Bayesian modelling

Computational strategies and diagnostics

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Outline

How do we assess convergence of a MCMC algorithm?

- the algorithm implementation must be correct,
- the chain must have converged to the target posterior.
- the effective sample size must be sufficiently large for inference.

Strategies

Many diagnostics require running multiple chains

- check within vs between variance,
- determine whether they converge to the same target.

Correct implementation

We can generate artificial data to check the procedure.

Simulation-based calibration (Talts et al., 2020) proceeds with, in order

1. $\boldsymbol{\theta}_0 \sim p(\boldsymbol{\theta})$,
2. $\boldsymbol{y}_0 \sim p(\boldsymbol{y} \mid \boldsymbol{\theta}_0)$,
3. $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_B \sim p(\boldsymbol{\theta} \mid \boldsymbol{y}_0)$.

Simulation-based calibration

- Conditional on the simulated $\boldsymbol{y}$, the distribution of $\boldsymbol{\theta}_0$ is the same as that of $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_B$.
- We do a dimension reduction step taking the test function $t(\cdot)$ to get the rank of the prior draw among the posterior ones, breaking ties at random if any.
- These steps are repeated K times, yielding K test functions $T_1, \ldots, T_K$. We then test for uniformity using results from Säilynoja et al. (2022).

Breaking down the Markov chain

We distinguish between three phases

- **burn in** period: initial draws allowing the algorithm to converge to it's stationary distribution (discarded)
- **warmup** adaptation period: tuning period for the proposal std. deviation, etc. (discarded)
- sampling period: draws post burn in and warmup that are kept for inference

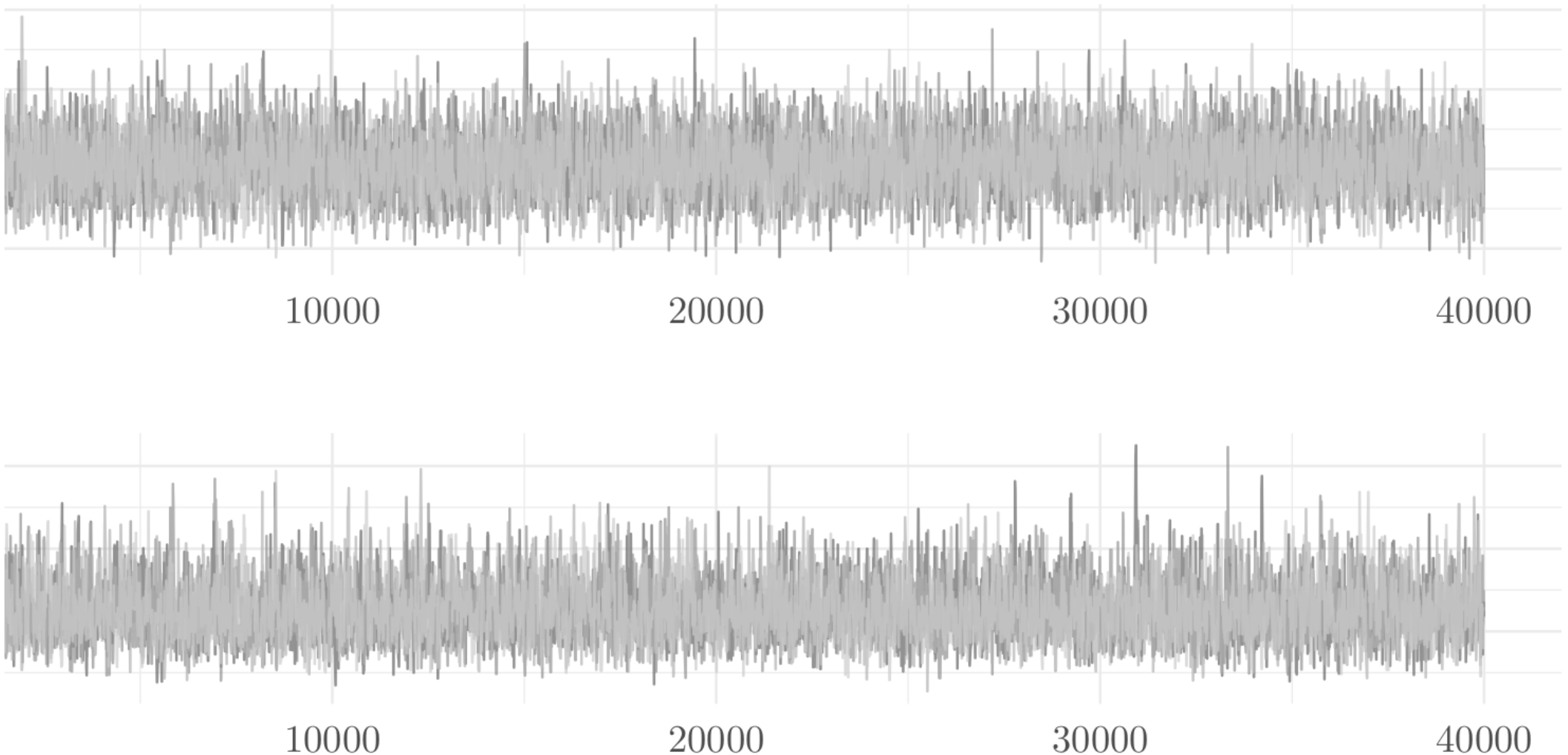
We can optionally **thin** by keeping one every k iterations from the sampling period to reduce the storage.

