Review: MCMC Idea

Situation:

- Given a target distribution $f(x)$
- Want to generate samples from $f(x)$

Idea:

- construct a Markov chain $\{X_i\}_{i=1}^{\infty}$ so that $\lim_{i\to\infty} P(X_i = x) = f(x)$
- simulate the Markov chain for many iterations
- for m large enough $x_m, x_{m+1}, \ldots$ are (essentially) from $f(x)$

Review: How to construct the Markov chain

How to construct such a Markov chain? ($x \in \Omega$ discrete)

- Markov chain transition probabilities: $P(y|x) = P(X_{i+1} = y|X_i = x)$
- Need to have

$$f(y) = \sum_{x \in \Omega} f(x)P(y|x) \text{ for all } y \in \Omega$$

- Sufficient condition: Detailed balance condition

$$f(x)P(y|x) = f(y)P(x|y) \text{for all} x, y \in \Omega$$

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Metropolis-Hastings setup for $P(y|x)$:

$$P(y|x) = Q(y|x)\alpha(y|x) \text{ when } y \neq x$$
$$P(x|x) = 1 - \sum_{y \neq x} Q(y|x)\alpha(y|x) \text{ when } y = x$$

where

$$\alpha(y|x) = \min\left\{1, \frac{f(y)}{f(x)}\frac{Q(x|y)}{Q(y|x)}\right\}$$

ï¿œ

Review: Common proposal types

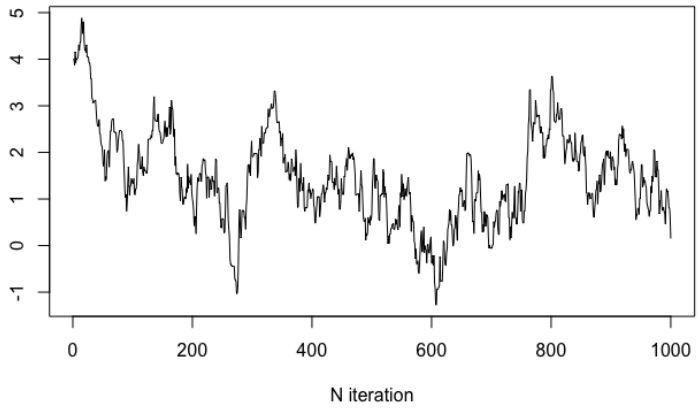
- Independent proposals: $Q(y|x) = q(y)$
  - usually not a good alternative (alone)
- Random walk proposals: $Q(y|x) = N(y|x, \sigma^2 I)$
  - is used a lot
  - includes a tuning parameter: σ
- Gibbs updates: $Q(y^j|x^j, \mathbf{x}^{-j}) = f(x^j|\mathbf{x}^{-j})$
  - is used a lot
  - the proposal density is the full conditional
  - no tuning paramter
  - acceptance rate 1
  - can be conbined with MH update

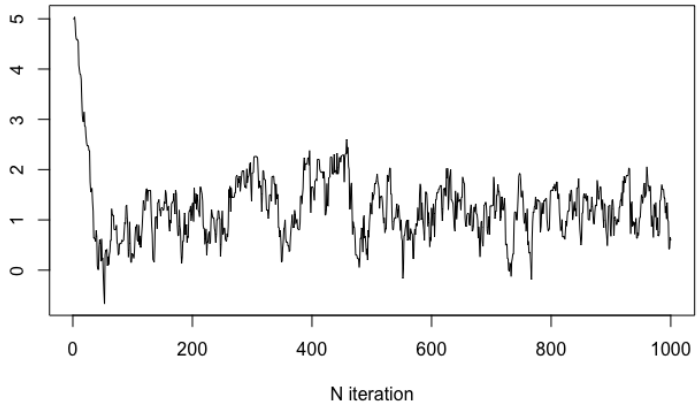
Review: Convergence diagnostic

Has the MC converged?

- Formal convergence diagnostics exists
  - some based on a single Markov chain run
  - some based on several Markov chain runs
- Standard way to assess convergence is to look at the traceplot
- If some properties of the target distribution is known: use it to check convergence!
- All convergence diagnostics can (and do) fail

Has bivariate this MC converged?





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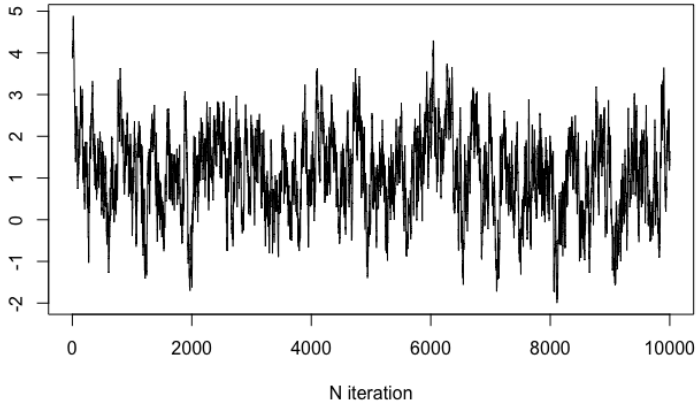

