Introduction to Bayesian analysis for medical studies – Part II: Bayesian computation

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Introduction

Estimating the *posterior* distribution is often costly

Bayesian computational statistics

Computational aspects of Bayesian inference can get sophisticated but are key to its successful application

Numerical integration – I

Real world applications: $\boldsymbol{\theta} = (\theta_1, \dots, \theta_d)$

⇒ joint *posterior* distribution of all d parameters

⚠ hard to compute:

- complexe likelihood
- integrating constant $f(\boldsymbol{y}) = \int_{\Theta^d} f(\boldsymbol{y}|\boldsymbol{\theta})\pi(\boldsymbol{\theta})\,\mathrm{d}\boldsymbol{\theta}$
- ...

Analytical form rarely available

⇒ numerical computations: integral of d multiplicity
– difficult when d is big (numerical issues as soon as $d > 4$)

Numerical integration – II

Even dimension 1 can be tough !

Example :

Let $x_1,\dots,x_n$ *iid* according to a Cauchy distribution $\mathscr{C}(\theta,1)$ with *prior* $\pi(\theta)=\mathcal{N}(\mu,\sigma^2)$ (μ and σ known)

$$\begin{aligned} p(\theta|x_1,\dots,x_n) &\propto f(x_1,\dots,x_n|\theta)\pi(\theta) \\ &\propto e^{-\frac{(\theta-\mu)^2}{2\sigma^2}}\prod_{i=1}^{n}(1+(x_i-\theta)^2)^{-1} \end{aligned}$$

⚠ normalizing constant has no analytical form ⇒ no analytical form for this *posterior* distibution

Marginal *posterior* distributions

Objective: draw conclusion based on the joint *posterior* distribution

⇒ probability of all possible values for each parameter (i.e. their marginal distribution – uni-dimensional)

⚠ Recovering all of the *posterior* density **numerically** requires the calculation of multidimensional integrals **for each possible value of the parameter**

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Algorithms based on **sampling simulations**
especially **Markov chain Monte Carlo** (MCMC)

Computational solutions

Bayes Theorem ⇒ *posterior* distribution

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How can one estimate the *posteriori* distribution ?

⇒ sample according to this posterior distribution

- direct **sampling**
- **Markov chain Monte Carlo** (MCMC)

Monte Carlo method

Monte Carlo : von Neumann & Ulam

(*Los Alamos Scientific Laboratory* – 1955)

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- **Law of Large Numbers** (LLN)
- so-called "**Monte Carlo sample**"

⇒ compute various functions from that sample distribution

Example : One wants to compute $\mathbb{E}[f(X)] = \int f(x) p_X(x) dx$

If $x_i \overset{iid}{\sim} p_X$, $\mathbb{E}[f(X)] = \frac{1}{N}\sum_{i=1}^{N} f(x_i)$ (LLN)

⇒ if one knows how to sample from p_X, one can then estimate $\mathbb{E}[f(X)]$

...

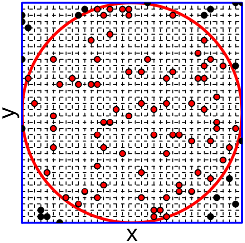
Monte Carlo method: illustration

π estimation:

Monte Carlo method: illustration

π estimation:

A casino *roulette* (in Monte Carlo ?)



A 36×36 grid

1. The probability of being inside the disk while in the square: $p_C = \frac{\pi R^2}{(2R)^2} = \frac{\pi}{4}$
2. n points $\{(x_{11},x_{21}),\dots,(x_{1n},x_{2n})\} = \{P_1,\dots,P_n\}$ on the 36×36 grid (generated with the *roulette*)
3. Count the number of points inside the disk

⇒ Compute the ratio (estimated probability of being inside the disk while in the square): $\widehat{p}_C = \frac{\sum P_i \in circle}{n}$

Monte Carlo method: illustration

π estimation:

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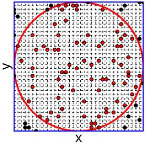

A 36×36 grid

If $n = 1000$ and 786 points are inside the disk : $\widehat{\pi} = 4 \times \frac{786}{1000} = 3.144$

One can improve the estimate by increasing:

- the **grid resolution**, and also
- the number of points sampled n: $\lim\limits_{n \to +\infty} \widehat{p}_C = p_C = \pi/4$ (LLN)

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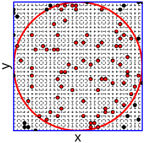

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Monte Carlo sample ⇒ compute various functions
e.g. π = 4 × the probability of being inside the disk

Your turn !

