

Bayesian Computation with R

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- ▶ Lecture:
 - ▶ Bayes approach
 - ▶ Bayesian computation
 - ▶ A hands-on example: Linear Model
 - ▶ Available tools in R
 - ▶ Example: Stochastic volatility models
- ▶ Exercises
- ▶ Projects

- ▶ Exercises:
 - ▶ Solutions handed in by e-mail to `gregor.kastner@wu.ac.at` in a .pdf-file together with the original .Rnw-file
 - ▶ Deadline: TBA
- ▶ Projects:
 - ▶ In groups of 2–3 students
 - ▶ Data analysis using Bayesian methods
 - ▶ Documentation of the analysis consisting of
 - (a) Problem description
 - (b) Model specification
 - (c) Model fitting: estimation and validation
 - (d) Interpretation
 - ▶ Report via e-mail as a .pdf-file (+ .Rnw-file)
Deadline: TBA
 - ▶ Presentation: TBA

- ▶ Lecture slides
- ▶ Further reading:
 - ▶ Meyer, R. and Yu J. (2000) BUGS for a Bayesian analysis of stochastic volatility models. *Econometrics Journal* 3, 198–215. DOI: 10.1111/1368-423X.00046
 - ▶ Carlin, B. P. and Louis, T. A. (2009) *Bayesian Methods for Data Analysis*. 3rd, CRC Press.

- ▶ JAGS: Just Another Gibbs Sampler
 - ▶ Available from sourceforge:
<http://sourceforge.net/projects/mcmc-jags/>
 - ▶ Current version: 3.4.0
 - ▶ Source code and binaries for Windows and Mac available
- ▶ R package **rjags** on CRAN:
 - ▶ Bayesian graphical models using MCMC with the JAGS library
 - ▶ Compatible version to JAGS: 3.11
 - ▶ `install.packages("rjags")`
- ▶ R package **coda** on CRAN:
 - ▶ Output analysis and diagnostics for MCMC
 - ▶ `install.packages("coda")`
- ▶ Further R packages on CRAN: **Ecdat**, **lme4**

- ▶ Plummer, M. (2013) JAGS Version 3.4.0 user manual. Available from sourceforge.
- ▶ Spiegelhalter, D., Thomas, A., Best, N. and Lunn, D. (2003) WinBUGS user manual. Version 1.4. Available at www.mrc-bsu.cam.ac.uk/bugs/winbugs/manual14.pdf.
- ▶ Spiegelhalter, D., Thomas, A., Best, N. and Lunn, D. (2003) Examples. Volume 1–3. Also available at www.mrc-bsu.cam.ac.uk/bugs/winbugs/ as Vol1.pdf, Vol2.pdf and Vol3.pdf.

What is the difference between classical frequentist and Bayesian statistics?

- ▶ To a frequentist, unknown model parameters are fixed and unknown, and only estimable by replications of data from some experiment.
- ▶ A Bayesian thinks of parameters as random, and thus having distributions for the parameters of interest. So Bayesian can think about unknown parameters θ for which no reliable frequentist experiment exist.

Idea of Bayes approach:

- ▶ A Bayesian writes down a prior guess for θ , $p(\theta)$, then combines this with the information that the data \mathbf{y} provide. This results in a posterior distribution of θ , $p(\theta|\mathbf{y})$.
- ▶ Inference is based on summaries of the posterior.
- ▶ posterior information \geq prior information ≥ 0 . The second \geq is replaced with $=$ if we have non-informative prior information.

The parameter θ is a **random** quantity with a **prior** distribution

$$\pi(\theta) \equiv \pi(\theta|\eta).$$

η are the **hyperparameters** which are assumed **fixed**.

Inference on the parameter θ is based on its **posterior** distribution given the data

$$\begin{aligned} p(\theta|\mathbf{y}) &= \frac{p(\mathbf{y}, \theta)}{p(\mathbf{y})} = \frac{p(\mathbf{y}, \theta)}{\int p(\mathbf{y}, \theta) d\theta} \\ &= \frac{f(\mathbf{y}|\theta)\pi(\theta)}{\int f(\mathbf{y}|\theta)\pi(\theta) d\theta}. \end{aligned}$$

- ▶ **Elicited priors:** based on expert knowledge.
- ▶ **Conjugate priors:** lead to a posterior distribution $p(\theta|\mathbf{y})$ belonging to the same distributional family as the prior.

Examples:

- ▶ Beta prior for the success probability parameter of a binomial likelihood.
- ▶ Gamma prior for the rate parameter of a Poisson likelihood.
- ▶ Normal prior for the mean parameter of a normal likelihood with known variance.
- ▶ Gamma prior for the inverse variance (aka precision) of a normal likelihood with known mean.

See http://en.wikipedia.org/wiki/Conjugate_prior.

- ▶ **Noninformative priors:** do not favor any values of θ if no a-priori information is available. E.g.:
 - ▶ Uniform distribution:
 - ▶ suitable if the parameter space is discrete and finite.
 - ▶ leads to **improper** priors (i.e., does not integrate to one) for continuous and infinite parameter space.
 - ▶ is not (always) invariant under reparameterization.
 - ▶ Jeffrey's prior: invariant under reparameterization.

$$\pi(\theta) \propto |I(\theta)|^{1/2},$$

where $I(\theta)$ is the expected Fisher information matrix with

$$I_{ij}(\theta) = -\mathbb{E}_{\mathbf{y}|\theta} \left[\frac{\partial^2}{\partial \theta_i \partial \theta_j} \log f(\mathbf{y}|\theta) \right].$$

- ▶ Exercise: Jeffrey's prior for binomial experiment.

► Point estimation:

- posterior mode (aka **generalized ML estimate**)
- posterior mean or median
- ...

► Interval estimation:

Definition

A $100 \times (1 - \alpha)\%$ **credible set** for θ is a subset C of Ω such that

$$1 - \alpha \leq P(C|\mathbf{y}) = \int_C p(\theta|\mathbf{y})d\theta.$$

The probability that θ lies in C given the observed data \mathbf{y} is at least $(1 - \alpha)$.