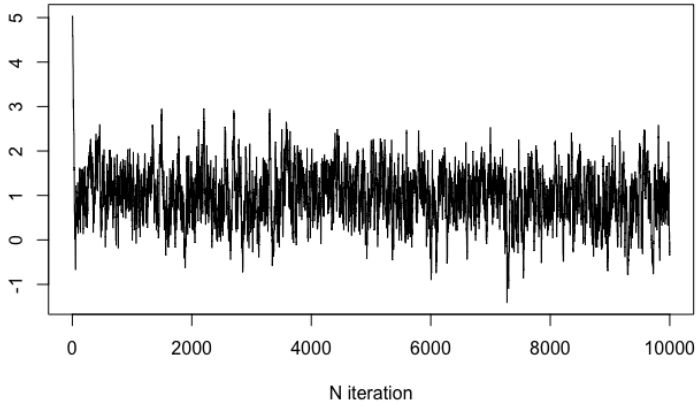

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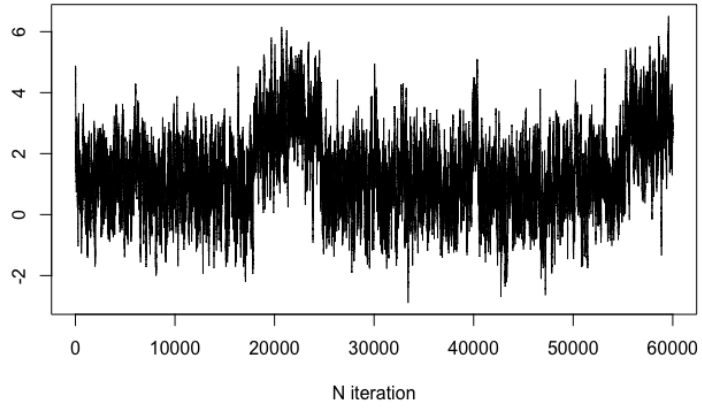

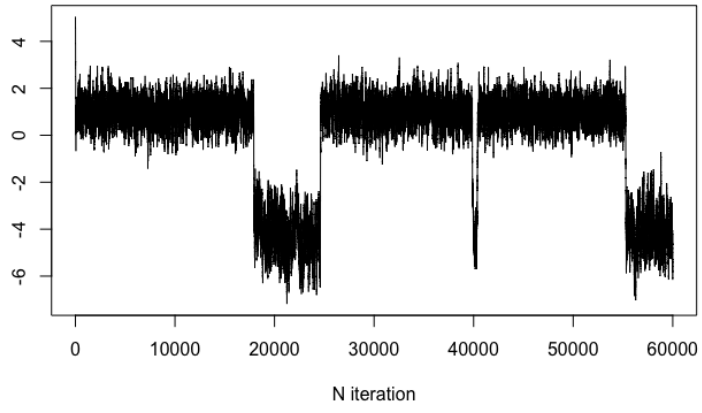

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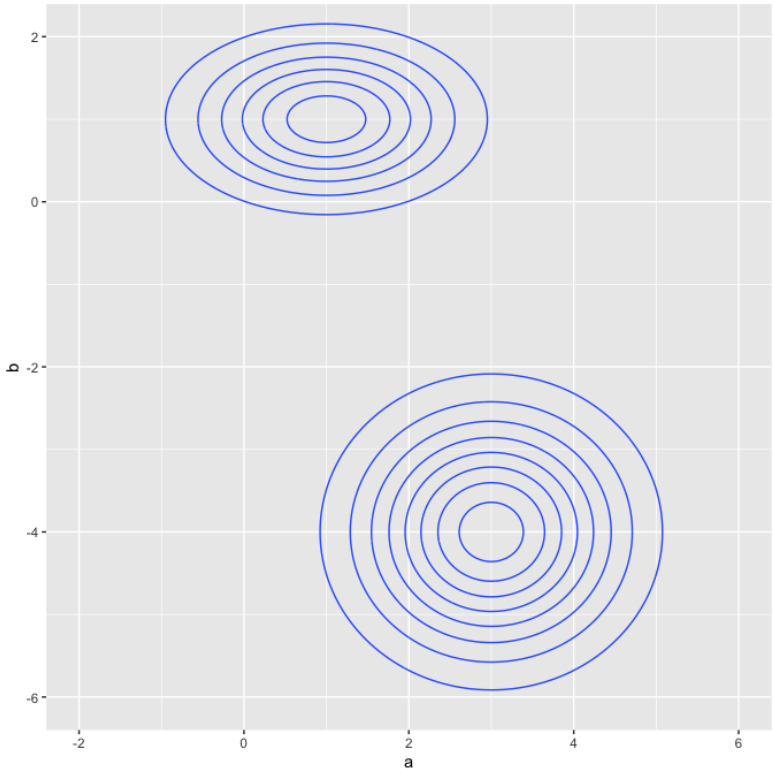


This is how the distribution looks like.

Used a RW proposal $\mathcal{N}(0, 0.3^2 I)$

Variance of the MCMC estimator

Recall: We want to estimate $\mu = \int g(x)\pi(x)\, dx$ with $\hat{\mu} = \frac{1}{n}\sum g(x_i)$ where $x_i \sim \pi(x)$.

In standard MC we have

$$x_1, x_2, \ldots, x_n \sim \pi(x), \text{ i.i.d.}$$

This gives

$$\mathrm{E}(\hat{\mu}) = \mu \text{ and } \mathrm{Var}(\hat{\mu}) = \frac{\mathrm{Var}(g(X))}{n}$$

We can estimate the variance $\mathrm{Var}(\hat{\mu})$ as

$$\widehat{\mathrm{Var}(\hat{\mu})} = \frac{\widehat{\mathrm{Var}(g(X))}}{n}$$

$$\widehat{\mathrm{Var}(g(X))} = \frac{1}{n-1}\sum(g(x_i) = \hat{\mu})$$

MCMC gives dependence samples, what is the variance then??