Practical: exercise 1

Direct sampling methods

Random & pseudo-random numbers

There exist several ways to generate so-called “random” numbers according to known distributions

NB: computer programs do not generate truly random numbers

Rather **pseudo-random**, which seem random but are actually generated by a deterministic process (depending on a “**seed**” parameter).

Uniform sample generation

Linear congruential algorithm: sample pseudo-random numbers according to the Uniform distribution on $[0,1]$ (Lehmer, 1948)

1. Generate a sequence of integers y_n such as:
   $y_{n+1} = (ay_n + b)$ mod. m
2. $x_n = \frac{y_n}{m-1}$

choose a, b and m so that y_n has a long period & $(x_1,\dots,x_n)$ can be considered *iid*

with y_0 the seed

<u>*Remark:*</u> $0 \leq y_n \leq m-1 \Rightarrow$ in practice m very large (e.g. 2^{19937}, default in R which uses the Mersenne-Twister variation)

In the following, sampling pseudo-random numbers uniformly on $[0,1]$ will be considered reliable and used by the different sampling algorithms

Other usual distributions

Relying on **relationships between the different usual distributions** starting from $U_i \sim \mathcal{U}_{[0,1]}$

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Binomial $Bin(n,p)$:

$$Y_i = \mathbb{1}_{U_i \leq p} \sim \text{Bernoulli}(p)$$
$$X = \sum_{i=1}^{n} Y_i \sim Bin(n,p)$$

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Normal $\mathcal{N}(0,1)$ (Box-Müller algorithm):

U_1 and U_2 are 2 independent uniform variables on $[0;1]$

$$Y_1 = \sqrt{-2\log U_1}\cos(2\pi U_2)$$
$$Y_2 = \sqrt{-2\log U_1}\sin(2\pi U_2)$$

⇒ Y_1 & Y_2 are independent random variables each following a $\mathcal{N}(0,1)$

Inverse transform sampling

Definition: For a function F defined on $\mathbb{R}$, its **generalized inverse** is defined as: $F^{-1}(u) = \inf\{x \text{ tq } F(x) > u\}$

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Property: Let

- F be a cumulative probability distribution function
- U be a uniform random variable on $[0,1]$

Then $F^{-1}(U)$ defines a random variable whith cumulative probability distribution function F

If

1. one knows F, the cumulative probability distribution function from which to sample
2. one can invert F

⇒ then one can sample this distribution from a uniform sample on $[0,1]$

Inverse transform sampling: illustration

Example: sample from the Exponential distribution with parameter λ

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- density of the Exponential distribution: $f(x) = \lambda \exp(-\lambda x)$
- its cumulative probability distribution function (its integral): $F(x) = 1 - \exp(-\lambda x)$

Let $F(x) = u$

Then $x = \dots$

Inverse transform sampling: illustration

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- density of the Exponential distribution: $f(x) = \lambda \exp(-\lambda x)$
- its cumulative probability distribution function (its integral): $F(x) = 1 - \exp(-\lambda x)$

Let $F(x) = u$

Then $x = -\dfrac{1}{\lambda} \log(1-u)$

$\Rightarrow$ and if $U \sim U_{[0;1]}$, then $X = F^{-1}(U) = -\frac{1}{\lambda}\log(1-U) \sim E(\lambda)$.

Your turn !

Practical: exercise 2

Acceptance-rejection method

Use an **instrumental distribution** g (which we know how to sample from)
⇒ to sample from the target distribution f

The general principle is to **choose** g **close to** f and to propose samples from g, to accept some and reject others to get a sample following f.

