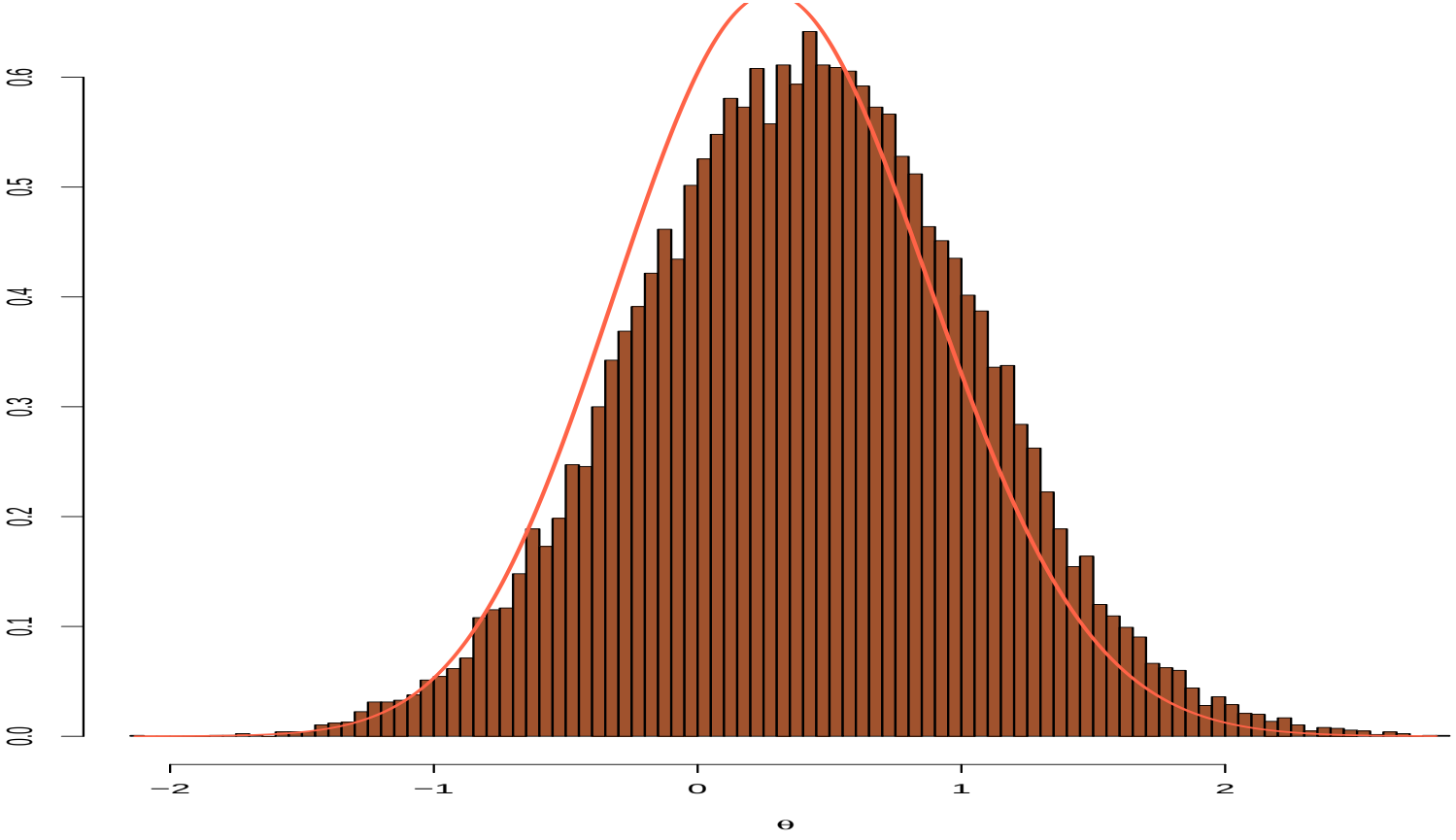
Example (Poly t distribution (2))

Invalid scheme:

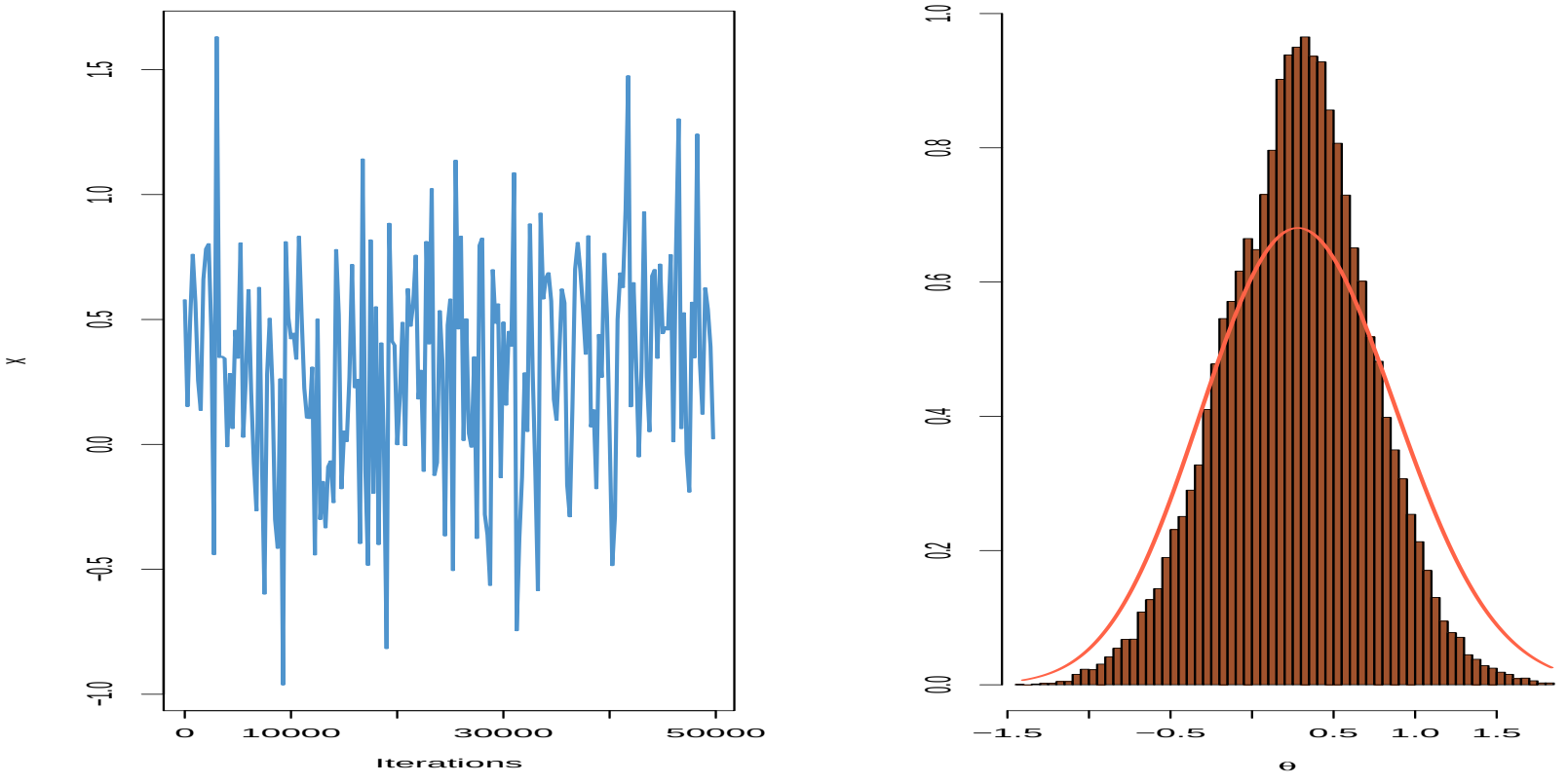
- when range of initial values too small, the $\theta^{(i)}$'s cannot converge to the target distribution and concentrates on too small a support.
- long-range dependence on past values modifies the distribution of the sequence.
- using past simulations to create a non-parametric approximation to the target distribution does not work either