Autocorrelation

To examine dependencies of successive MCMC samples, the autocorrelation function can be used. Let $x_1, \ldots, x_N$, where N denotes the number of samples, denote our MCMC chain.

The lag k autocorrelation $\rho(k)$ is the correlation between every draw and its k-th lag. For N reasonably large

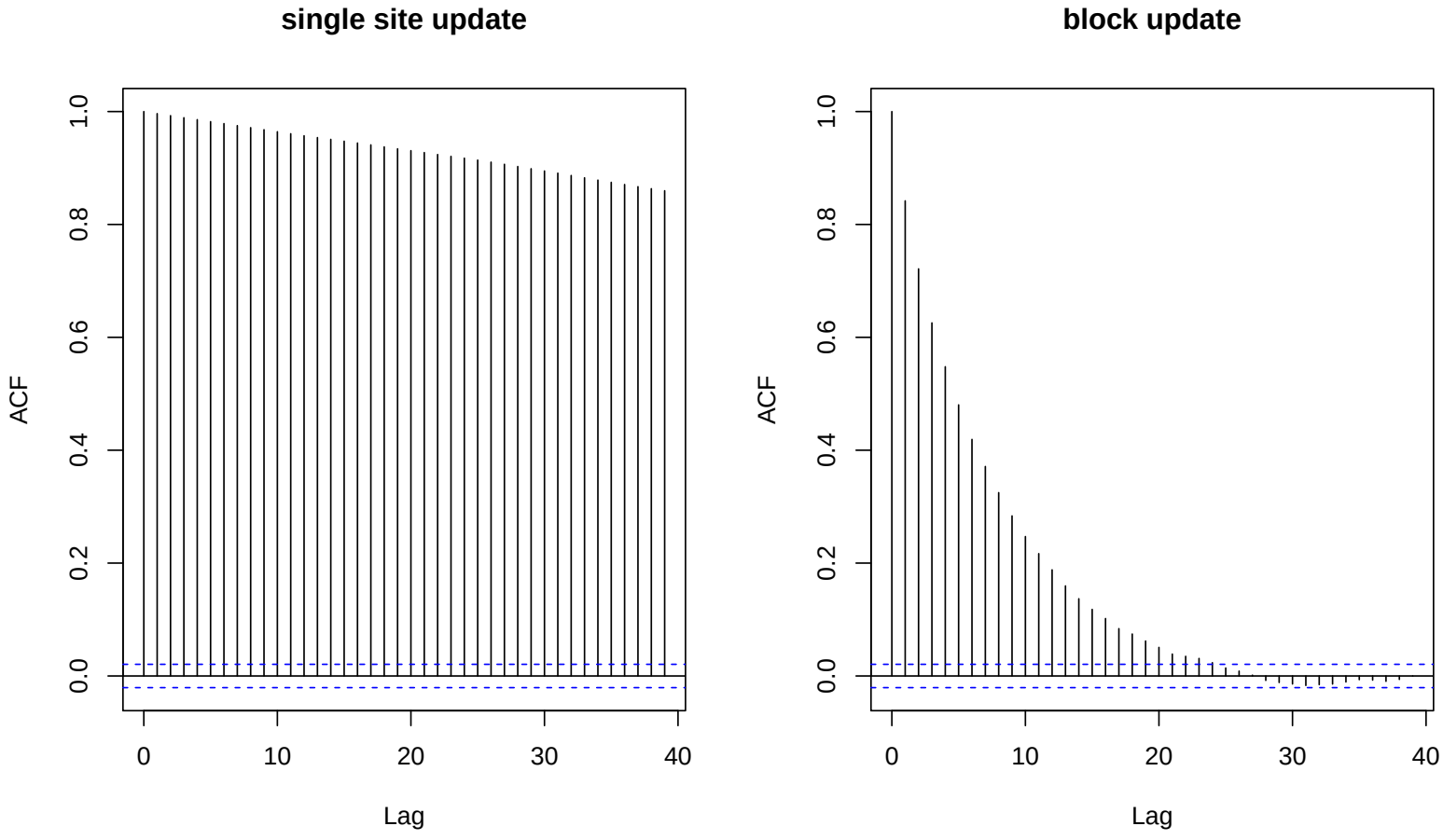
$$\rho(k) \approx \frac{\sum_{i=1}^{N-k}(x_i - \bar{x})(x_{i+k} - \bar{x})}{\sum_{i=1}^{N}(x_i - \bar{x})^2},$$

where $\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$ is the overall mean.

- With increasing lag k we expect lower autocorrelations.
- If autocorrelation is still relatively high for higher values of k, this indicates high degree of correlation between our draws and slow mixing.

Example: Korsbetningen

Autocorrelation function for N (after discarding the burn-in period)



Effective sample size

A useful measure to compare the performance of different MCMC samplers is the effective sample size (ESS) Kass et al. (1998) American Statistician 52, 93–100..

- The ESS is the estimated number of independent samples needed to obtain a parameter estimate with the same precision as the MCMC estimate based on N dependent samples.

$$\text{ESS} = \frac{N}{\tau}, \quad \tau = 1 + 2 \cdot \sum_{k=1}^{\infty} \rho(k),$$

where τ is the autocorrelation time and $\rho(k)$ the autocorrelation at lag k.

Estimate of ESS

$$\text{ESS} = \frac{N}{\tau}, \quad \tau = 1 + 2 \cdot \sum_{k=1}^{\infty} \rho(k),$$

Estimate τ as

$$\tau = 1 + 2 \cdot \sum_{k=1}^{m} \hat{\rho}(k)$$

where $\hat{\rho}(k)$ is the sample autocorrelation function at lag k, and m is choosen to fullfill some criteria.