Visual diagnostic: trace plots

Display the Markov chain sample path as a function of the number of iterations.

- Ideally, run multiple chains to see if they converge to the same mode (for multimodal behaviour).
- Markov chains should look like a fat hairy caterpillar!
- Check the `bayesplot` and `coda` **R** packages (trace plot, trace rank, correlograms, marginal densities, etc.)

Checking convergence with multiple chains



Four healthy parallel chains for parameters.

Trace rank plot

A **trace rank** plot compares the rank of the values of the different chain at a given iteration.

- With good mixing, the ranks should switch frequently and be distributed uniformly across integers.

Effective sample size

Are my chains long enough to compute reliable summaries?

Compute the sample size we would have with independent draws by taking

$$\text{ESS} = \frac{B}{\{1 + 2\sum_{t=1}^{\infty} \gamma_t\}}$$

where γ_t is the lag t autocorrelation.

The relative effective sample size is simply ESS/B: small values indicate pathological or inefficient samplers.

How many samples?

We want our average estimate to be reliable!

- We probably need ESS to be several hundred
- We can estimate the variance of the target to know the precision
- (related question: how many significant digits to report?)

Estimating the variance (block method)

1. Break the chain of length B (after burn in) in K blocks of size $\approx K/B$.
2. Compute the sample mean of each segment. These values form a Markov chain and should be approximately uncorrelated.
3. Compute the standard deviation of the segments mean. Rescale by $K^{-1/2}$ to get standard error of the global mean.

More efficient methods using overlapping blocks exists.