- ▶ The comparison of predictors made by alternative scientific explanations is a mainstay of statistics.
- ▶ **Hypothesis testing:** After determining an appropriate test statistics $T(y)$, we get:

$$\text{p-value} = \mathbb{P}[T(y) \text{ more extreme than } T(y_{\text{obs}}) | \theta, H_0]$$

- ▶ Classical hypothesis testing has some disadvantages:
 - ▶ H_0 must be a simplification of H_a , like in nested models.
 - ▶ We can only offer evidence against the null hypothesis.
 - ▶ The p-value itself offers no direct interpretation as a “weight of evidence”.

The Bayesian approach to hypothesis testing is much simpler:

- ▶ As in the case for interval estimation, it requires some prior knowledge.
- ▶ Based on the data that each of the hypotheses is supported to predict, one applies Bayes' Theorem and computes the posterior probability that the first hypothesis is correct.

► Bayes factors:

- The Bayes factor BF is the ratio of the posterior odds of model M_1 to the prior odds of M_1 :

$$\begin{aligned} BF &= \frac{P(M_1|\mathbf{y})/P(M_2|\mathbf{y})}{P(M_1)/P(M_2)} \\ &= \frac{p(\mathbf{y}|M_1)}{p(\mathbf{y}|M_2)}, \end{aligned}$$

i.e., the ratio of the observed marginal densities for the two models.

- For two **a priori** equally probable models the BF equals the posterior odds of M_1 . BF captures the change in the odds in favor of model 1 as we move from prior to posterior.

- ▶ Jeffrey's scale for interpretation:

BF	Strength of evidence
< 1	Negative (support of M_2)
1–3	Barely worth mentioning
3–10	Substantial
10–30	Strong
30–100	Very strong
> 100	Decisive

- ▶ A fun reference: Wagenmakers, E.-J., Wetzels R., Borsboom D. and van der Maas, H. (2011). Why Psychologists Must Change the Way They Analyze Their Data: The Case of Psi. *Journal of Personality and Social Psychology* 100(3), 426–432.

- ▶ 16 consumers have been recruited by a fast food chain to compare the flavour of ground beef patties.
- ▶ The patties were kept frozen for eight months in different freezers:
 - ▶ a high-quality freezer consistently maintaining the temperature at 0°F (-18°C)
 - ▶ a freezer where the temperature varies between 0 and 15°F (-18 to -9°C).
- ▶ In a double-blind study (neither consumers nor waiters know where the patties were stored) each consumer evaluated patties from both fridges.
- ▶ The food chain executives are interested in whether the higher-quality freezer leads to a substantial improvement in taste.
- ▶ The study result is that 13 out of 16 consumers prefer the more expensive patty.

For a Bayesian analysis we need two components:

► **Likelihood:**

- We assume that consumers are independent and that the probability θ of preferring the more expensive patty is constant over the consumers.
- Their decisions form a sequence of Bernoulli trials.

Denoting the number of consumers preferring the more expensive patty by Y gives

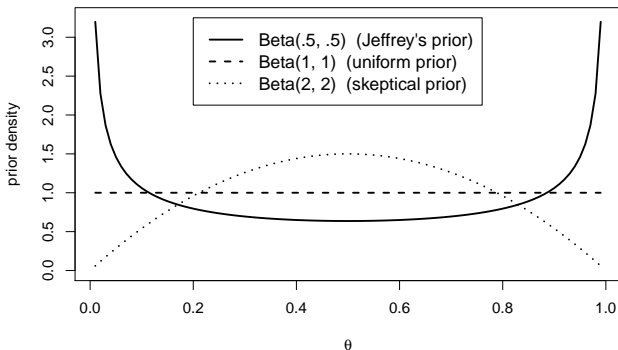
$$Y|\theta \sim \text{Bin}(16, \theta),$$

which is equivalent to

$$f(y|\theta) = \binom{16}{y} \theta^y (1 - \theta)^{16-y}.$$

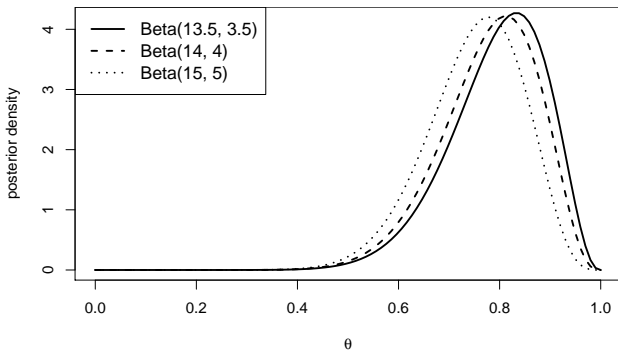
- **Prior:** The Beta distribution is a conjugate family for the binomial distribution.

$$\pi(\theta) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \theta^{\alpha-1} (1 - \theta)^{\beta-1}.$$



Thanks to the conjugacy the posterior distribution for θ is

$$\begin{aligned} p(\theta|y) &\propto f(y|\theta)\pi(\theta) \propto \theta^{y+\alpha-1}(1-\theta)^{16-y+\beta-1} \\ &\propto \text{Beta}(y + \alpha, 16 - y + \beta) \end{aligned}$$



- ▶ We return to the executives' question concerning a substantial improvement in taste.
- ▶ We select 0.6 as the critical value that θ must exceed in order for the improvement to be regarded as “substantial”.
- ▶ Given this cutoff value, we compare the hypotheses $M_1 : \theta \geq 0.6$ and $M_2 : \theta < 0.6$.
- ▶ Using a uniform prior we get for $\mathbb{P}(\theta > .6|x)$:

```
> (p1 <- round(pbeta(0.6, 14, 4, lower.tail = FALSE),  
+             digits = 3))
```

```
[1] 0.954
```

The Bayes factor is then given by

$$BF = \frac{0.954/0.046}{0.4/0.6} = 31.1.$$

This implies a reasonable strong preference for M_1 .