Different criteria exists.

Example: Korsbetningen - Effective sample size (ESS)

```
> library(coda)
> nsamples

[1] 8000

> ## single site
> effectiveSize(as.mcmc(res1))

       N    theta
18.46377 13.65231

> ## block update
> effectiveSize(as.mcmc(res2))

       N    theta
564.3797 925.7764

>
```

The precision of the MCMC estimate of the posterior mean of N based on 8000 samples from a single site update is a good as taking 16 independent samples!

Geweke diagnostics

The MCMC chain is divided into two windows

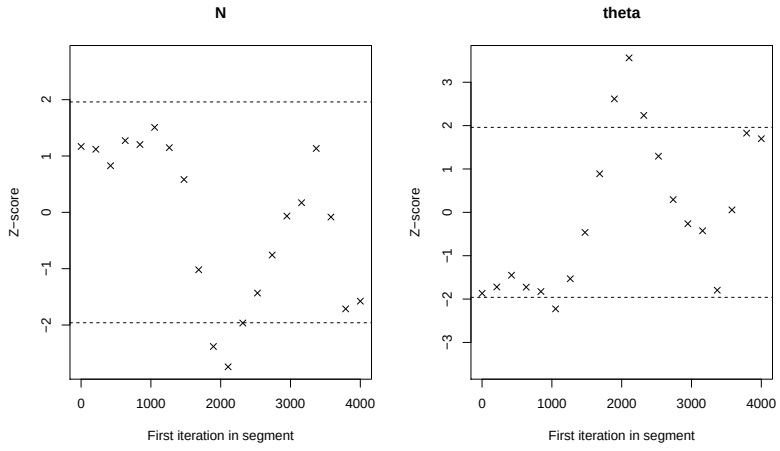
- the first x%, and
- the last y% of the iterates

(`coda` default: $x = 10$, $y = 50$). For both windows the mean is calculated.

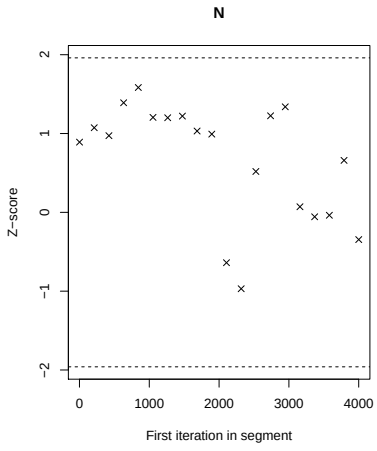
If the chain is stationary both values should be equal and Geweke's test statistic (z-score) follows an asymptotical standard normal distribution.

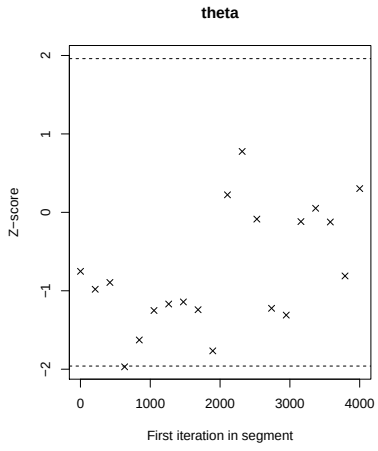
Example: Korsbetningen - Geweke plot

Single Site



Block Update





Further reading

There are several convergence diagnostics:

- some are based on a single Markov chain run
- some are based on several Markov chain runs

There are no guarantees!

For further reading see for example

- Gilks, W. R., Richardson, S. and Spiegelhalter, D.J. (1996) *Markov Chain Monte Carlo in Practice, Chapman & Hall, London*,

Different approaches are implemented in the

- R-package `coda`. (Plummer et al., 2006)

Summary

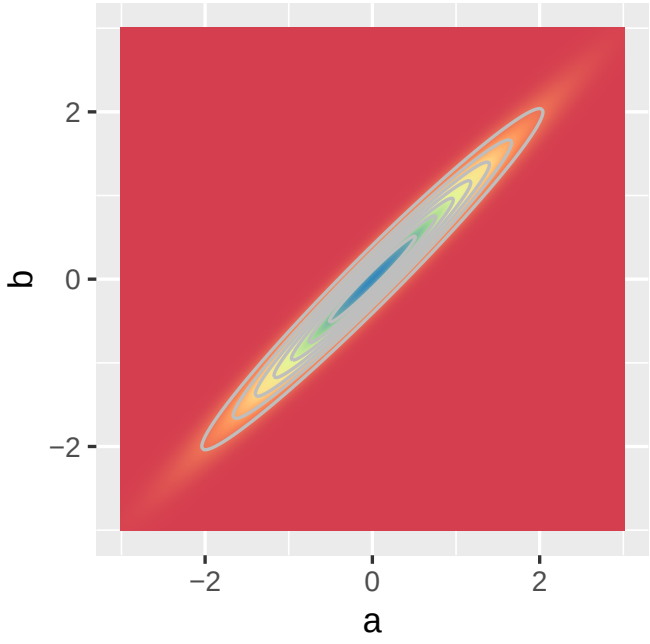
- Diagnostics cannot guarantee that chain has converged
- Can indicate that it has not converged

Solutions?

- Run longer and thin output
- Reparametrize model
- "Block" correlated variables together
  - Joint update might be more efficient however for some parameter combination the acceptance rate can be very slow!
- integrate out variables
- ...