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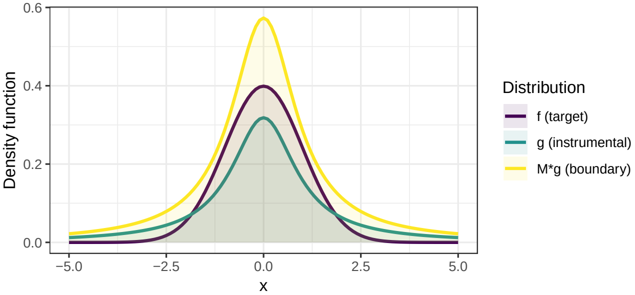
```
Let $f$ be the targeted density function
Let $g$ be a proposal density function (from which one knows how to sample)
such that, for all $x$: $f(x) \leq Mg(x)$
While $i \leq n$:
    1 Sample $x_i \sim g$ and $u_i \sim \mathcal{U}_{[0,1]}$
    2 If $u_i \leq \frac{f(x_i)}{Mg(x_i)}$, accept the draw:
      $y_i := x_i$
      else reject it and return to 1.
```

$\Rightarrow$ $(y_1, \dots, y_n) \overset{iid}{\sim} f$

Acceptance-rejection: importance of the proposal



Example of a proposal and a target ditribution for the accept−reject algorithm

Remarque : The smaller M, the greater acceptance rate

⇒ the more the algorithm is efficient at sampling from f (less iterations for a sample size n)

So one wishes g the as close as possible to f !

⚠ g will necessarily have heavier tail than the target

⇒ when the number of parameters increases, acceptance rate decrease svery rapidly *(curse of dimension)*

MCMC Algorithms

Markov chain definition

Markov chain: discrete time stochastic process

Definition: a series of random variables X_0, X_1, X_2, ... (all valued over the same state space) with the "memoryless" **Markov property**:

$$p(X_i = x | X_0 = x_0, X_1 = x_1, \ldots, X_{i-1} = x_{i-1}) = p(X_i = x | X_{i-1} = x_{i-1})$$

The set E of all possible values of X_i is called the **state space**

2 parameters:

1. initial distribution $p(X_0)$
2. tansition probabilities $T(x, A) = p(X_i \in A | X_{i-1} = x)$

NB: only **homogeneous** Markov chains considered here:
$p(X_{i+1} = x | X_i = y) = p(X_i = x | X_{i-1} = y)$

Markov chains properties

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Property: a Markov chain is **aperiodic** if nothing induces periodic behavior of the trajectories

Stationary law & ergodic theorem

Definition: A probability distribution $\tilde{p}$ is called **invariant law** (or **stationary law**) for a Markov chain if it verifies the following property:

if $X_i \sim \tilde{p}$, then $X_{i+j} \sim \tilde{p} \; \forall j \geq 1$

Remark: a Markov chain can admit several stationary laws

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Ergodic theorem (infinite space): A positive irreducible and recurrent Markov chain admits a single invariant probability distribution $\tilde{p}$ and converges towards it

Markov chain example (discrete state space)– I

Doudou (a hamster) follows a Markov chain every minute with 3 states:

- S sleep
- E eat
- W work out

⇒ its activity in 1min only depends on its current activity

Matrix of transition probabilities:

$$P = \begin{pmatrix} X_i/X_{i+1} & S & E & W \\ S & 0.9 & 0.05 & 0.05 \\ E & 0.7 & 0 & 0.3 \\ W & 0.8 & 0 & 0.2 \end{pmatrix}$$

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1) Is the Markov chain irreducible ? recurrent ? aperiodic ?

2) Suppose Doudou is now asleep. What about in 2 min ? in 10 min ?

3) Suppose now that Doudou is working out. What about in 10 min ?