- ▶ Asymptotic methods
- ▶ Noniterative Monte Carlo methods
- ▶ Markov chain Monte Carlo methods

- ▶ **prehistory (1763–1960):** Conjugate priors.
- ▶ **1960's:** Numerical quadrature (Newton-Cotes methods, Gaussian quadrature, etc.).
- ▶ **1970's:** Expectation-Maximization (EM) algorithm (iterative mode finder).
- ▶ **1980's:** Asymptotic methods.
- ▶ **1980's:** Noniterative Monte Carlo methods (direct posterior sampling and indirect methods, e.g., importance sampling, rejection).
- ▶ **1990's:** Markov chain Monte Carlo (MCMC; Gibbs sampling, Metropolis Hastings algorithm, etc.). \Rightarrow broadly applicable, but require care in parametrization and convergence diagnosis!
- ▶ **2000's:** Sequential Monte Carlo (SMC)

When n is large, $f(y|\theta)$ will be quite peaked relative to $\pi(\theta)$, and so $p(\theta|y)$ will be approximately normal.

Theorem (Bayesian Central Limit Theorem)

Suppose $Y_1, \dots, Y_n \stackrel{iid}{\sim} f_i(y_i|\theta)$ and that the prior $\pi(\theta)$ and the likelihood $f(\mathbf{y}|\theta)$ are positive and twice differentiable near $\hat{\theta}^\pi$, the posterior mode of θ .

Then for large n

$$p(\theta|\mathbf{y}) \sim N(\hat{\theta}^\pi, [I^\pi(\mathbf{y})]^{-1}),$$

where $[I^\pi(\mathbf{y})]^{-1}$ is the “generalized” observed Fisher information matrix for θ , i.e., minus the inverse Hessian of the log posterior evaluated at the mode.

Using a flat prior on θ , we have

$$l(\theta) = \log(f(x|\theta)\pi(\theta)) = x \log \theta + (n - x) \log(1 - \theta) + C.$$

The first derivative is given by

$$\frac{\partial l(\theta)}{\partial \theta} = \frac{x}{\theta} - \frac{n - x}{1 - \theta}.$$

Equating to zero and solving for θ gives the posterior mode by

$$\hat{\theta}^{\pi} = \frac{x}{n}.$$

The second derivative is given by

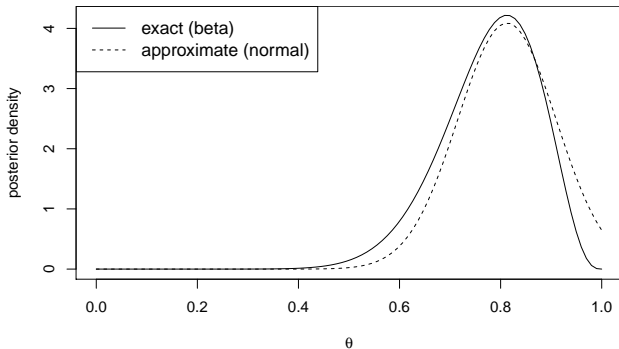
$$\frac{\partial^2 l(\theta)}{\partial \theta^2} = -\frac{x}{\theta^2} - \frac{n - x}{(1 - \theta)^2}.$$

Evaluating at the estimate $\hat{\theta}^\pi$ gives

$$\left. \frac{\partial^2 l(\theta)}{\partial \theta^2} \right|_{\theta=\hat{\theta}^\pi} = -\frac{n}{\hat{\theta}^\pi(1-\hat{\theta}^\pi)}.$$

Thus the posterior can be approximated by

$$p(\theta|x) \sim N(\hat{\theta}^\pi, \frac{\hat{\theta}^\pi(1-\hat{\theta}^\pi)}{n}).$$



Similar modes, but very different tail behavior.

► **Advantages:**

- Deterministic, noniterative algorithm.
- Substitutes differentiation for integration.
- Facilitates studies of Bayesian robustness.

► **Disadvantages:**

- Requires well-parametrized, unimodal posterior.
- θ must be of at most moderate dimension.
- n must be large, but is beyond our control.

- ▶ Direct sampling
- ▶ Indirect methods
 - ▶ Importance sampling
 - ▶ Rejection sampling

We begin with the most basic definition of Monte Carlo integration:

- ▶ Suppose $\theta \sim p(\theta)$ and we seek $\gamma := \mathbb{E}[c(\theta)] = \int c(\theta)p(\theta)d\theta$.
- ▶ Then if $\theta_1, \dots, \theta_N \stackrel{iid}{\sim} p(\theta)$, we have

$$\hat{\gamma} = \frac{1}{N} \sum_{j=1}^N c(\theta_j),$$

which converges to $\mathbb{E}[c(\theta)]$ with probability 1 as $N \rightarrow \infty$.

- ▶ Hence the computation of posterior expectations requires only a sample size of N from the posterior.

- ▶ Suppose we wish to approximate

$$\mathbb{E}[h(\theta)|\mathbf{y}] = \frac{\int h(\theta)f(\mathbf{y}|\theta)\pi(\theta)d\theta}{\int f(\mathbf{y}|\theta)\pi(\theta)d\theta}.$$

Suppose further we can roughly approximate the normalized likelihood times prior, $cf(\mathbf{y}|\theta)\pi(\theta)$, by some density $g(\theta)$ from which we can easily sample.

- ▶ Then defining the weight function $w(\theta) = f(\mathbf{y}|\theta)\pi(\theta)/g(\theta)$,

$$\mathbb{E}[h(\theta)|\mathbf{y}] = \frac{\int h(\theta)w(\theta)g(\theta)d\theta}{\int w(\theta)g(\theta)d\theta} \approx \frac{\frac{1}{N} \sum_{j=1}^N h(\theta_j)w(\theta_j)}{\frac{1}{N} \sum_{j=1}^N w(\theta_j)},$$

where $\theta_j \stackrel{iid}{\sim} g(\theta)$.