Adaptive scheme for a sample of 10 $x_j \sim \mathcal{T}_\ni$ and initial variances of (top) 0.1, (middle) 0.5, and (bottom) 2.5.



Comparison of the distribution of an adaptive scheme sample of $25,000$ points with initial variance of 2.5 and of the target distribution.



Sample produced by $50,000$ iterations of a nonparametric adaptive MCMC scheme and comparison of its distribution with the target distribution.

Simply forget about it!

Warning:

One should not constantly adapt the proposal on past performances

Either adaptation ceases after a period of *burnin*
or the adaptive scheme must be theoretically assessed on its own right.

Importance sampling revisited

Approximation of integrals

back to basic importance

$$\mathfrak{I} = \int h(x)\pi(x)dx$$

by *unbiased estimators*

$$\hat{\mathfrak{I}} = \frac{1}{n}\sum_{i=1}^{n} \varrho_i h(x_i)$$

when

$$x_1, \ldots, x_n \overset{iid}{\sim} q(x) \qquad \text{and} \qquad \varrho_i \overset{\text{def}}{=} \frac{\pi(x_i)}{q(x_i)}$$

Markov extension

For densities f and g, and importance weight

$$\omega(x) = f(x)/g(x)\,,$$

for any kernel $K(x, x')$ with stationary distribution f,

$$\int \omega(x)\, K(x, x')\, g(x) dx = f(x')\,.$$

[McEachern, Clyde, and Liu, 1999]

Consequence: An importance sample transformed by MCMC transitions keeps its weights

Unbiasedness preservation:

$$\begin{aligned}\mathbb{E}\left[\omega(X)h(X')\right] &= \int \omega(x)\, h(x')\, K(x, x')\, g(x)\, dx\, dx' \\ &= \mathbb{E}_f\left[h(X)\right]\end{aligned}$$

Not so exciting!

The weights do not change!

If x has small weight

$$\omega(x) = f(x)/g(x)\,,$$

then

$$x' \sim K(x, x')$$

keeps this small weight.

Pros and cons of importance sampling vs. MCMC

- Production of a sample (IS) vs. of a Markov chain (MCMC)
- Dependence on importance function (IS) vs. on previous value (MCMC)
- Unbiasedness (IS) vs. convergence to the true distribution (MCMC)
- Variance control (IS) vs. learning costs (MCMC)
- Recycling of past simulations (IS) vs. progressive adaptability (MCMC)
- Processing of moving targets (IS) vs. handling large dimensional problems (MCMC)
- **Non-asymptotic validity (IS) vs. difficult asymptotia for adaptive algorithms (MCMC)**

Dynamic importance sampling

Idea

It is possible to generalise importance sampling using random weights ω_t such that

$$\mathbb{E}[\omega_t | x_t] = \pi(x_t)/g(x_t)$$

(a) Self-regenerative chains

[Sahu & Zhigljavsky, 1998; Gasemyr, 2002]

Proposal

$$Y \sim p(y) \propto \tilde{p}(y)$$

and target distribution $\pi(y) \propto \tilde{\pi}(y)$
Ratios

$$\omega(x) = \pi(x)/p(x) \quad \text{and} \quad \tilde{\omega}(x) = \tilde{\pi}(x)/\tilde{p}(x)$$

Unknown **Known**

Acceptance function

$$\alpha(x) = \frac{1}{1 + \kappa\tilde{\omega}(x)} \qquad \kappa > 0$$

Geometric jumps

Theorem

If

$$Y \sim p(y)$$

and

$$W|Y = y \sim \mathscr{G}(\alpha(y))\,,$$

then

$$X_t = \cdots = X_{t+W-1} = Y \neq X_{t+W}$$

defines a Markov chain with stationary distribution π

Plusses

- Valid for any choice of κ [κ small = large variance and κ large = slow convergence]
- Only depends on current value [Difference with Metropolis]
- Random integer weight W [Similarity with Metropolis]
- Saves on the rejections: always accept [Difference with Metropolis]
- Introduces geometric noise compared with importance sampling

$$\sigma^2_{SZ} = 2\,\sigma^2_{IS} + (1/\kappa)\sigma^2_{\pi}$$

- Can be used with a sequence of proposals p_k and constants κ_k [Adaptativity]

A generalisation

[Gåsemyr, 2002]

Proposal density $p(y)$ and probability $q(y)$ of accepting a jump.