Markov chain example (discrete state space) – II

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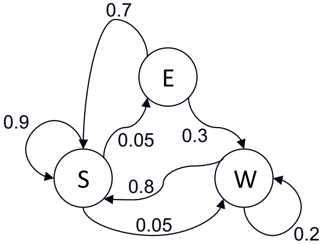

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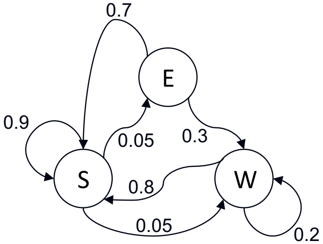

2) Suppose Doudou is now asleep. What about in 2 min ? in 10 min ?

$$x_0 = \begin{pmatrix}1\\0\\0\end{pmatrix}^T \quad x_2 = x_0 P^2 = \begin{pmatrix}0.885\\0.045\\0.070\end{pmatrix}^T \quad x_{10} = x_2 P^8 = x_0 P^{10} = \begin{pmatrix}0.884\\0.044\\0.072\end{pmatrix}^T$$

Markov chain example (discrete state space) – II

3) Suppose now that Doudou is working out. What about in 10 min ?

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3) Suppose now that Doudou is working out. What about in 10 min ?

$$x_0 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}^T \qquad x_{10} = x_0 P^{10} = \begin{pmatrix} 0.884 \\ 0.044 \\ 0.072 \end{pmatrix}^T$$

Here, the Markov chain being aperiodic, recurrent and irreducible, there is a stationary law: $\tilde{p} = \tilde{p}P$.

MCMC algorithms: general principle

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1. the Markov chain must first converge to its stationary distribution:

$$\forall\, X_0\,,\, X_n \xrightarrow[n\to+\infty]{\mathscr{L}} \tilde{p}$$

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2. then Monte Carlo convergence must also happen:

$$\frac{1}{N}\sum_{i=1}^{N} f(X_{n+i}) \xrightarrow[N\to+\infty]{} \mathbb{E}[f(X)]$$

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$$\overbrace{X_0 \to X_1 \to X_2 \to \cdots \to X_n}^{\text{Markov chain convergence}} \to \overbrace{X_{n+1} \to X_{n+2} \to \cdots \to X_{n+N}}^{\text{Monte Carlo sample}}$$

General framework of MCMC algorithms

MCMC algorithms uses an acceptance-rejection framework

```
1 Initialise $x^{(0)}$
2 For $t = 1 \dots n+N$ :
    a Propose a new candidate $y^{(t)} \sim q(y^{(t)}|x^{(t-1)})$
    b Accept $y^{(t)}$ with probability $\alpha(x^{(t-1)}, y^{(t)})$:
        $x^{(t)} := y^{(t)}$
      if $t > n$, “save” $x^{(t)}$ (as part of the final Monte Carlo sample)
```

where q is the instrumental distribution for proposing new samples and α is the acceptance probability.

Choosing the instrumental distribution

Not absolutely optimal choice for the instrumental distribution q proposing new samples

$\Rightarrow$ infinite possibilities: some better than others

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To guaranty convergence towards the target $\tilde{p}$:

- the support of q has to cover the support of $\tilde{p}$
- q must not generate periodic values

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To guaranty convergence towards the target $\tilde{p}$:

- the support of q has to cover the support of $\tilde{p}$
- q must not generate periodic values

NB: *ideally* q is **easy** and **fast** to **compute**

Metropolis-Hastings algorithm

1. Initialise $x^{(0)}$
2. For $t = 1, \dots, n+N$:
   a. Sample $y^{(t)} \sim q(y^{(t)}|x^{(t-1)})$
   b. Compute the acceptance probability
   $$\alpha^{(t)} = \min\left\{1, \frac{\tilde{p}(y^{(t)})}{q(y^{(t)}|x^{(t-1)})} \Big/ \frac{\tilde{p}(x^{(t-1)})}{q(x^{(t-1)}|y^{(t)})}\right\}$$
   c. Acceptance-rejection step: sample $u^{(t)} \sim \mathscr{U}_{[0;1]}$
   $$x^{(t)} = \begin{cases} y^{(t)} & \text{if } u^{(t)} \leq \alpha^{(t)} \\ x^{(t-1)} & \text{else} \end{cases}$$

$$\alpha^{(t)} = \min\left\{1, \frac{\tilde{p}(y^{(t)})}{\tilde{p}(x^{(t-1)})} \frac{q(x^{(t-1)}|y^{(t)})}{q(y^{(t)}|x^{(t-1)})}\right\}$$