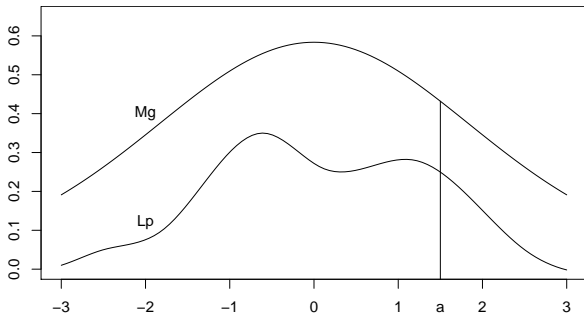
- ▶ Here, $g(\theta)$ is called the importance function; a good match to $cf(\mathbf{y}|\theta)\pi(\theta)$ will produce roughly equal weights.

- ▶ Instead of trying to approximate the posterior

$$p(\theta|\mathbf{y}) = \frac{f(\mathbf{y}|\theta)\pi(\theta)}{\int f(\mathbf{y}|\theta)\pi(\theta)d\theta},$$

we try to find a majorizing function.

- ▶ Suppose there exists a constant $M > 0$ and a smooth density $g(\theta)$, called the envelope function, such that $f(\mathbf{y}|\theta)\pi(\theta) < Mg(\theta)$ for all θ .
- ▶ The algorithm proceeds as follows:
 - (i) Generate $\theta_j \sim g(\theta)$.
 - (ii) Generate $U \sim \text{Unif}(0, 1)$.
 - (iii) If $MUg(\theta_j) < f(\mathbf{y}|\theta_j)\pi(\theta_j)$, accept θ_j . Otherwise reject θ_j .
 - (iv) Return to step (i) and repeat, until the desired sample size is obtained.
- ▶ The final sample consists of random draws from $p(\theta|\mathbf{y})$.



- ▶ Consider the θ_j samples in the histogram bar centered at a : the rejection step “slices off” the top portion of the bar.
- ▶ Repeat for all a : accepted θ_j s mimic the lower curve!
- ▶ Need to choose M as small as possible (efficiency), and watch for “envelope violations”!

- ▶ Iterative MC methods are useful when it is difficult or impossible to find a feasible importance or envelope density.
- ▶ **Algorithms:**
 - ▶ Gibbs sampler
 - ▶ Metropolis-Hastings algorithm
 - ▶ Slice sampler
- ▶ **Performance evaluation:**
 - ▶ Convergence monitoring and diagnostics
 - ▶ Variance estimation

- ▶ Given two unknowns x and y , we can often write

$$p(x) = \int p(x|y)p(y)dy \quad \text{and} \quad p(y) = \int p(y|x)p(x)dx,$$

where $p(x|y)$ and $p(y|x)$ are known.

- ▶ Seeking $p(x)$ the analytical solution via **substitution** is:

$$p(x) = \int p(x|y) \int p(y|x')p(x')dx'dy = \int h(x, x')p(x')dx',$$

where $h(x, x') = \int p(x|y)p(y|x')dy$.

- ▶ This determines a **fixed point** system which converges under mild conditions.

$$p_{i+1}(x) = \int h(x, x')p_i(x')dx'$$

- ▶ Tanner and Wong (1987) showed that one can also use a sampling-based approach which they refer to as **data augmentation**.
 1. Draw $X^{(0)} \sim p_0(x)$.
 2. Draw $Y^{(1)} \sim p(y|x^{(0)})$.
 3. Finally, $X^{(1)} \sim p(x|y^{(1)})$.
- ▶ Then $X^{(1)}$ has marginal distribution

$$p_1(x) = \int p(x|y)p_1(y)dy = \int h(x, x')p_0(x')dx'.$$

- ▶ Repeating this process produces pairs $(X^{(i)}, Y^{(i)})$ such that $X^{(i)} \xrightarrow{d} X \sim p(x)$ and $Y^{(i)} \xrightarrow{d} Y \sim p(y)$.
- ▶ The luxury of avoiding the integration above has come at the price of obtaining not the marginal density $p(x)$ itself, but only a **sample** from this density.

- ▶ Suppose the joint distribution of $\boldsymbol{\theta} = (\theta_1, \dots, \theta_K)$ is uniquely determined by the full conditional distributions, $\{p_i(\theta_i | \theta_{j \neq i}), i = 1, \dots, K\}$.
- ▶ Given an arbitrary set of starting values $\{\theta_1^{(0)}, \dots, \theta_K^{(0)}\}$,

Draw $\theta_1^{(1)} \sim p_1(\theta_1 | \theta_2^{(0)}, \dots, \theta_K^{(0)})$,

Draw $\theta_2^{(1)} \sim p_2(\theta_2 | \theta_1^{(1)}, \theta_2^{(0)}, \dots, \theta_K^{(0)})$,

\vdots

Draw $\theta_K^{(1)} \sim p_K(\theta_K | \theta_1^{(1)}, \dots, \theta_{K-1}^{(1)})$.

- ▶ Under mild conditions,

$$(\theta_1^{(t)}, \dots, \theta_K^{(t)}) \xrightarrow{d} (\theta_1, \dots, \theta_K) \sim p \quad \text{as } t \rightarrow \infty.$$

- ▶ For T sufficiently large (say, bigger than t_0), $\{\theta^{(t)}\}_{t=t_0+1}^T$ is a (correlated) sample from the true posterior.
- ▶ We might use a sample mean to estimate the posterior mean

$$\mathbb{E}(\theta_i|\mathbf{y}) \approx \frac{1}{T - t_o} \sum_{t=t_0+1}^T \theta_i^{(t)}.$$

- ▶ The time from $t = 0$ to $t = t_0$ is commonly known as the **burn-in** period.
- ▶ We may also run m parallel Gibbs sampling chains and obtain

$$\mathbb{E}(\theta_i|\mathbf{y}) \approx \frac{1}{m(T - t_o)} \sum_{j=1}^m \sum_{t=t_0+1}^T \theta_i^{(j,t)},$$

where the index j indicates chain number.