Algorithm (Gåsemyr's dynamic weights)

Generate a sequence of random weights W_n by

1. Generate $Y_n \sim p(y)$
2. Generate $V_n \sim \mathcal{B}(q(y_n))$
3. Generate $S_n \sim \mathcal{G}eo(\alpha(y_n))$
4. Take $W_n = V_n S_n$

Validation

▸ direct to PMC

$$\phi(y) = \frac{p(y)q(y)}{\int p(y)q(y)dy}\,,$$

the chain (X_t) associated with the sequence (Y_n, W_n) by

$$Y_1 = X_1 = \cdots = X_{1+W_1-1}, Y_2 = X_{1+W_1} = \cdots$$

is a Markov chain with transition

$$K(x, y) = \alpha(x)\phi(y)$$

which has a point mass at $y = x$ with weight $1 - \alpha(x)$.

Ergodicity for Gåsemyr's scheme

Necessary and sufficient condition

π is stationary for (X_t) iff

$$\alpha(y) = q(y)/(\kappa\pi(y)/p(y)) = q(y)/(\kappa w(y))$$

for some constant κ.

Implies that

$$\mathbb{E}[W^n|Y^n = y] = \kappa w(y)\,.$$

[Average importance sampling]

Special case: $\alpha(y) = 1/(1+\kappa w(y))$ of Sahu and Zhigljavski (2001)

Properties

Constraint on κ: for $\alpha(y) \leq 1$, κ must be such that

$$\frac{p(y)q(y)}{\pi(y)} \leq \kappa$$

Reverse of accept-reject conditions (!)
Variance of

$$\sum_n W_n h(Y_n) / \sum_n W_n \tag{4}$$

is

$$2 \int \frac{(h(y) - \mu)^2}{q(y)} w(y)\pi(y)dy - (1/\kappa)\sigma_\pi^2 \,,$$

by Cramer-Wold/Slutsky
Still worse than importance sampling.

(b) Dynamic weighting

[Wong & Liang, 1997; Liu, Liang & Wong, 2001; Liang, 2002]

▸ direct to PMC

Generalisation of the above: simultaneous generation of points and weights, (θ_t, ω_t), under the constraint

$$\mathbb{E}[\omega_t|\theta_t] \propto \pi(\theta_t) \tag{5}$$

Same use as importance sampling weights

Algorithm (Liang's dynamic importance sampling)

1. Generate $y \sim K(x, y)$ and compute

$$\varrho = \omega \, \frac{\pi(y)K(y, x)}{\pi(x)K(x, y)}$$

2. Generate $u \sim \mathcal{U}(0, 1)$ and take

$$(x', \omega') = \begin{cases} (y, (1+\delta)\varrho/a) & \text{if } u < a \\ (x, (1+\delta)\omega/(1-a)) & \text{otherwise} \end{cases}$$

where $a = \varrho/(\varrho + \theta)$, $\theta = \theta(x, \omega)$, and $\delta > 0$ constant or independent rv

Preservation of the equilibrium equation

If g_- and g_+ denote the distributions of the augmented variable (X, W) before the step and after the step, respectively, then

$$
\begin{aligned}
&\int_0^\infty \omega' \, g_+(x', \omega') \, d\omega' = \\
&\int (1+\delta) \left[\varrho(\omega, x, x') + \theta\right] \, g_-(x, \omega) \, K(x, x') \, \frac{\varrho(\omega, x, x')}{\varrho(\omega, x, x') + \theta} \, dx \, d\omega \\
&+ \int (1+\delta) \, \frac{\omega(\varrho(\omega, x', z) + \theta)}{\theta} \, g_-(x', \omega) \, K(x, z) \, \frac{\theta}{\varrho(\omega, x', z) + \theta} \, dz \, d\omega \\
&= (1+\delta) \left\{ \int \omega \, g_-(x, \omega) \, \frac{\pi(x') K(x', x)}{\pi(x)} \, dx \, d\omega \right. \\
&\left. + \int \omega \, g_-(x', \omega) \, K(x', z) \, dz \, d\omega \right\} \\
&= (1+\delta) \left\{ \pi(x') \int c_0 \, K(x', x) \, dx + c_0 \pi(x') \right\} \\
&= 2(1+\delta) c_0 \pi(x') \,,
\end{aligned}
$$

where c_0 proportionality constant

Expansion phenomenon

$$\mathbb{E}[\omega_{t+1}] = 2(1+\delta)\mathbb{E}[\omega_t]$$

Special case: R-move

[Liang, 2002]

$\delta = 0$ and $\theta \equiv 1$, and thus

$$(x', \omega') = \begin{cases} (y, \varrho + 1) & \text{if } u < \varrho/(\varrho + 1) \\ (x, \omega(\varrho + 1)) & \text{otherwise,} \end{cases}$$

[Importance sampling]

Special case: W-move

$\theta \equiv 0$, thus $a = 1$ and

$$(x', \omega') = (y, \varrho)\,.$$

Q-move

[Liu & al, 2001]

$$(x', \omega') = \begin{cases} (y, \theta \vee \varrho) & \text{if } u < 1 \wedge \varrho/\theta\,, \\ (x, a\omega) & \text{otherwise,} \end{cases}$$

with $a \geq 1$ either a constant or an independent random variable.

Notes

- Updating step in Q and R schemes written as

$$(x_{t+1}, \omega_{t+1}) = \{x_t, \omega_t / \mathsf{Pr}(R_t = 0)\}$$

with probability $\mathsf{Pr}(R_t = 0)$ and

$$(x_{t+1}, \omega_{t+1}) = \{y_{t+1}, \omega_t r(x_t, y_{t+1}) / \mathsf{Pr}(R_t = 1)\}$$

with probability $\mathsf{Pr}(R_t = 1)$, where R_t is the move indicator and

$$y_{t+1} \sim K(x_t, y)$$

Notes (2)

- Geometric structure of the weights

$$\Pr(R_t = 0) = \frac{\omega_t}{\omega_{t+1}}\,.$$

and

$$\Pr(R_t = 0) = \frac{\omega_t\, r(x_t, y_t)}{\omega_t\, r(x_t, y_t) + \theta}, \quad \theta > 0\,,$$

for the R scheme

- Number of steps T before an acceptance (a jump) such that

$$\begin{aligned}\Pr\left(T \geq t\right) &= P(R_1 = 0, \ldots, R_{t-1} = 0) \\ &= \mathbb{E}\left[\prod_{j=0}^{t-1} \frac{\omega_j}{\omega_{j+1}}\right] \propto \mathbb{E}[1/\omega_t]\,.\end{aligned}$$