$\Rightarrow$ computable even if $\tilde{p}$ is known only up to a constant !
(like the posterior)

Metropolis-Hastings: particular cases

Sometimes $\alpha^{(t)}$ computation simplifies:

- **independent Metropolis-Hastings**: $q(y^{(t)}|x^{(t-1)}) = q(y^{(t)})$
- **random walk Metropolis-Hastings**: $q(y^{(t)}|x^{(t-1)}) = g(y^{(t)} - x^{(t-1)})$
  If g is symetric $\big(g(-x) = g(x)\big)$, then:

$$\frac{\tilde{p}(y^{(t)})}{\tilde{p}(x^{(t-1)})}\frac{q(y^{(t)}|x^{(t-1)})}{q(x^{(t-1)}|y^{(t)})} = \frac{\tilde{p}(y^{(t)})}{\tilde{p}(x^{(t-1)})}\frac{\cancel{g(y^{(t)} - x^{(t-1)})}}{\cancel{g(x^{(t-1)} - y^{(t)})}} = \frac{\tilde{p}(y^{(t)})}{\tilde{p}(x^{(t-1)})}$$

Pro and cons of Metropolis-Hastings

- 😁 very simple & very general
- 😁 allow sampling from uni- or multi-dimensional distributions
- ☹ choice of the proposal is crucial, but hard
  ⇒ huge impact on algorithm performances
- ☹ quickly becomes inefficient dimension is too high

NB: a high rejection rate often implies important computation timings

Simulated annealing

Change $\alpha^{(t)}$ computation during the algorithm:

1. $\alpha^{(t)}$ must first be large to explore all of the state space
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    c Acceptance-rejection step: sample $u^{(t)} \sim \mathcal{U}_{[0;1]}$
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```

Ex: $T(t) = T_0 \left(\frac{T_f}{T_0}\right)^{\frac{t}{n}}$ ⇒ particularly useful for avoiding local optima

Gibbs sampler

When the dimension ↗ ⇒ very hard to propose probable values

Gibbs samplers: re-actualisation coordinate by coordinate, while conditioning on the most recent values (no acceptance-rejection)

1. Initialise $x^{(0)} = (x_1^{(0)}, \dots, x_d^{(0)})$
2. For $t = 1, \dots, n+N$:
   - a. Sample $x_1^{(t)} \sim p(x_1 | x_2^{(t-1)}, \dots, x_d^{(t-1)})$
   - b. Sample $x_2^{(t)} \sim p(x_2 | x_1^{(t)}, x_3^{(t-1)}, \dots, x_d^{(t-1)})$
   - c. ...
   - d. Sample $x_i^{(t)} \sim p(x_i | x_1^{(t)}, \dots, x_{i-1}^{(t)}, x_{i+1}^{(t-1)}, \dots, x_d^{(t-1)})$
   - e. ...
   - f. Sample $x_d^{(t)} \sim p(x_d | x_2^{(t)}, \dots, x_{d-1}^{(t)})$

NB: if the conditional distribution is unknown for some coordinates, an acceptance-rejection step can be included for this coordinate only (*Metropolis within gibbs*)

Your turn !

Practical: exercise 3

MCMC in practice

MCMC softwares

- **BUGS** : *Bayesian inference Using Gibbs Sampling*

  1989 MRC BSU University of Cambridge (UK)

  ⇒ flexible software for Bayesian analysis in complex statistical models through MCMC algorithms

  - WinBUGS: ⚠ clic + *Windows only* + stopped development
    https://www.mrc-bsu.cam.ac.uk/software/bugs/the-bugs-project-winbugs/
  - OpenBUGS: ⚠ clic + *Windows only* + *Linux partially*
    https://www.mrc-bsu.cam.ac.uk/software/bugs/openbugs/
  - JAGS: 😁 command line + R interface
    http://mcmc-jags.sourceforge.net/

- **STAN**: specialized for high-dimensional problems
  http://mc-stan.org/

rjags

JAGS software is modern and efficient :

- relies on the BUGS language to specify a Bayesian model
- R interface thanks to rjags package
- results analysis with R packages
  - coda
  - HDInterval

Markov chain convergence

In Bayesian analysis, MCMC algorithms are used to obtain a **Monte Carlo sample** from the *posterior* distribution

⇒ requires **Markov chain convergence** towards its stationary law (*posterior* distribution).