- ▶ What happens if the full conditional $p(\theta_i|\theta_{j \neq i}, \mathbf{y})$ is not available in closed form?
- ▶ Typically, $p(\theta_i|\theta_{j \neq i}, \mathbf{y})$ will be available up to a proportionality constant, since it is proportional to the part of the Bayesian model (likelihood times prior) that involves θ_i .
- ▶ Suppose the true joint posterior for $\boldsymbol{\theta}$ has unnormalized density $p(\boldsymbol{\theta})$.
- ▶ Choose a candidate density $q(\boldsymbol{\theta}^*|\boldsymbol{\theta}^{(t-1)})$ that is a valid density function for every possible value of the conditioning variable $\boldsymbol{\theta}^{(t-1)}$, and satisfies

$$q(\boldsymbol{\theta}^*|\boldsymbol{\theta}^{(t-1)}) = q(\boldsymbol{\theta}^{(t-1)}|\boldsymbol{\theta}^*),$$

i.e., q is symmetric in its arguments.

- ▶ Given a starting value $\theta^{(0)}$ at iteration $t = 0$, the algorithm proceeds as follows.

For $t = 1, \dots, T$ repeat:

1. Draw θ^* from $q(\cdot | \theta^{(t-1)})$.
2. Compute the ratio

$$r = \frac{p(\theta^*)}{p(\theta^{(t-1)})}.$$

3. If $r \geq 1$, set $\theta^{(t)} = \theta^*$;
If $r < 1$, set $\theta^{(t)} = \begin{cases} \theta^* & \text{with probability } r \\ \theta^{(t-1)} & \text{with probability } 1 - r \end{cases}$.

- ▶ Then a draw $\theta^{(t)}$ converges in distribution to a draw from the true posterior density $p(\theta | \mathbf{y})$.
- ▶ **Note:** When used as a substep in a larger (e.g., Gibbs) algorithm, we often use $T = 1$ (convergence still OK).

- ▶ How to choose the candidate density?
- ▶ The usual approach (after θ has been transformed to have support \mathbb{R}^K , if necessary) is to set

$$q(\theta^*|\theta^{(t-1)}) = N(\theta^*|\theta^{(t-1)}, \tilde{\Sigma}).$$

In one dimension $\tilde{\Sigma}$ is often chosen to provide an observed acceptance ratio near 50%:

- ▶ Very small steps \Rightarrow High acceptance rate, but also high auto-correlation.
- ▶ Very large steps \Rightarrow Low acceptance rate and also high auto-correlation.

- ▶ **Metropolis-Hastings algorithm:**

Hastings (1970) showed we can drop the requirement that q be symmetric, provided we use

$$r = \frac{p(\theta^*)q(\theta^{(t-1)}|\theta^*)}{p(\theta^{(t-1)})q(\theta^*|\theta^{(t-1)})}.$$

This is useful for asymmetric target densities.

- ▶ Ease and/or accelerate sampling from $p(\theta)$ by adding an **auxiliary** (or **latent**) variable $U \sim p(u|\theta)$.
- ▶ Suppose we want to sample a univariate θ from $p(\theta|\mathbf{y}) \propto h(\theta)$. We add an auxiliary variable U such that $U|\theta \sim \text{Unif}(0, h(\theta))$. The joint distribution of θ and U is

$$p(\theta, u) \propto h(\theta) \frac{1}{h(\theta)} I(u < h(\theta)) = I(u < h(\theta)),$$

where I denotes the indicator function.

- ▶ The Gibbs sampler for this joint distribution is given by
 1. $u|\theta \sim \text{Unif}(0, p(\theta))$, and
 2. $\theta|u \sim \text{Unif}(\theta : p(\theta) \geq u)$.
- ▶ The second update (over the “slice” defined by u) requires $p(\theta)$ to be invertible, either analytically or numerically.

When is it safe to stop and summarize MCMC output?

- ▶ We would like to ensure that $\int |\hat{p}_t(\theta) - p(\theta)| d\theta < \epsilon$.
But all we can hope to see is $\int |\hat{p}_t(\theta) - \hat{p}_{t+k}(\theta)| d\theta < \epsilon$.
- ▶ One can never “prove” convergence of a MCMC algorithm using only a finite realization from the chain.
- ▶ A slowly converging sampler may be indistinguishable from one that will never converge (e.g., due to nonidentifiability)!
- ▶ Does the eventual mixing of “initially overdispersed” parallel sampling chains provide worthwhile information on convergence?
 - ▶ Poor mixing of parallel chains can help discover extreme forms of **nonconvergence**.

Various summaries of MCMC output, such as

- ▶ **Sample auto-correlations** in one or more chains:
 - ▶ Close to 0 indicates near-independence → Chain should quickly traverse the entire parameter space.
 - ▶ Close to 1 indicates that the sampler is “stuck”.
- ▶ Diagnostic tests requiring several chains include for example Gelman & Rubin's shrink factor.
- ▶ Other tests for convergence requiring only one chain include among others Heidelberger & Welch's, Raftery & Lewis's and Geweke's diagnostics.

- ▶ Run a few (3 to 5) parallel chains, with starting points believed to be overdispersed.
 - ▶ E.g., covering ± 3 prior standard deviations from the prior mean.
- ▶ Overlay the resulting sample traces for the parameters or a representative subset (if there are many parameters or a hierarchical model is fitted).
- ▶ Annotate each plot with **lag 1 sample autocorrelations** and perhaps Gelman & Rubin's diagnostics.
- ▶ Look at convergence diagnostic tests output.
- ▶ Investigate bivariate plots and **crosscorrelations** among parameters suspected of being confounded, just as one might do regarding collinearity in linear regression.