Alternative scheme

Preservation of weight expectation:

$$(x_{t+1}, \omega_{t+1}) = \begin{cases} (x_t, \alpha_t \omega_t / \mathsf{Pr}(R_t = 0)) \\ \quad \text{with probability } \mathsf{Pr}(R_t = 0) \text{ and} \\ (y_{t+1}, (1 - \alpha_t)\omega_t r(x_t, y_{t+1}) / \mathsf{Pr}(R_t = 1)) \\ \quad \text{with probability } \mathsf{Pr}(R_t = 1). \end{cases}$$

Alternative scheme (2)

Then

$$\begin{aligned}\Pr(T=t) &= P(R_1=0,\ldots,R_{t-1}=0,R_t=1)\\ &= \mathbb{E}\left[\prod_{j=0}^{t-1}\alpha_j\frac{\omega_j}{\omega_{j+1}}(1-\alpha_t)\frac{\omega_{t-1}r(x_0,Y_t)}{\omega_t}\right]\end{aligned}$$

which is equal to

$$\alpha^{t-1}(1-\alpha)\mathbb{E}[\omega_o\, r(x,Y_t)/\omega_t]$$

when α_j constant and deterministic.

Example

Choose a function $0 < \beta(\cdot, \cdot) < 1$ and to take, while in (x_0, ω_0),

$$(x_1, \omega_1) = \left(y_1, \frac{\omega_0 r(x_0, y_1)}{\alpha(x_0, y_1)} (1 - \beta(x_0, y_1) \right)$$

with probability

$$\min(1, \omega_0 r(x_0, y_1)) \stackrel{\Delta}{=} \alpha(x_0, y_1)$$

and

$$(x_1, \omega_1) = \left(x_0, \frac{\omega_0}{1 - \alpha(x_0, y_1)} \times \beta(x_0, y_1) \right)$$

with probability $1 - \alpha(x_0, y_1)$.

Population Monte Carlo

Idea

Simulate from the product distribution

$$\pi^{\bigotimes n}(x_1, \ldots, x_n) = \prod_{i=1}^{n} \pi(x_i)$$

and apply dynamic importance sampling to the sample (*a.k.a.* population)

$$\mathbf{x}^{(t)} = (x_1^{(t)}, \ldots, x_n^{(t)})$$

Iterated importance sampling

As in Markov Chain Monte Carlo (MCMC) algorithms, introduction of a *temporal dimension* :

$$x_i^{(t)} \sim q_t(x|x_i^{(t-1)}) \qquad i = 1, \ldots, n, \quad t = 1, \ldots$$

and

$$\hat{\mathfrak{I}}_t = \frac{1}{n} \sum_{i=1}^{n} \varrho_i^{(t)} h(x_i^{(t)})$$

is still unbiased for

$$\varrho_i^{(t)} = \frac{\pi_t(x_i^{(t)})}{q_t(x_i^{(t)}|x_i^{(t-1)})}, \qquad i = 1, \ldots, n$$

Fundamental importance equality

Preservation of unbiasedness

$$\mathbb{E}\left[h(X^{(t)})\ \frac{\pi(X^{(t)})}{q_t(X^{(t)}|X^{(t-1)})}\right]$$
$$= \int h(x)\,\frac{\pi(x)}{q_t(x|y)}\,q_t(x|y)\,g(y)\,dx\,dy$$
$$= \int h(x)\,\pi(x)\,dx$$

for **any distribution** g on $X^{(t-1)}$

Sequential variance decomposition

Furthermore,

$$\operatorname{var}\left(\hat{\mathfrak{I}}_t\right) = \frac{1}{n^2} \sum_{i=1}^{n} \operatorname{var}\left(\varrho_i^{(t)} h(x_i^{(t)})\right) ,$$

if $\operatorname{var}\left(\varrho_i^{(t)}\right)$ exists, because the $x_i^{(t)}$'s are conditionally uncorrelated

Note

This decomposition is still valid for correlated [in i] $x_i^{(t)}$'s when incorporating weights $\varrho_i^{(t)}$

Simulation of a population

The importance distribution of the sample (*a.k.a.* particles) $\mathbf{x}^{(t)}$

$$q_t(\mathbf{x}^{(t)}|\mathbf{x}^{(t-1)})$$

can depend on the previous sample $\mathbf{x}^{(t-1)}$ in any possible way as long as marginal distributions

$$q_{it}(x) = \int q_t(\mathbf{x}^{(t)})\, d\mathbf{x}_{-i}^{(t)}$$

can be expressed to build importance weights

$$\varrho_{it} = \frac{\pi(x_i^{(t)})}{q_{it}(x_i^{(t)})}$$

Special case of the product proposal

If

$$q_t(\mathbf{x}^{(t)}|\mathbf{x}^{(t-1)}) = \prod_{i=1}^{n} q_{it}(x_i^{(t)}|\mathbf{x}^{(t-1)})$$

[Independent proposals]

then

$$\text{var}\left(\hat{\mathfrak{I}}_t\right) = \frac{1}{n^2} \sum_{i=1}^{n} \text{var}\left(\varrho_i^{(t)} h(x_i^{(t)})\right) ,$$

Validation

skip validation

$$\begin{aligned}
&\mathbb{E}\left[\varrho_i^{(t)} h(X_i^{(t)})\ \ \varrho_j^{(t)} h(X_j^{(t)})\right] \\
&\quad = \int h(x_i) \frac{\pi(x_i)}{q_{it}(x_i|\mathbf{x}^{(t-1)})} \frac{\pi(x_j)}{q_{jt}(x_j|\mathbf{x}^{(t-1)})} h(x_j) \\
&\qquad\qquad q_{it}(x_i|\mathbf{x}^{(t-1)})\, q_{jt}(x_j|\mathbf{x}^{(t-1)})\, dx_i\, dx_j\, g(\mathbf{x}^{(t-1)}) d\mathbf{x}^{(t-1)} \\
&\quad = \mathbb{E}_\pi\left[h(X)\right]^2
\end{aligned}$$

whatever the distribution g on $\mathbf{x}^{(t-1)}$

Self-normalised version

In general, π is unscaled and the weight

$$\varrho_i^{(t)} \propto \frac{\pi(x_i^{(t)})}{q_{it}(x_i^{(t)})}\,, \qquad i = 1, \ldots, n\,,$$

is scaled so that

$$\sum_i \varrho_i^{(t)} = 1$$

Self-normalised version properties

- Loss of the unbiasedness property and the variance decomposition
- Normalising constant can be estimated by

$$\varpi_t = \frac{1}{tn} \sum_{\tau=1}^{t} \sum_{i=1}^{n} \frac{\pi(x_i^{(\tau)})}{q_{i\tau}(x_i^{(\tau)})}$$