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⇒ **study the convergence empirically for each analysis**

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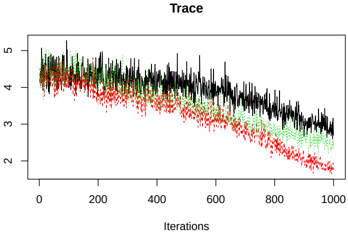
💡 Initialisation of **several** **Markov chains** from different initial values
⇒ If **convergence is reached**, then these **chains must be overlapping**

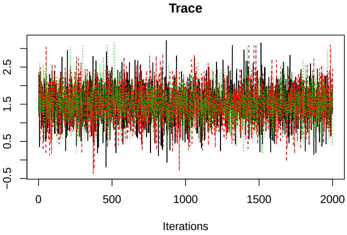
Graphical diagnostics

- Trace
- *Posterior* density
- Running Quantiles
- Gelman-Rubin diagram
- Auto-correlogram

Trace

`coda::traceplot()`



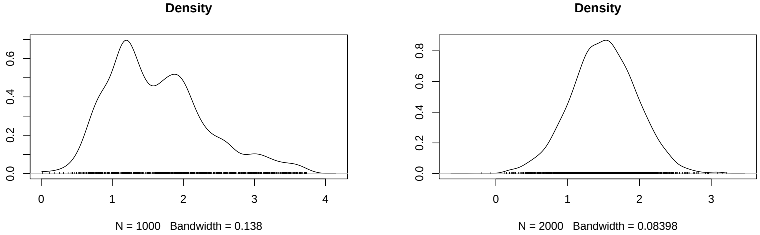


😁 chain traces must overlap and mix

☹️ ↗ `n.iter` and/or ↗ burn-in

Posterior density

`coda::densplot()`

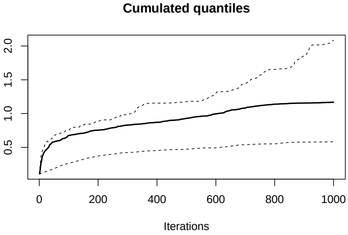


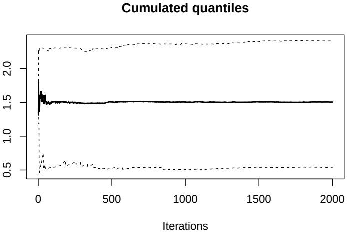
😁 density must be smooth and uni-modal

☹ ↗ `n.iter` and/or ↗ burn-in

Running quantiles

`coda::cumuplot()`


Cumulated quantiles


Cumulated quantiles

😁 running quantiles must be stable across iterations

🙁 ↗ `n.iter` and/or ↗ burn-in

Gelman-Rubin statistic

- variation between the different chains
- variation within a given chain

If the algorithm has properly converged, the between-chain variation must be close to zero

$\theta_{[c]} = (\theta_{[c]}^{(1)}, \dots, \theta_{[c]}^{(N)})$ the N-sample from chain number $c = 1, \dots, C$