How good is our MCMC estimate once we get it?

- ▶ Suppose we have a single long chain of (post-convergence) MCMC samples $\{\theta^{(t)}\}_{t=1}^T$. Let

$$\hat{\theta}_T = \hat{\mathbb{E}}[\theta|\mathbf{y}] = \frac{1}{T} \sum_{t=1}^T \theta^{(t)}.$$

- ▶ Then by the CLT, under iid sampling we could take

$$\hat{\mathbb{V}}_{\text{iid}}[\hat{\theta}_T] = \frac{s_{\hat{\theta}}^2}{T} = \frac{1}{T(T-1)} \sum_{t=1}^T (\theta^{(t)} - \hat{\theta}_T)^2.$$

But this is likely an **underestimate** due to positive autocorrelation in the MCMC samples.

- ▶ To avoid wasteful parallel sampling or “thinning”, compute the effective sample size,

$$\text{ESS} = \frac{T}{\kappa(\theta)},$$

where $\kappa(\theta) = 1 + 2 \sum_{k=1}^{\infty} \rho_k(\theta)$ is the **autocorrelation time**, and we cut off the sum when $\rho_k(\theta) < \epsilon$.

Then

$$\hat{\mathbb{V}}_{\text{ESS}}(\hat{\theta}_T) = \frac{s_{\hat{\theta}}^2}{\text{ESS}(\theta)}.$$

Note: $\kappa(\theta) \geq 1$, so $\text{ESS}(\theta) \leq T$, and so we have that $\hat{\mathbb{V}}_{\text{ESS}} \geq \hat{\mathbb{V}}_{\text{iid}}$ as expected.

► Another alternative: **Batching**

Divide the run into m successive batches of length k with batch means b_1, \dots, b_m . Then $\hat{\theta}_T = \bar{b} = \frac{1}{m} \sum_{i=1}^m b_i$, and

$$\hat{\mathbb{V}}_{\text{batch}}(\hat{\theta}_T) = \frac{1}{m(m-1)} \sum_{i=1}^m (b_i - \hat{\theta}_T)^2,$$

provided that k is large enough so that the correlation between batches is negligible.

- For any $\hat{\mathbb{V}}$ used to approximate $\mathbb{V}(\hat{\theta}_N)$, a 95% CI for $\mathbb{E}[\theta|\mathbf{y}]$ is then given by

$$\hat{\theta}_T \pm z_{0.025} \sqrt{\hat{\mathbb{V}}}.$$

- ▶ Observation equation: $\mathbf{y}|\boldsymbol{\beta}, \sigma^2 \sim N(\mathbf{X}\boldsymbol{\beta}, \sigma^2\mathbf{I})$

- ▶ Observation equation: $\mathbf{y}|\boldsymbol{\beta}, \sigma^2 \sim N(\mathbf{X}\boldsymbol{\beta}, \sigma^2\mathbf{I})$
- ▶ Prior distributions: $\boldsymbol{\beta}|\sigma^2 \sim N(\mathbf{b}_0, \sigma^2\mathbf{B}_0)$, $\sigma^2 \sim \mathcal{G}^{-1}(c_0, C_0)$

- ▶ Observation equation: $\mathbf{y}|\beta, \sigma^2 \sim N(\mathbf{X}\beta, \sigma^2\mathbf{I})$
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$$\begin{aligned} p(\beta, \sigma^2|\mathbf{y}) &\propto \underbrace{p(\mathbf{y}|\beta, \sigma^2)}_{\text{likelihood}} \underbrace{p(\beta, \sigma^2)}_{\text{prior}} = p(\mathbf{y}|\beta, \sigma^2)p(\beta|\sigma^2)p(\sigma^2) \\ &\propto \left(\frac{1}{\sigma}\right)^n \exp\left\{-\frac{1}{2\sigma^2}(\mathbf{y} - \mathbf{X}\beta)'(\mathbf{y} - \mathbf{X}\beta)\right\} \times \\ &\quad \left(\frac{1}{\sigma}\right)^p \exp\left\{-\frac{1}{2\sigma^2}(\beta - \mathbf{b}_0)'\mathbf{B}_0^{-1}(\beta - \mathbf{b}_0)\right\} \times \\ &\quad \left(\frac{1}{\sigma^2}\right)^{c_0+1} \exp\left\{-\frac{C_0}{\sigma^2}\right\} \end{aligned}$$

The posterior $\beta, \sigma^2 | \mathbf{y}$ follows a so-called “normal-inverse-gamma” distribution, for which it can be shown that

$$\hat{\beta}_{\text{Bayes}} := \mathbb{E}[\beta | \mathbf{y}] = (\mathbf{X}'\mathbf{X} + \mathbf{B}_0^{-1})^{-1}(\mathbf{B}_0^{-1}\mathbf{b}_0 + \mathbf{X}'\mathbf{y})$$

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Setting $\mathbf{A} = (\mathbf{X}'\mathbf{X} + \mathbf{B}_0^{-1})^{-1}\mathbf{X}'\mathbf{X}$, we can interpret $\hat{\beta}_{\text{Bayes}}$ as the weighted mean of prior expectation \mathbf{b}_0 and OLS estimate $\hat{\beta}_{\text{OLS}}$:

$$\hat{\beta}_{\text{Bayes}} = (\mathbf{I} - \mathbf{A})\mathbf{b}_0 + \mathbf{A}\hat{\beta}_{\text{OLS}}$$

Note that when the diagonal elements of \mathbf{B}_0 are large, \mathbf{A} approaches \mathbf{I} and thus $\hat{\beta}_{\text{Bayes}}$ approaches $\hat{\beta}_{\text{OLS}}$. Vice versa, when \mathbf{B}_0 has small diagonal elements, \mathbf{A} approaches $\mathbf{0}$, thus $\hat{\beta}_{\text{Bayes}}$ approaches \mathbf{b}_0 .

What to do if you don't speak normal-inverse-gamma-ish, or you want to find a more flexible way of learning about the posterior distribution?