- Variance decomposition (approximately) recovered if ϖ_{t-1} is used instead

Sampling importance resampling

Importance sampling from g can **also** produce samples from the target π

[Rubin, 1987]

Theorem (Bootstraped importance sampling)

If a sample $(x_i^\star)_{1\leq i\leq m}$ is derived from the weighted sample $(x_i, \varrho_i)_{1\leq i\leq n}$ by multinomial sampling with weights ϱ_i, then

$$x_i^\star \sim \pi(x)$$

Note

Obviously, the $x_i^\star$'s are **not iid**

Iterated sampling importance resampling

This principle can be extended to iterated importance sampling:
After each iteration, resampling produces a sample from π
[Again, not iid!]

Incentive

Use previous sample(s) to learn about π and q

Generic Population Monte Carlo

Algorithm (Population Monte Carlo Algorithm)

For $t = 1, \ldots, T$

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

1. Select the generating distribution $q_{it}(\cdot)$
2. Generate $\tilde{x}_i^{(t)} \sim q_{it}(x)$
3. Compute $\varrho_i^{(t)} = \pi(\tilde{x}_i^{(t)})/q_{it}(\tilde{x}_i^{(t)})$

Normalise the $\varrho_i^{(t)}$'s into $\bar{\varrho}_i^{(t)}$'s

Generate $J_{i,t} \sim \mathcal{M}((\bar{\varrho}_i^{(t)})_{1 \le i \le N})$ and set $x_{i,t} = \tilde{x}_{J_{i,t}}^{(t)}$

D-kernels in competition

A general adaptive construction:

Construct $q_{i,t}$ as a mixture of D different transition kernels depending on $x_i^{(t-1)}$

$$q_{i,t} = \sum_{\ell=1}^{D} p_{t,\ell} \mathfrak{K}_\ell(x_i^{(t-1)}, x), \qquad \sum_{\ell=1}^{D} p_{t,\ell} = 1\,,$$

and adapt the weights $p_{t,\ell}$.

Example

Take $p_{t,\ell}$ proportional to the survival rate of the points (*a.k.a.* particles) $x_i^{(t)}$ generated from $\mathfrak{K}_\ell$

Implementation

Algorithm (D-kernel PMC)

For $t = 1, \ldots, T$

generate $(K_{i,t})_{1 \leq i \leq N} \sim \mathscr{M}((p_{t,k})_{1 \leq k \leq D})$

for $1 \leq i \leq N$, generate

$$\tilde{x}_{i,t} \sim \mathfrak{K}_{K_{i,t}}(x)$$

compute and renormalize the importance weights $\omega_{i,t}$

generate $(J_{i,t})_{1 \leq i \leq N} \sim \mathscr{M}((\overline{\omega}_{i,t})_{1 \leq i \leq N})$

take $x_{i,t} = \tilde{x}_{J_{i,t},t}$ and $p_{t+1,d} = \sum_{i=1}^{N} \bar{\omega}_{i,t} \mathbb{I}_d(K_{i,t})$

Links with particle filters

- Usually setting where $\pi = \pi_t$ changes with t: Population Monte Carlo also adapts to this case
- Can be traced back all the way to Hammersley and Morton (1954) and the self-avoiding random walk problem
- Gilks and Berzuini (2001) produce iterated samples with (SIR) resampling steps, and add an MCMC step: this step must use a π_t invariant kernel
- Chopin (2001) uses iterated importance sampling to handle large datasets: this is a special case of PMC where the q_{it}'s are the posterior distributions associated with a portion k_t of the observed dataset

Links with particle filters (2)

- Rubinstein and Kroese's (2004) *cross-entropy* method is parameterised importance sampling targeted at rare events
- Stavropoulos and Titterington's (1999) *smooth bootstrap* and Warnes' (2001) *kernel coupler* use nonparametric kernels on the previous importance sample to build an improved proposal: this is a special case of PMC
- West (1992) mixture approximation is a precursor of smooth bootstrap
- Mengersen and Robert (2002) "pinball sampler" is an MCMC attempt at population sampling
- Del Moral and Doucet (2003) sequential Monte Carlo samplers also relates to PMC, with a Markovian dependence on the past sample $\mathbf{x}^{(t)}$ but (limited) stationarity constraints

Things can go wrong

Unexpected behaviour of the mixture weights when the number of particles increases

$$\sum_{i=1}^{N} \bar{\omega}_{i,t} \mathbb{I}_{K_{i,t}=d} \longrightarrow P \frac{1}{D}$$

Conclusion

At *each* iteration, every weight converges to $1/D$:
the algorithm fails to learn from experience!!

Saved by Rao-Blackwell!!

Modification: Rao-Blackwellisation (=conditioning)

Use the whole mixture in the importance weight:

$$\omega_{i,t} = \pi(\tilde{x}_{i,t}) \sum_{d=1}^{D} p_{t,d} \mathfrak{K}_d(x_{i,t-1}, \tilde{x}_{i,t})$$

instead of

$$\omega_{i,t} = \frac{\pi(\tilde{x}_{i,t})}{\mathfrak{K}_{K_{i,t}}(x_{i,t-1}, \tilde{x}_{i,t})}$$

Adapted algorithm

Algorithm (Rao-Blackwellised D-kernel PMC)

At time t ($t = 1, \ldots, T$),

Generate
$$(K_{i,t})_{1 \leq i \leq N} \overset{iid}{\sim} \mathcal{M}((p_{t,d})_{1 \leq d \leq D});$$

Generate
$$(\tilde{x}_{i,t})_{1 \leq i \leq N} \overset{\text{ind}}{\sim} \mathfrak{K}_{K_{i,t}}(x_{i,t-1}, x)$$

and set $\omega_{i,t} = \pi(\tilde{x}_{i,t}) \Big/ \sum_{d=1}^{D} p_{t,d} \mathfrak{K}_d(x_{i,t-1}, \tilde{x}_{i,t})$;

Generate
$$(J_{i,t})_{1 \leq i \leq N} \overset{iid}{\sim} \mathcal{M}((\bar{\omega}_{i,t})_{1 \leq i \leq N})$$

and set $x_{i,t} = \tilde{x}_{J_{i,t},t}$ and $p_{t+1,d} = \sum_{i=1}^{N} \bar{\omega}_{i,t} p_{t,d}$.