Gelman-Rubin statistic: $R = \dfrac{\frac{N-1}{N} W \frac{1}{N} B}{W}$

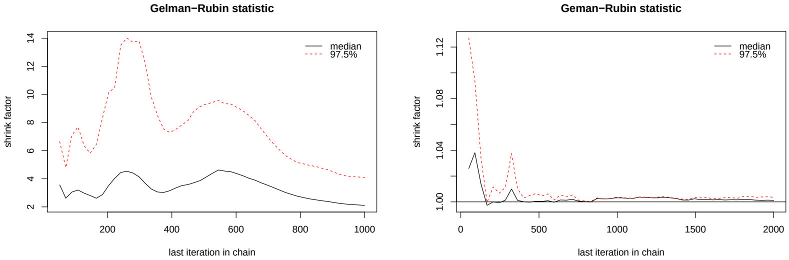
- between-chain variance: $B = \frac{N}{C-1} \sum_{c=1}^{C} (\bar{\theta}_{[C]} - \bar{\theta}.)^2$
- chain average: $\bar{\theta}_{[c]} = \frac{1}{N} \sum_{t=1}^{N} \theta_{[c]}^{(t)}$
- global average: $\bar{\theta}. = \frac{1}{C} \sum_{c=1}^{C} \bar{\theta}_{[C]}$
- within-chain variance: $s_{[c]}^2 = \frac{1}{N-1} \sum_{t=1}^{N} (\theta_{[c]}^{(t)} - \bar{\theta}_{[C]})^2$

$$N \to +\infty \ \& \ B \to 0 \Rightarrow R \to 1$$

Other statistics exist. . .

Gelman-Rubin diagram

`coda::gelman.plot()`



😁 Gelman-Rubin statistic median must remain under the $1{,}01$ threshold (or $1{,}05$)

☹ ↗ `n.iter` and/or ↗ burn-in

Effective Sample Size (ESS)

Markov property ⇒ **auto-correlation** between values sampled after one another (dependent sampling) :

- reduce the amount of information available within a sample size n
- slows down LLN convergence

Effective sample size quantifies this:

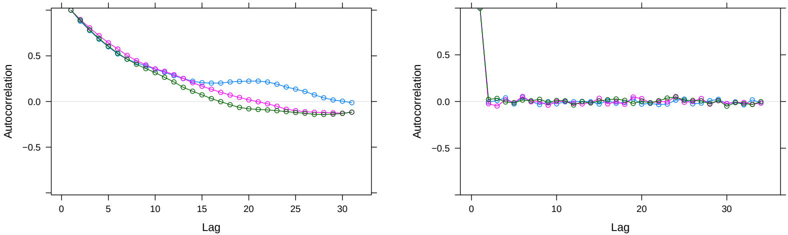
$$ESS = \frac{N}{1 + 2\sum_{k=1}^{+\infty} \rho(k)}$$

where $\rho(k)$ is the auto-correlation with lag k.

Space out saved samples (e.g. every 2, 5, or 10 iterations)
⇒ reduces dependency within the Monte Carlo sample generated

Auto-correlation

`coda::acfplot()`



😁 auto-correlations must decrease rapidly to oscillate around zero

☹ ↗ `thin` and/or ↗ `n.iter` and/or ↗ burn-in

Monte Carlo error

For a given parameter, quantifies the error introduced through the Monte Carlo method

(standard deviation of the Monte Carlo estimator across the chains)

- That error must be consistent from one chain to another
- The larger N (number of iterations), the smaller the Monte Carlo error will be

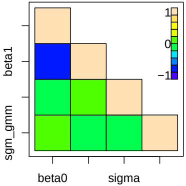
⚠ This **Monte Carlo error** must be small with respect to the estimated variance of the *posterior* distribution

Estimation

Thanks to MCMC algorithms, one can obtain **a Monte Carlo sample from the *posterior* distribution** for a **Bayesian model**

Monte Carlo method can then be used to get ***posterior* estimates** :

- Point estimates (*posterior* mean, *posterior* median, . . .)
- Credibility interval (shortest: *Highest Density Interval – HDI* with R package `HDInterval`)
- Correlations between parameters
- . . .



Deviance Information Criterion (*DIC*)

Deviance is: $D(\theta) = -2\log(p(\theta|\mathbf{y})) + C$ with C a constant

Deviance Information Criterion is then:

$$DIC = \overline{D(\theta)} + p_D$$

where $p_D = \left(D(\overline{\theta}) - \overline{D(\theta)}\right)$ represents a penalty for the effective number of parameters

⇒ DIC allows to compare different models estimated on the same data

the smaller the DIC, the better the model !

[M Plummer, Penalized loss functions for Bayesian model comparison, *Biostatistics*, 2008]

Your turn !

Practical: exercise 4

Questions ?