What to do if you don't speak normal-inverse-gamma-ish, or you want to find a more flexible way of learning about the posterior distribution?



Use the **Gibbs-sampler** to “surf the posterior” by alternately simulating values from the (full) conditional parameter densities $\beta|\mathbf{y}, \sigma^2$ and $\sigma^2|\mathbf{y}, \beta$.

- $\beta | \mathbf{y}, \sigma^2 \sim N(\mathbf{b}_n, \mathbf{B}_n)$ with

$$\begin{aligned}\mathbf{B}_n &= \left(\frac{1}{\sigma^2} \mathbf{X}'\mathbf{X} + \frac{1}{\sigma^2} \mathbf{B}_0^{-1} \right)^{-1} \\ \mathbf{b}_n &= \mathbf{B}_n \left(\frac{1}{\sigma^2} \mathbf{X}'\mathbf{y} + \frac{1}{\sigma^2} \mathbf{B}_0^{-1} \mathbf{b}_0 \right)\end{aligned}$$

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- ▶ $\sigma^2 | \mathbf{y}, \beta \sim \mathcal{G}^{-1}(c_n, C_n)$ with

$$\begin{aligned}c_n &= c_0 + \frac{n}{2} + \frac{p}{2} \\ C_n &= C_0 + \frac{1}{2}(\mathbf{y} - \mathbf{X}\beta)'(\mathbf{y} - \mathbf{X}\beta) + \frac{1}{2}(\beta - \mathbf{b}_0)' \mathbf{B}_0^{-1}(\beta - \mathbf{b}_0)\end{aligned}$$

- ▶ General purpose estimation tools are provided by the BUGS family:
 1. WinBUGS
 2. OpenBUGS
 3. JAGS
- ▶ Models are specified via variants of the BUGS language.
- ▶ The software parses the model and determines the samplers automatically to generate draws from the posterior.

- ▶ **Estimation:**

- ▶ **R2WinBUGS** allows to run WinBUGS & OpenBUGS from R.
- ▶ **rjags** provides an interface to the JAGS library.

- ▶ **Post-processing, convergence diagnostics:**

- ▶ **coda** (Convergence Diagnosis and Output Analysis):
 - ▶ contains a suite of functions that can be used to summarize, plot, and and diagnose convergence from MCMC samples.
 - ▶ can easily import MCMC output from WinBUGS, OpenBUGS, and JAGS, or from plain matrices.
 - ▶ provides the Gelman & Rubin, Geweke, Heidelberger & Welch, and Raftery & Lewis diagnostics.

For more information see the CRAN Task View: Bayesian Inference.

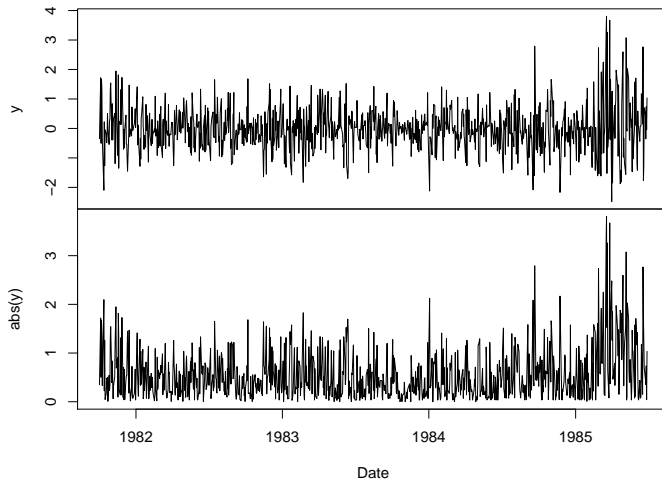
- ▶ The data consists of a time series of daily Pound/Dollar exchange rates $\{x_t\}$ from 01/10/81 to 28/06/85. We have this data available in package **Ecdat** in R.

```
> data("Garch", package = "Ecdat")
> Garch <- subset(Garch,
+                 date >= 811001 & date <= 850628,
+                 c(date, bp))
> x <- Garch$bp
```

- ▶ The series of interest are the daily mean-corrected returns times hundred, $\{y_t\}$ for $t = 1, \dots, n$.

$$y_t = 100 \left[\log x_t - \log x_{t-1} - \frac{1}{n} \sum_{i=1}^n (\log x_t - \log x_{t-1}) \right],$$

```
> y <- 100 * diff(log(x))
> y <- y - mean(y)
```

- ▶ The stochastic volatility model can be written in the form of a nonlinear state-space model.
- ▶ A state-space model specifies the conditional distributions of the observations given unknown states, here the underlying latent volatilities, θ_t , in the observation equations for $t = 1, \dots, n$

$$y_t | \theta_t = \exp\left(\frac{1}{2}\theta_t\right) u_t, \quad u_t \stackrel{iid}{\sim} N(0, 1).$$

- ▶ The unknown states are assumed to follow a Markovian transition over time given by the state equations for $t = 1, \dots, n$

$$\theta_t | \theta_{t-1}, \mu, \phi, \tau^2 = \mu + \phi(\theta_{t-1} - \mu) + \nu_t, \quad \nu_t \stackrel{iid}{\sim} N(0, \tau^2).$$

with $\theta_0 \sim N(\mu, \tau^2)$.

- ▶ The state θ_t determines the amount of volatility on day t .
- ▶ ϕ measures the autocorrelation present in the logged squared data and is restricted to be $-1 < \phi < 1$. It can be interpreted as the persistence in the volatility.
- ▶ The constant scaling factor $\beta = \exp(\mu/2)$ can be seen as the modal volatility.
- ▶ τ^2 is the volatility of log-volatilities.
- ▶ **Remark:** For Bayesian estimation the parameterization of the normal distribution is in general with respect to mean μ and precision τ , i.e.,

$$y \sim \text{dnorm}(\mu, \tau),$$

where $\tau = \sigma^{-2}$, i.e., the precision is the inverse of the variance. The conjugate prior for the precision is the Gamma distribution.