Convergence properties

Theorem (LLN)

Under regularity assumptions, for $h \in L^1_\Pi$ *and for every* $t \geq 1$,

$$\frac{1}{N}\sum_{k=1}^{N} \bar{\omega}_{i,t} h(x_{i,t}) \overset{N\to\infty}{\longrightarrow}_P \Pi(h)$$

and

$$p_{t,d} \overset{N\to\infty}{\longrightarrow}_P \alpha_d^t$$

The limiting coefficients $(\alpha_d^t)_{1\leq d\leq D}$ *are defined recursively as*

$$\alpha_d^t = \alpha_d^{t-1} \int \left(\frac{\mathfrak{K}_d(x,x')}{\sum_{j=1}^{D} \alpha_j^{t-1} \mathfrak{K}_j(x,x')} \right) \Pi \otimes \Pi(dx, dx').$$

Recursion on the weights

Set F as

$$F(\alpha) = \left(\alpha_d \int \left[\frac{\mathfrak{K}_d(x, x')}{\sum_{j=1}^{D} \alpha_j \mathfrak{K}_j(x, x')} \right] \Pi \otimes \Pi(dx, dx') \right)_{1 \le d \le D}$$

on the simplex

$$S = \left\{ \alpha = (\alpha_1, \ldots, \alpha_D);\ \forall d \in \{1, \ldots, D\},\ \alpha_d \ge 0 \quad \text{and} \sum_{d=1}^{D} \alpha_d = 1 \right\}.$$

and define the sequence

$$\boldsymbol{\alpha}^{t+1} = F(\boldsymbol{\alpha}^t)$$

Kullback divergence

Definition (Kullback divergence)

For $\alpha \in S$,

$$\mathrm{KL}(\boldsymbol{\alpha}) = \int \left[\log \left(\frac{\pi(x)\pi(x')}{\pi(x) \sum_{d=1}^{D} \alpha_d \mathfrak{K}_d(x, x')} \right) \right] \Pi \otimes \Pi(dx, dx').$$

Kullback divergence between Π and the mixture.

Goal: Obtain the mixture closest to Π, i.e., that minimises $\mathrm{KL}(\boldsymbol{\alpha})$

Connection with RBDPMCA ??

Theorem

Under the assumption

$$\forall d \in \{1, \ldots, D\}, -\infty < \int \log(\mathfrak{K}_d(x, x'))\Pi \otimes \Pi(dx, dx') < \infty$$

for every $\boldsymbol{\alpha} \in \mathfrak{S}_D$,

$$KL(F(\boldsymbol{\alpha})) \leq KL(\boldsymbol{\alpha}).$$

Conclusion

The Kullback divergence decreases at every iteration of RBDPMCA

An integrated EM interpretation

skip interpretation

We have

$$\boldsymbol{\alpha}^{\min} = \arg\min_{\boldsymbol{\alpha}\in S} KL(\boldsymbol{\alpha}) = \arg\max_{\boldsymbol{\alpha}\in S} \int \log p_{\boldsymbol{\alpha}}(\bar{x})\Pi\otimes\Pi(d\bar{x})$$
$$= \arg\max_{\boldsymbol{\alpha}\in S} \int \log \int p_{\boldsymbol{\alpha}}(\bar{x},K)dK\,\Pi\otimes\Pi(d\bar{x})$$

for $\bar{x} = (x, x')$ and $K \sim \mathcal{M}((\alpha_d)_{1\le d\le D})$. Then $\boldsymbol{\alpha}^{t+1} = F(\boldsymbol{\alpha}^t)$ means

$$\boldsymbol{\alpha}^{t+1} = \arg\max_{\boldsymbol{\alpha}} \iint \mathbb{E}_{\boldsymbol{\alpha}^t}(\log p_{\boldsymbol{\alpha}}(\bar{X},K)|\bar{X}=\bar{x})\Pi\otimes\Pi(d\bar{x})$$

and

$$\lim_{t\to\infty} \boldsymbol{\alpha}^t = \boldsymbol{\alpha}^{\min}$$

Illustration

Example (A toy example)

Take the target

$$1/4\mathcal{N}(-1, 0.3)(x) + 1/4\mathcal{N}(0, 1)(x) + 1/2\mathcal{N}(3, 2)(x)$$