Typical MCMC problems

- Note: If you knows the solution, it is easy to solve a problem!
- Properties of $f(x)$ that may make MCMC difficult
  - strong dependency between variables



Typical MCMC problems

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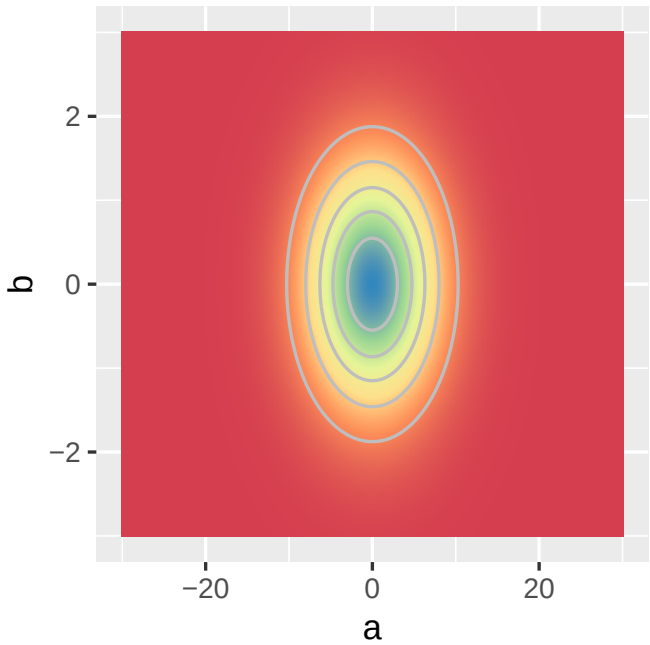

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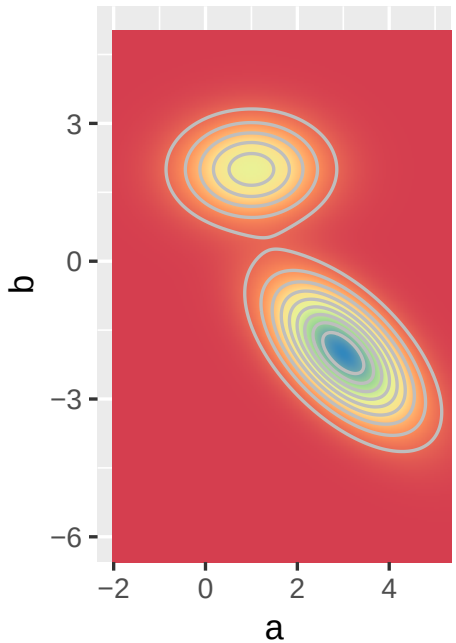

Typical MCMC problems

- Note: If you knows the solution, it is easy to solve a problem!
- Properties of $f(x)$ that may make MCMC difficult
  - strong dependency between variables
  - different scales on different variables
  - several modes
- In toy examples: this is not a problem
  - we know how $f(x)$ looks like
- In real problems: this may be difficult
  - we have a formula for $f(x)$
  - we don't know how $f(x)$ looks like

MCMC

- Since the advent of simulation-based techniques (notably MCMC), Bayesian computation has enjoyed incredible development
- This has certainly been helped by dedicated software (eg BUGS and then WinBUGS, OpenBUGS, JAGS, Stan)
- MCMC methods are very general and can effectively be applied to "any" model

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- This has certainly been helped by dedicated software (eg BUGS and then WinBUGS, OpenBUGS, JAGS, Stan)
- MCMC methods are very general and can effectively be applied to "any" model
- However:
  - Even if in theory, MCMC can provide (nearly) exact inference, given perfect convergence and MC error $\to 0$, in practice, this has to be balanced with model complexity and running time
  - This is particularly an issue for problems characterised by large data or very complex structure (eg hierarchical models)
  - This is also a problem if one wants to, for example, test the sensitivity of the model to the prior choice

What it INLA?

Integrated Nested Laplace Approximation

The short answer:

> *INLA is a fast method to do Bayesian inference with latent Gaussian models and* `R-INLA` *is an R-package that implements this method with a flexible and simple interface*

A (much) longer answer can be found in:

Rue, Martino, and Chopin (2009) "Approximate Bayesian inference for latent Gaussian models by using integrated nested Laplace approximations." *Journal of the royal statistical society*: Series B. 319-392

Ingredients of INLA

- Latent Gaussian Models
  - Class of models where INLA can be applied
- Gaussian Markov Random Fieds
  - Sparse matrix computations
- Laplace Approximation
  -

Hierarchical Bayesian models

Hierarchical models are an extremely useful tool in Bayesian model building.

Three parts:

- Observation model $\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta}$: Encodes information about observed data.
- The latent model $\boldsymbol{x}|\boldsymbol{\theta}$: The unobserved process.
- Hyperpriors for $\boldsymbol{\theta}$: Models for all of the parameters in the observation and latent processes.