Block means in pictures

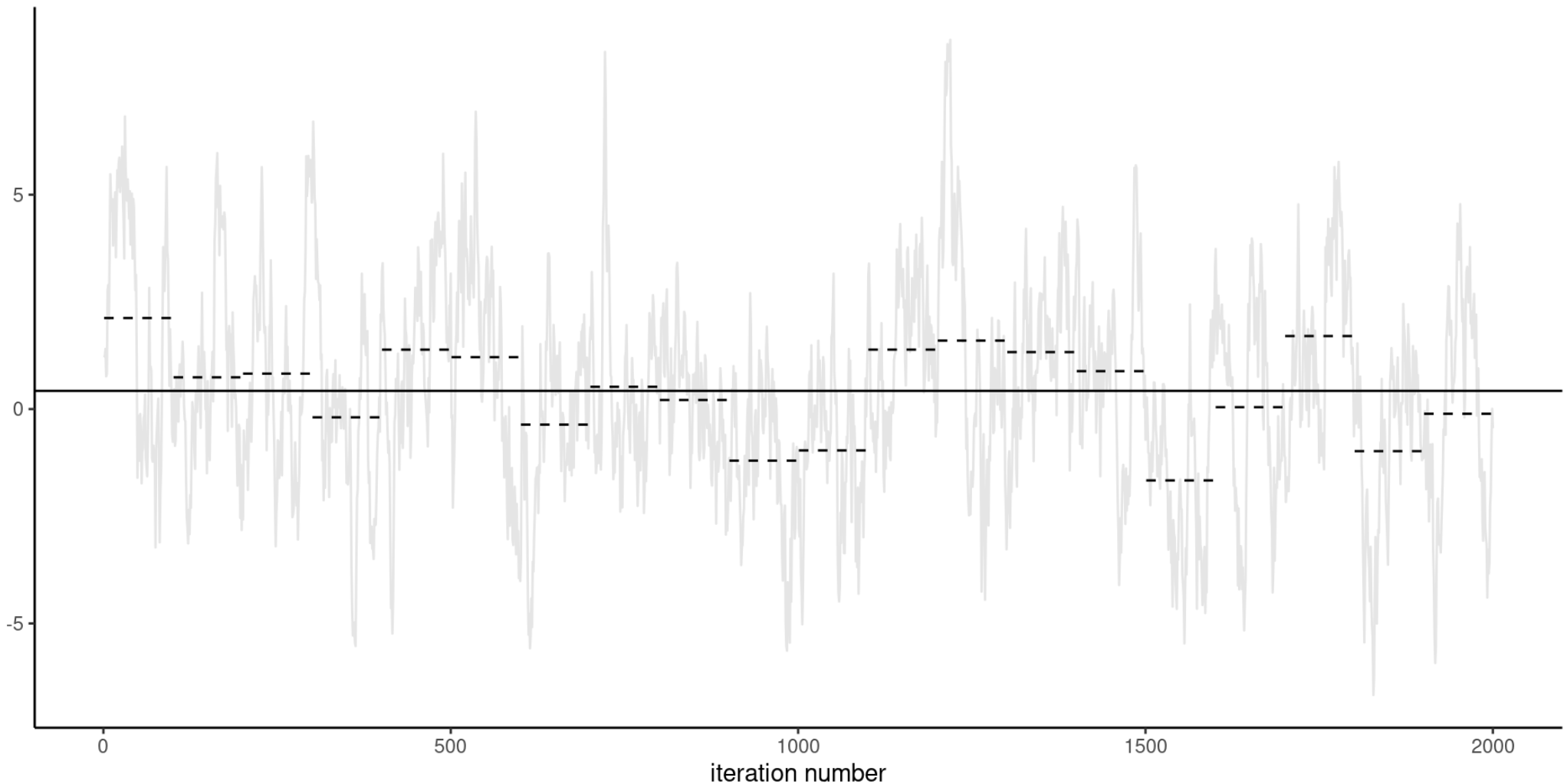


Figure 1: Calculation of the standard error of the posterior mean using the batch method.

Cautionary warning about stationarity

Batch means only works if the chain is sampling from the stationary distribution!

The previous result (and any estimate) will be unreliable and biased if the chain is not (yet) sampling from the posterior.