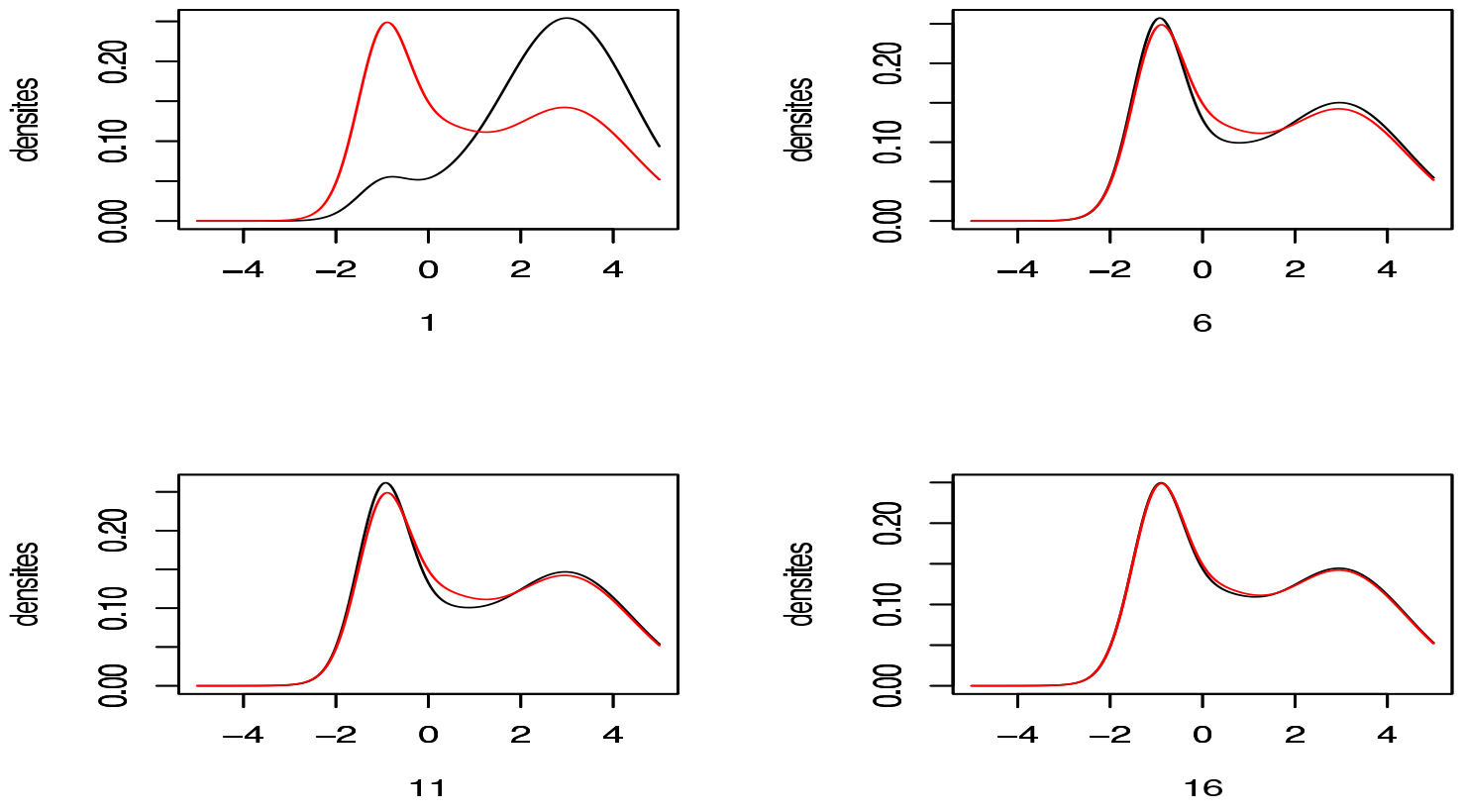
and use 3 proposals: $\mathcal{N}(-1, 0.3)$, $\mathcal{N}(0, 1)$ and $\mathcal{N}(3, 2)$

[Surprise!!!]

Then

1	0.0500000	0.05000000	0.9000000
2	0.2605712	0.09970292	0.6397259
6	0.2740816	0.19160178	0.5343166
10	0.2989651	0.19200904	0.5090259
16	0.2651511	0.24129039	0.4935585

Weight evolution



Target and mixture evolution

Example : PMC for mixtures

Observation of an iid sample $\mathbf{x} = (x_1, \ldots, x_n)$ from

$$p\mathcal{N}(\mu_1, \sigma^2) + (1-p)\mathcal{N}(\mu_2, \sigma^2),$$

with $p \neq 1/2$ and $\sigma > 0$ known.
Usual $\mathcal{N}(\theta, \sigma^2/\lambda)$ prior on μ_1 and μ_2:

$$\pi(\mu_1, \mu_2|\mathbf{x}) \propto f(\mathbf{x}|\mu_1, \mu_2)\, \pi(\mu_1, \mu_2)$$

Algorithm (Mixture PMC)

Step 0: Initialisation

For $j = 1, \ldots, n = pm$, choose $(\mu_1)_j^{(0)}, (\mu_2)_j^{(0)}$

For $k = 1, \ldots, p$, set $r_k = m$

Step i: Update $(i = 1, \ldots, I)$

For $k = 1, \ldots, p$,

1. generate a sample of size r_k as

$$(\mu_1)_j^{(i)} \sim \mathcal{N}\left((\mu_1)_j^{(i-1)}, v_k\right) \quad \text{and} \quad (\mu_2)_j^{(i)} \sim \mathcal{N}\left((\mu_2)_j^{(i-1)}, v_k\right)$$

2. compute the weights

$$\varrho_j \propto \frac{f\left(\mathbf{x} \middle| (\mu_1)_j^{(i)}, (\mu_2)_j^{(i)}\right) \pi\left((\mu_1)_j^{(i)}, (\mu_2)_j^{(i)}\right)}{\varphi\left((\mu_1)_j^{(i)} \middle| (\mu_1)_j^{(i-1)}, v_k\right) \varphi\left((\mu_2)_j^{(i)} \middle| (\mu_2)_j^{(i-1)}, v_k\right)}$$

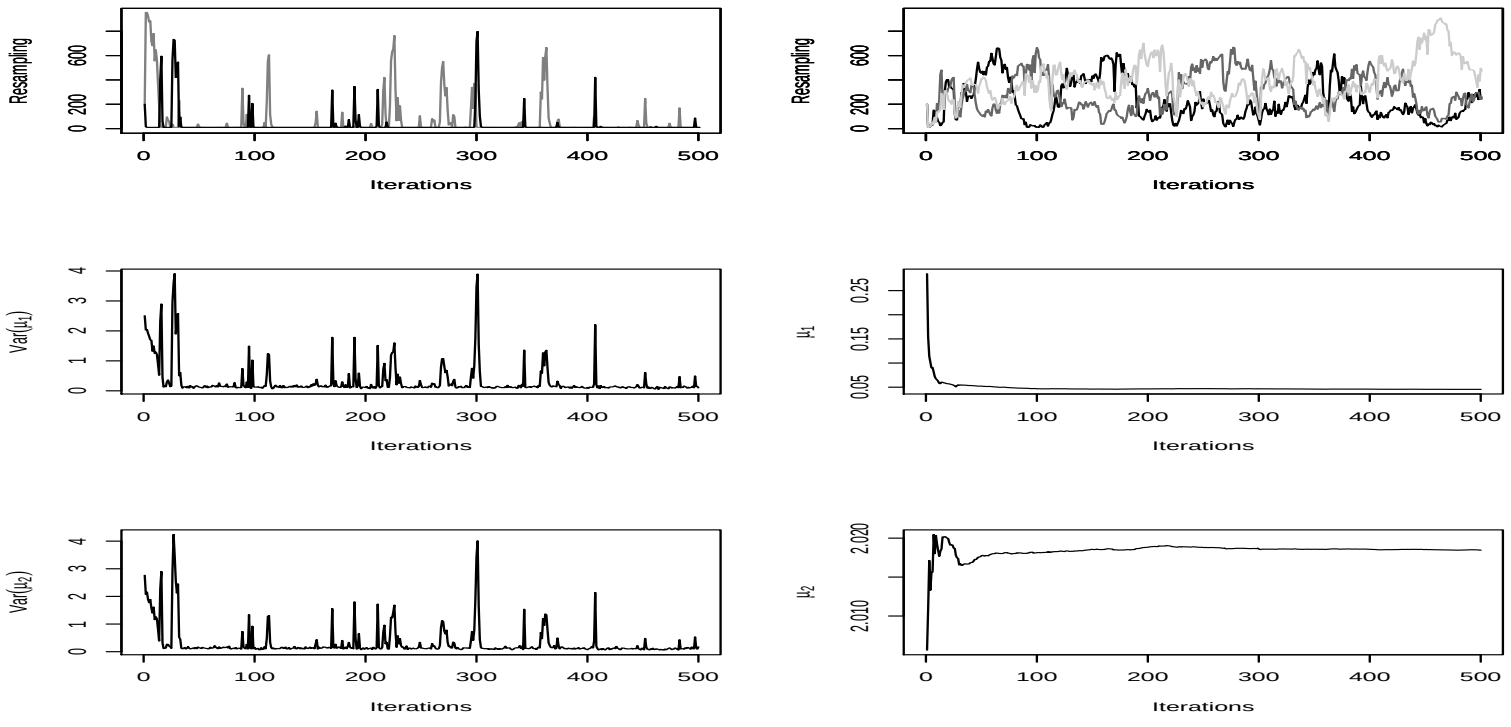
Resample the $\left((\mu_1)_j^{(i)}, (\mu_2)_j^{(i)}\right)_j$ using the weights ϱ_j,