Latent Gaussian models

A very general way of specifying the problem is by modelling the mean for the i-th unit by means of an additive linear predictor, defined on a suitable scale (e.g. logistic for binomial data)

$$\eta_i = \alpha + \sum_{l=1}^{L} f_l(u_{li}) + \sum_{k=1}^{K} \beta_k z_{ki} + \epsilon_i$$

where

- α is the intercept
- $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_K)$ quantify the effect of $\boldsymbol{x} = (x_1, \ldots, x_K)$ on the response
- $\boldsymbol{f} = (f_1, \ldots, f_L)$ is a set of functions defined in terms of some covariates $\boldsymbol{z} = (z_1, \ldots, z_K)$

And assume

$$\boldsymbol{x} = (\alpha, \boldsymbol{\beta}, \boldsymbol{f}) \sim \mathcal{N}(0, \boldsymbol{Q}(\theta)^{-1})$$

Many commonly used models can be written as LGM:

- Multiple regression
- Generalized linear model (GLM)
- Generalized additive model (GAM)
- Generalized additive mixed model (GAMM, GLMM)

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$$\eta_i = E(y_i) = \alpha + \sum_{k=1}^{K} \beta_k z_{ki}$$

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$$\eta_i = g(\mu_i) = \alpha + \sum_{k=1}^{K} \beta_k z_{ki}$$

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  - $\{f_l(\cdot)\}$: Non-linear smooth effects of covariates u_l
- Generalized additive mixed model (GAMM, GLMM)

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  - $g(\cdot)$: link function
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  - β: Linear effects of covariates z

Some more example of LGM

- Disease Mapping
- Geostatistical models
- Survival models
- Stochastic volatility models
- Spatial and spatio-temporal models
- Spline smoothing
- +++

Unified framework

Observations: $\boldsymbol{y}$

Latent field: $\boldsymbol{x}$

Hyperparameters: $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$

Unified framework

Observations: $\boldsymbol{y}$ Assumed conditionally independent given $\boldsymbol{x}$ and $\boldsymbol{\theta}_1$

$$\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta}_1 \sim \prod_i \pi(y_i|x_i, , \boldsymbol{\theta}).$$

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$$\boldsymbol{x}|\boldsymbol{\theta}_1 \sim \mathcal{N}(0, \boldsymbol{Q}(\boldsymbol{\theta}_2)^{-1})$$

The latent field $\boldsymbol{x}$ can be large $(10^1 - 10^6)$

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The latent field $\boldsymbol{x}$ can be large $(10^1 - 10^6)$

Hyperparameters: $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ Precision parameters of the Gaussian field and parameters of the likelihood

$$\boldsymbol{\theta} \sim \pi(\boldsymbol{\theta})$$

The vector $\boldsymbol{\theta}$ is usually small (1-10)

Main interest

The posterior distribution is given by

$$\pi(\boldsymbol{x}, \boldsymbol{\theta}|\boldsymbol{y}) \propto \pi(\boldsymbol{\theta})\pi(\boldsymbol{x}|\boldsymbol{\theta}) \prod_i \pi(y_i|x_i, \boldsymbol{\theta})$$

Main interest

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$$\pi(\boldsymbol{x}, \boldsymbol{\theta}|\boldsymbol{y}) \propto \pi(\boldsymbol{\theta})\pi(\boldsymbol{x}|\boldsymbol{\theta}) \prod_i \pi(y_i|x_i, \boldsymbol{\theta})$$

We are mainly interested in the posterior marginals

$$\pi(x_i|\boldsymbol{y}) = \int_{\boldsymbol{\theta}} \underbrace{\int_{\boldsymbol{x}_{-i}} \pi(\boldsymbol{x}, \boldsymbol{\theta}|\boldsymbol{y}) d\boldsymbol{x}_{-i}}_{\pi(x_i, \boldsymbol{\theta}|\boldsymbol{y})} d\boldsymbol{\theta} = \int_{\boldsymbol{\theta}} \pi(x_i, \boldsymbol{\theta}|\boldsymbol{y}) d\boldsymbol{\theta} = \int_{\boldsymbol{\theta}} \pi(x_i|\boldsymbol{\theta}, \boldsymbol{y})\pi(\boldsymbol{\theta}|\boldsymbol{y}) d\boldsymbol{\theta}$$

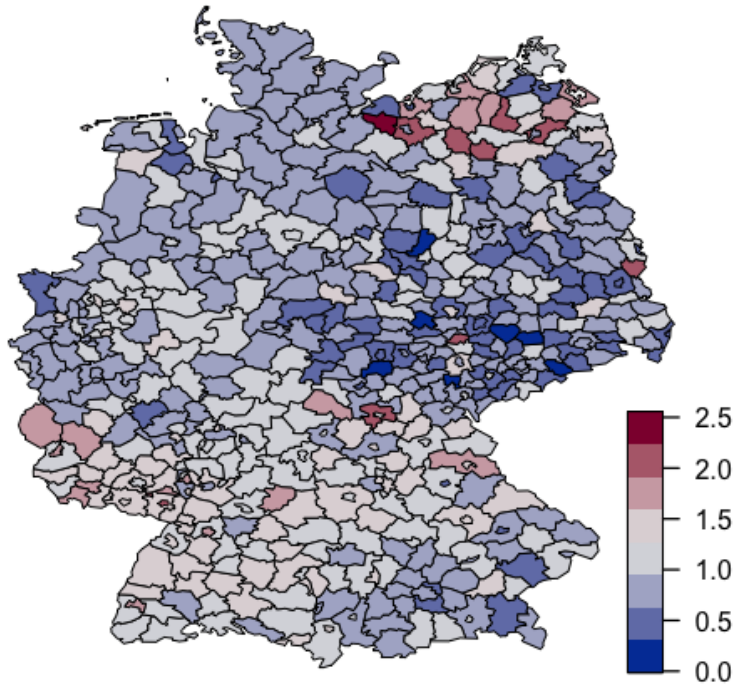
$$\pi(\theta_j|\boldsymbol{y}) = \int_{\boldsymbol{\theta}_{-j}} \underbrace{\int_{\boldsymbol{x}} \pi(\boldsymbol{x}, \boldsymbol{\theta}|\boldsymbol{y}) d\boldsymbol{x}}_{\pi(\boldsymbol{\theta}|\boldsymbol{y})} d\boldsymbol{\theta}_{-j} = \int_{\boldsymbol{\theta}_{-j}} \pi(\boldsymbol{\theta}|\boldsymbol{y}) d\boldsymbol{\theta}_{-j}$$

Example: Disease Mapping in Germany

We observed larynx cancer mortality counts for males in 544 district of Germany from 1986 to 1990 and want to make a model.