Lack of stationarity

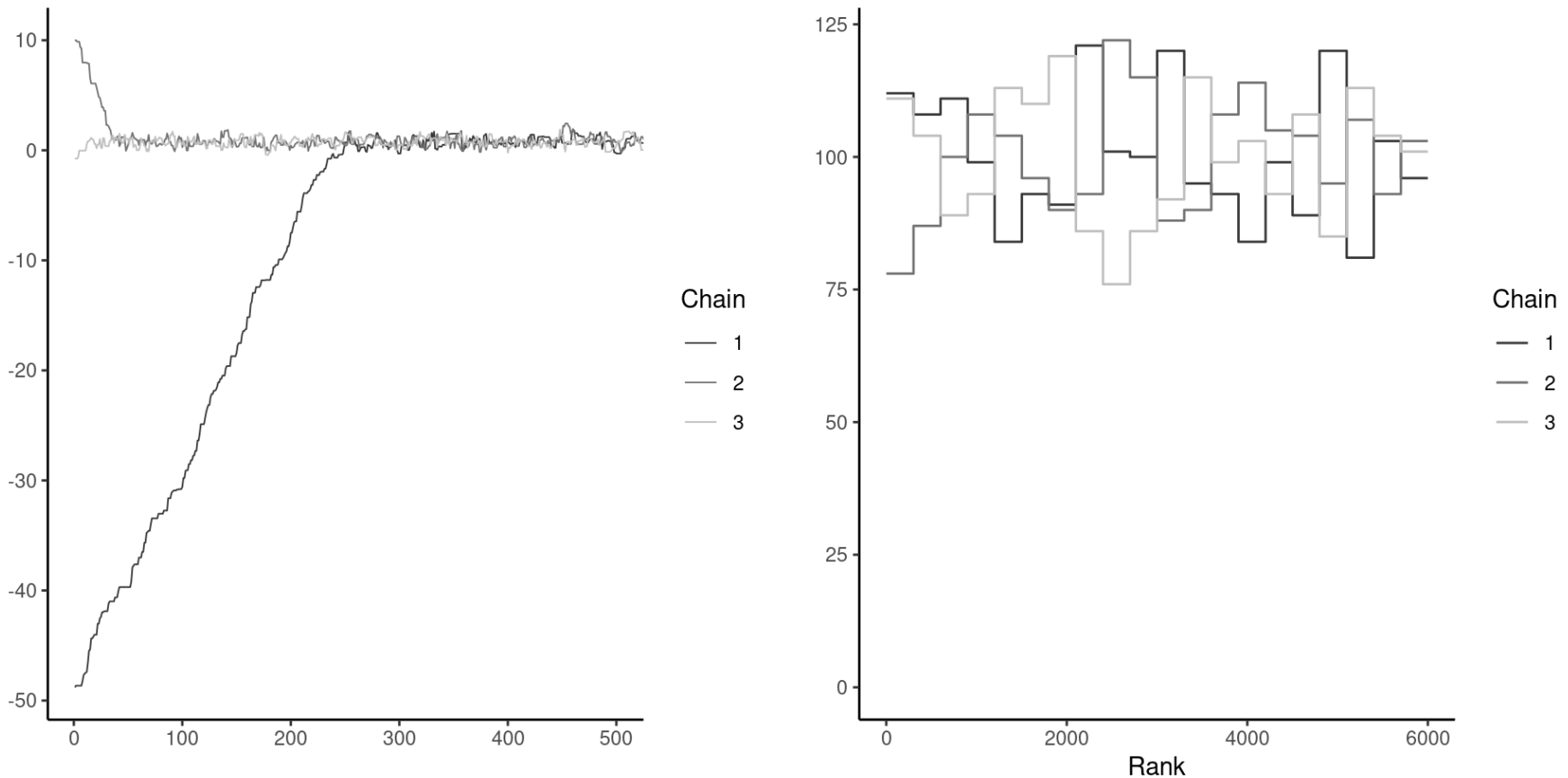


Figure 2: Traceplots of three Markov chains for the same target with different initial values for the first 500 iterations (left) and trace rank plot after discarding these (right). The latter is indicative of the speed of mixing.

Gelman–Rubin diagnostic

Suppose we run M chains for B iterations, post burn in.

Denote by θ_{bm} the bth draw of the mth chain, we compute the global average

$$\bar{\theta} = \frac{1}{BM} \sum_{b=1}^{B} \sum_{m=1}^{m} \theta_{bm}$$

and similarly the chain-specific sample average and variances, respectively $\bar{\theta}_m$ and $\widehat{\sigma}^2_m$ ($m = 1, \ldots, M$).

Sum of square decomposition

The between-chain variance and within-chain variance estimator are

$$\mathsf{Va}_{\text{between}} = \frac{B}{M-1}\sum_{m=1}^{M}(\bar{\theta}_m - \bar{\theta})^2$$

$$\mathsf{Va}_{\text{within}} = \frac{1}{M}\sum_{m=1}^{m}\widehat{\sigma}_m^2$$

Potential scale reduction statistic

The Gelman–Rubin diagnostic, denoted $\widehat{R}$, is obtained by running multiple chains and considering the difference between within-chain and between-chains variances,

$$\widehat{R} = \left(\frac{\mathsf{Va}_{\text{within}}(B-1) + \mathsf{Va}_{\text{between}}}{B\mathsf{Va}_{\text{within}}} \right)^{1/2}$$

Any value of $\widehat{R}$ larger 1 is indicative of problems of convergence.