Details

After an arbitrary initialisation, use of the previous (importance) sample (after resampling) to build random walk proposals,

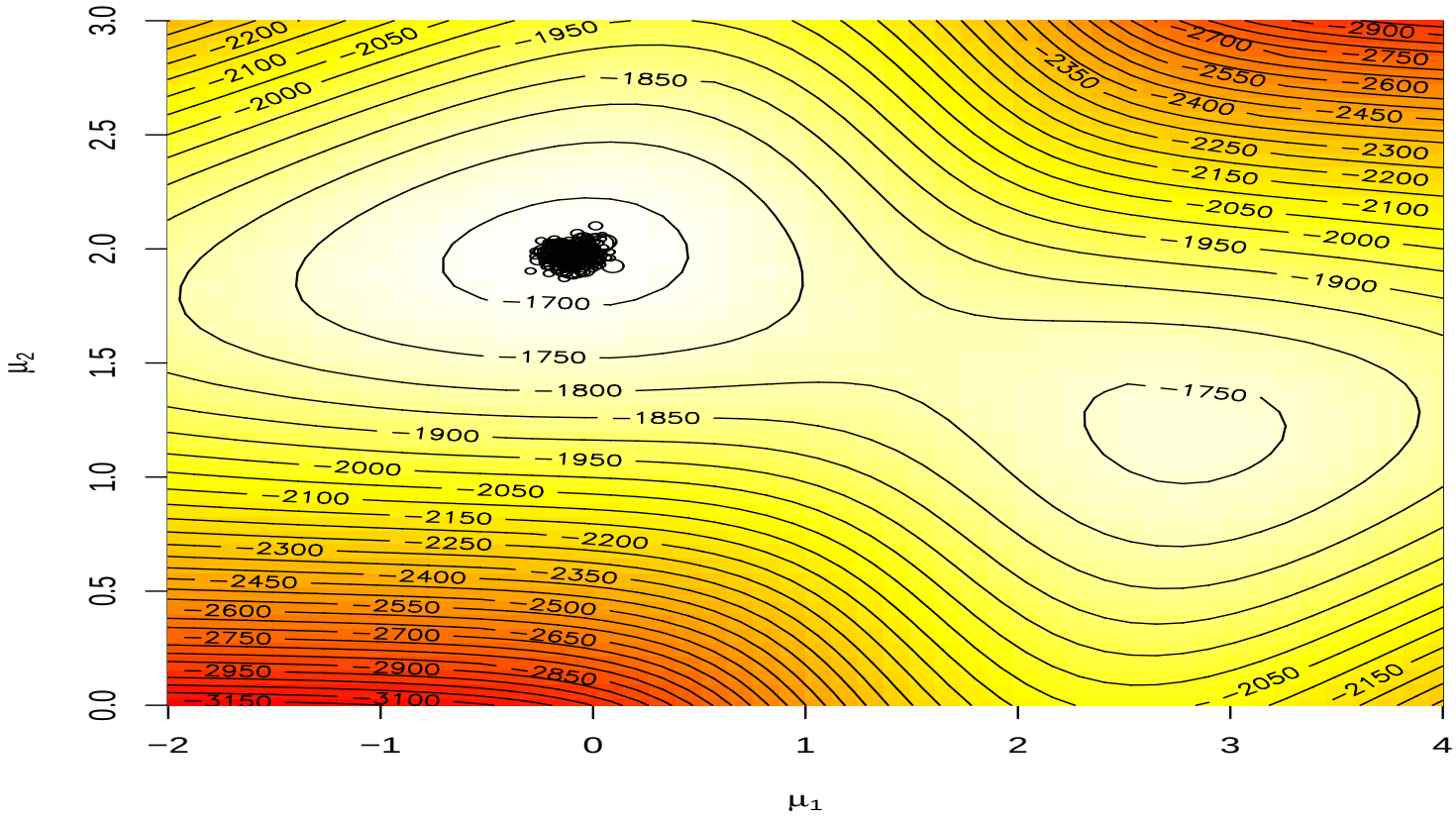
$$\mathcal{N}((\mu)_j^{(i-1)}, v_j)$$

with a multiscale variance v_j within a predetermined set of p scales ranging from 10^3 down to 10^{-3}, whose importance is proportional to its survival rate in the resampling step.



(u.left)

Number of resampled points for $v_1 = 5$ (darker) and $v_2 = 2$; *(u.right)* Number of resampled points for the other variances; *(m.left)* Variance of the μ_1's along iterations; *(m.right)* Average of the μ_1's over iterations; *(l.left)* Variance of the μ_2's along iterations; *(l.right)* Average of the simulated μ_2's over iterations.



Log-posterior distribution and sample of means