Information available:

- y_i The count in disctrict i
- E_i An offset, expected number of cases in district i
- c_i A covariate (level of smoking consumption in district i)
- s_i Spatial location i (district)



Level 1: The data

We have to decide on the likelihood of our data $\boldsymbol{y}$

- The responses are counts
- We choose a Poisson model

$$y_i|\eta_i \sim \text{Poisson}(E_i \exp(\eta_i))$$

- η_i is a linear function of the latent components

Level 2: The Latent Model

The latent field $\boldsymbol{x}$ consists of two parts:

- One fixed effect: the intercept μ
- Three random effects:
  - The spatially structured effect f_s.
  - The unstructured effect u which accounts for non-observed variability
  - The unknown effect $f(c_i)$ of the exposure covariate which assumes value c_i for district i.

These are combined for each location to give a linear predictor

$$\eta_i = \mu + f_s(s_i) + f(c_i) + u_i$$

The latent field is $\boldsymbol{x} = \{\mu, (f_s(\cdot)), (f(\cdot)), u_1, \ldots, u_n\}$

Level 3: The hyperparameters

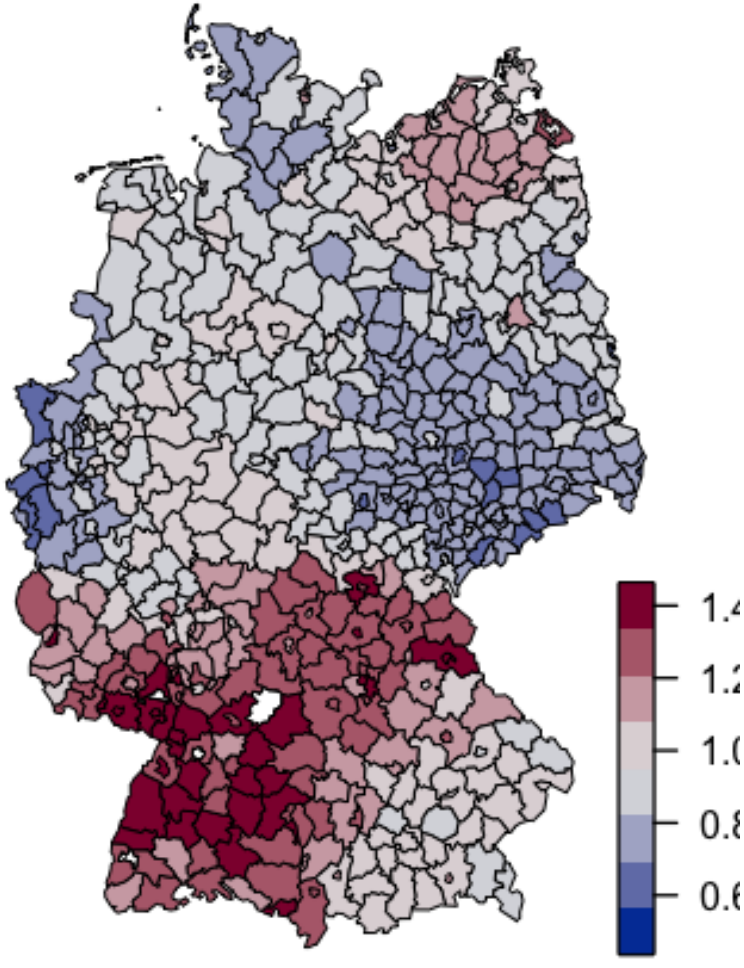
The structured and unstructured spatial effect as well as the smooth covariate effect will be each controlled by one parameter

- τ_c , τ_f , τ_η : The precisions (inverse variances) of the covariate effect, spatial effect and unstructured effect, respectively.

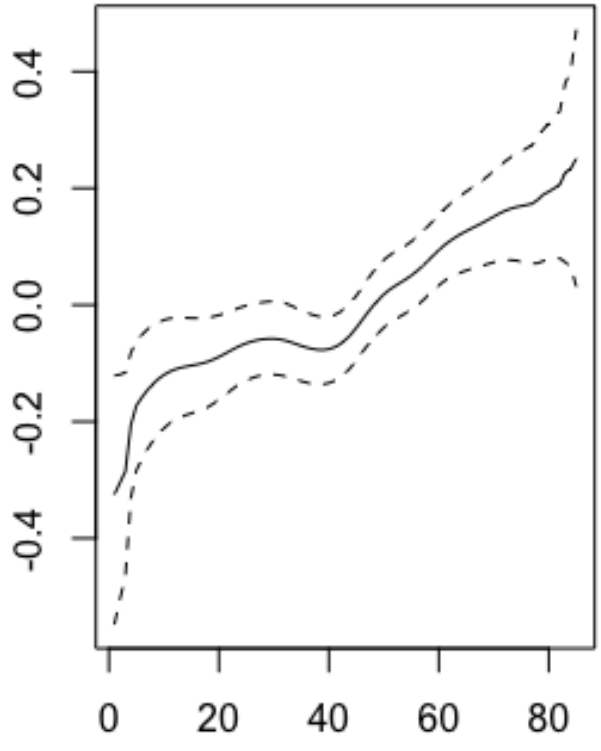
The hyperparameters are $\boldsymbol{\theta} = (\tau_c, \tau_f, \tau_\eta)$, and must be given a prior $\pi(\tau_c, \tau_f, \tau_\eta)$

What are we interested in?