The full Bayesian model consists of

- ▶ a prior for the unobservables
 - ▶ 3 parameters: μ, ϕ, τ^2
 - ▶ unknown states: $\theta_0, \dots, \theta_n$

$$p(\mu, \phi, \tau^2, \theta_0, \dots, \theta_n) = p(\mu, \phi, \tau^2)p(\theta_0|\mu, \tau^2) \prod_{t=1}^n p(\theta_t|\theta_{t-1}, \mu, \phi, \tau^2),$$

- ▶ a joint distribution for the observables y_1, \dots, y_n

$$p(y_1, \dots, y_n|\mu, \phi, \tau^2, \theta_0, \dots, \theta_n) = \prod_{t=1}^n p(y_t|\theta_t).$$

```
model {  
  for (t in 1:length(y)) {  
    y[t] ~ dnorm(0, 1/exp(theta[t]));  
  }  
  theta0 ~ dnorm(mu, itau2);  
  theta[1] ~ dnorm(mu + phi * (theta0 - mu), itau2);  
  for (t in 2:length(y)) {  
    theta[t] ~ dnorm(mu + phi * (theta[t-1] - mu), itau2);  
  }  
  ## prior  
  mu ~ dnorm(0, 0.1);  
  phistar ~ dbeta(20, 1.5);  
  itau2 ~ dgamma(2.5, 0.025);  
  ## transform  
  beta <- exp(mu/2);  
  tau <- sqrt(1/itau2);  
  phi <- 2 * phistar - 1  
}
```

- ▶ Given the model specification a graphical model is constructed to determine the parents and direct children of each variable/node.
- ▶ Based on these relationships suitable samplers are selected (from the **base** and **bugs** module):
 - ▶ **Conjugate sampler:** for Gibbs sampling.
 - ▶ **Finite sampler:** discrete valued node with fixed support of less than 20 possible values, not bounded using truncation.
 - ▶ **Discrete slice sampler:** for any scalar discrete-valued stochastic node.
 - ▶ **Real slice sampler:** for any scalar real-valued stochastic node.

```
> library("rjags")
> initials <-
+   list(list(phistar = 0.975, mu = 10, itau2 = 300),
+         list(phistar = 0.5, mu = 0, itau2 = 50),
+         list(phistar = 0.025, mu = -10, itau2 = 1))
> initials <- lapply(initials, "c",
+                     list(.RNG.name = "base::Wichmann-Hill",
+                           .RNG.seed = 2207))
> model <- jags.model("volatility.bug", data = list(y = y),
+                     inits = initials, n.chains = 3)
> update(model, n.iter = 10000)
> draws <- coda.samples(model, c("phi", "tau", "beta"),
+                           n.iter = 100000, thin = 20)
> summary(draws)
```

Iterations = 11020:111000

Thinning interval = 20

Number of chains = 3

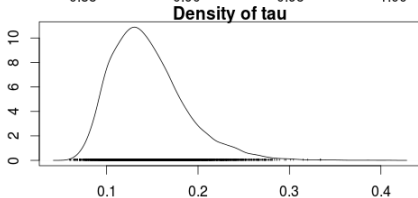
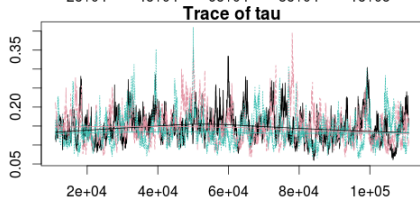
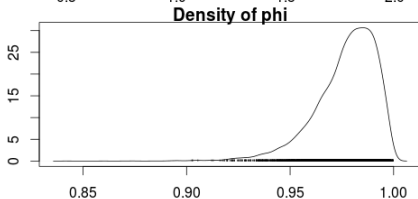
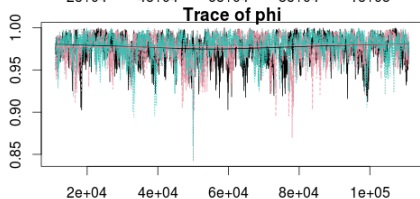
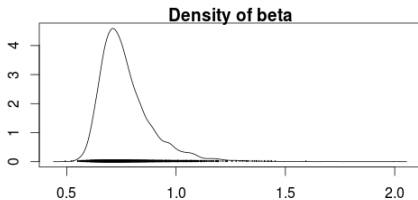
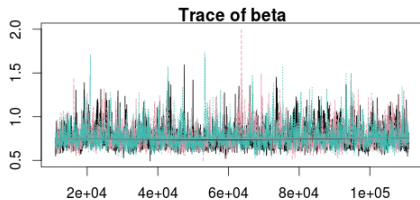
Sample size per chain = 5000

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

	Mean	SD	Naive SE	Time-series SE
beta	0.770	0.1231	0.001005	0.003436
phi	0.977	0.0150	0.000122	0.000676
tau	0.145	0.0408	0.000333	0.002469

2. Quantiles for each variable:

	2.5%	25%	50%	75%	97.5%
beta	0.611	0.689	0.744	0.821	1.084
phi	0.940	0.969	0.980	0.988	0.997
tau	0.085	0.116	0.139	0.167	0.243



- ▶ Auto- and crosscorrelation: `autocorr.diag`, `autocorr.plot`, `crosscorr`
- ▶ Gelman and Rubin diagnostics: `gelman.diag`
- ▶ Heidelberger and Welch diagnostics: `heidel.diag`
- ▶ Geweke diagnostics: `geweke.diag`, `geweke.plot`
- ▶ Raftery and Lewis diagnostics: `raftery.diag`

For more information see the CODA manual at <http://www.mrc-bsu.cam.ac.uk/bugs/documentation/Download/cdaman03.pdf> and the addendum to the manual at <http://www.mrc-bsu.cam.ac.uk/bugs/documentation/Download/cdaman04.pdf>

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