Structured spatial effect $\exp(f_s(s_i))$



Covariate effect $\exp(f(c_i))$



INLA computing scheme

We want to approximate:

$$\pi(x_i|\boldsymbol{y}) = \int_{\boldsymbol{\theta}} \pi(x_i|\boldsymbol{\theta}, \boldsymbol{y})\pi(\boldsymbol{\theta}|\boldsymbol{y})d\boldsymbol{\theta}$$

$$\pi(\theta_j|\boldsymbol{y}) = \int_{\boldsymbol{\theta}_{-j}} \pi(\boldsymbol{\theta}|\boldsymbol{y})d\boldsymbol{\theta}_{-j}$$

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- Approximate $\pi(x_i|\boldsymbol{\theta}, \boldsymbol{y})$ as $\widetilde{\pi}(x_i|\boldsymbol{\theta}, \boldsymbol{y})$
- Use numerical integration (a finite sum) to compute
  - $$\widetilde{\pi}(x_i|\boldsymbol{y}) = \sum_k \widetilde{\pi}(x_i|\boldsymbol{\theta}_k, \boldsymbol{y})\ \widetilde{\pi}(\boldsymbol{\theta}_k|\boldsymbol{y})\ \Delta_k.$$
  - $$\widetilde{\pi}(\boldsymbol{\theta}_j|\boldsymbol{y})$$

Gaussian Markov Random Fields

A GMRF $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)$ is a random vector following a multivariate Gaussian distribution

$$\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{Q}^{-1}) \text{ where } \boldsymbol{Q}^{-1} = \boldsymbol{\Sigma}$$

and that is endowed with some Markov properties like

$$x_j \perp x_i | \boldsymbol{x}_{-ij}$$

where $\boldsymbol{x}_{-ij}$ indicates "all elements of $\boldsymbol{x}$ other than i and j"

The easiest example is a AR(1) model

Gaussian Markov Random Fields

If $\boldsymbol{\Sigma}$ is the covariance matrix of a Gaussian vector and $\boldsymbol{Q} = \boldsymbol{\Sigma}^{-1}$ is the precision matrix, we have that

$$x_i \perp x_j \iff \Sigma_{ij} = 0$$

and

$$x_i \perp x_j \iff Q_{ij} = 0$$

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GMRF have sparse precision matrices....this means it is "easy" to compute determinant and invert $\boldsymbol{Q}$

The GMRF approximation

Let $\boldsymbol{x}$ denote a GMRF with precision matrix $\boldsymbol{Q}$ and mean $\boldsymbol{\mu}$. Approximate

$$\pi(\boldsymbol{x}|\boldsymbol{\theta}, \boldsymbol{y}) \propto \exp\left(-\frac{1}{2}\boldsymbol{x}^\top \boldsymbol{Q}\boldsymbol{x} + \sum_{i=1}^{n} \log \pi(y_i|x_i)\right)$$

by using a second-order Taylor expansion of $\log \pi(y_i|x_i)$ around $\boldsymbol{\mu}_0$, say.

Recall

$$f(x) \approx f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2}f''(x_0)(x - x_0)^2 = a + bx - \frac{1}{2}cx^2$$

with $b = f'(x_0) - f''(x_0)x_0$ and $c = -f''(x_0)$.

The GMRF approximation (II)

Thus,

$$\tilde{\pi}(\boldsymbol{x}|\boldsymbol{\theta},\boldsymbol{y}) \propto \exp\left(-\frac{1}{2}\boldsymbol{x}^\top \boldsymbol{Q}\boldsymbol{x} + \sum_{i=1}^{n}(a_i + b_i x_i - 0.5 c_i x_i^2)\right)$$
$$\propto \exp\left(-\frac{1}{2}\boldsymbol{x}^T(\boldsymbol{Q} + \text{diag}(\boldsymbol{c}))\boldsymbol{x} + \boldsymbol{b}^T\boldsymbol{x}\right)$$

to get a Gaussian approximation with precision matrix $\boldsymbol{Q} + \text{diag}(\boldsymbol{c})$ and mean given by the solution of $(\boldsymbol{Q} + \text{diag}(\boldsymbol{c}))\boldsymbol{\mu} = \boldsymbol{b}$. The canonical parameterization is

$$\mathcal{N}_C(\mathbf{b}, \boldsymbol{Q} + \text{diag}(\boldsymbol{c}))$$

which corresponds to

$$\mathcal{N}((\boldsymbol{Q} + \text{diag}(\boldsymbol{c}))^{-1}\mathbf{b}, (\boldsymbol{Q} + \text{diag}(\boldsymbol{c}))^{-1}).$$

The GMFR approximation - One dimensional example

Assume

$$y|\lambda \sim \text{Poisson}(\lambda) \text{ Likelihood}$$
$$\lambda = \exp(x) \text{ Likelihood}$$
$$x \sim \mathcal{N}(0, 1) \text{ Latent Model}$$

we have that

$$\pi(x|y) \propto \pi(y|x)\pi(x) \propto \exp\{-\frac{1}{2}x^2 + \underbrace{xy - exp(x)}_{\text{non-gaussian part}}\}$$

(Show R-code `Taylor_expansion.R`)

The GMRF approximation