Bad chains

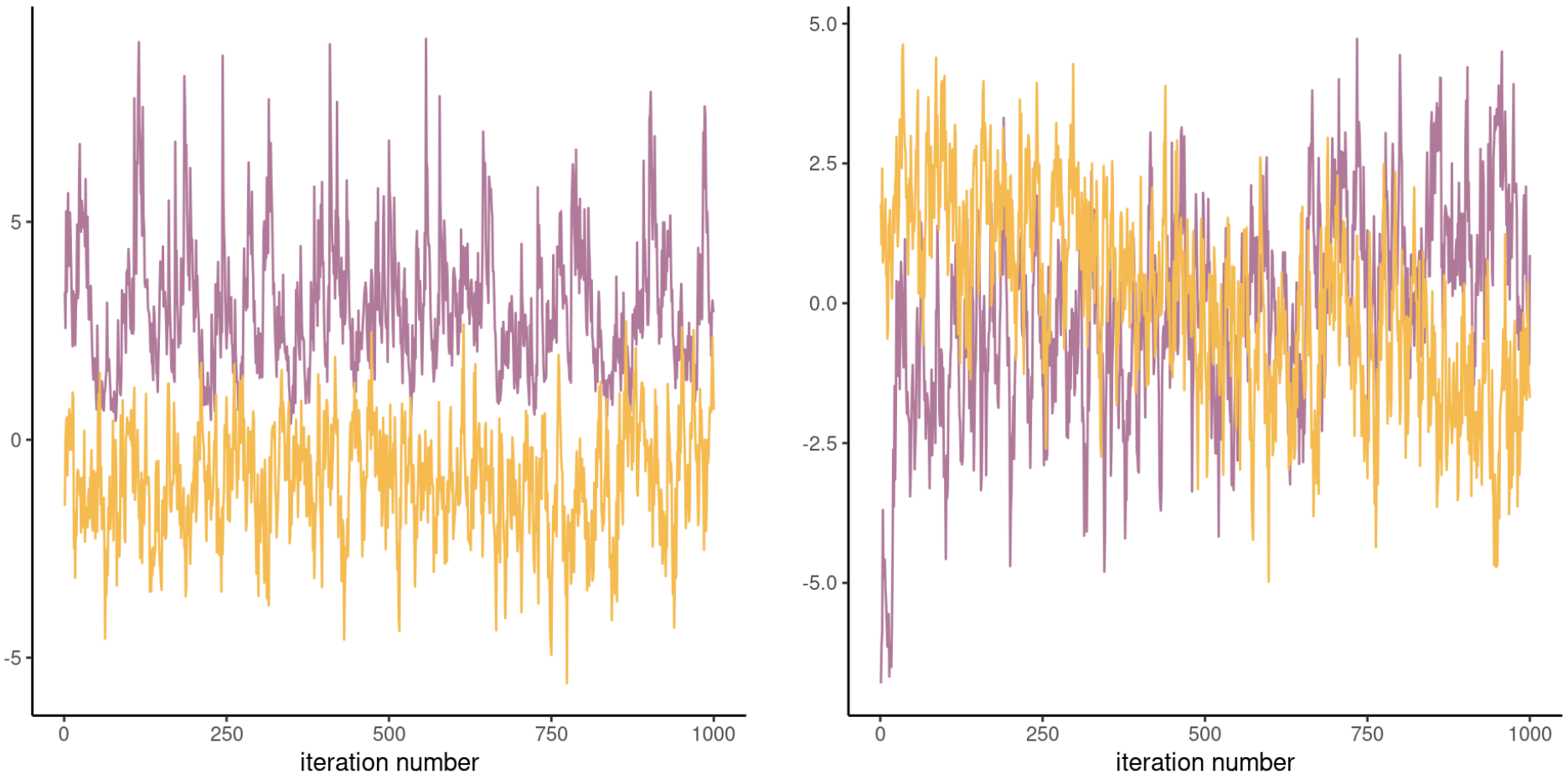


Figure 3: Two pairs of Markov chains: the top ones seem stationary, but with different modes and $\widehat{R} \approx 3.4$. The chains on the right hover around zero, but do not appear stable, with $\widehat{R} \approx 1.6$.

One chain or multiple chains?

Generally, it is preferable to run a single chain for a longer period than run multiple chains sequentially

- there is a cost to initializing multiple times with different starting values since we must discard initial draws.
- but with parallel computations, multiple chains are more frequent nowadays.
- multiple diagnostics require running several chains.

Posterior predictive checks

1. For each of the B draws from the posterior, simulate n observations from the posterior predictive $p(\tilde{\boldsymbol{y}} \mid \boldsymbol{y})$
2. For each replicate, compute a summary statistics (median, quantiles, std. dev., etc.)
3. Compare it with the same summary computed for the sample $\boldsymbol{y}$.

Posterior predictive checks

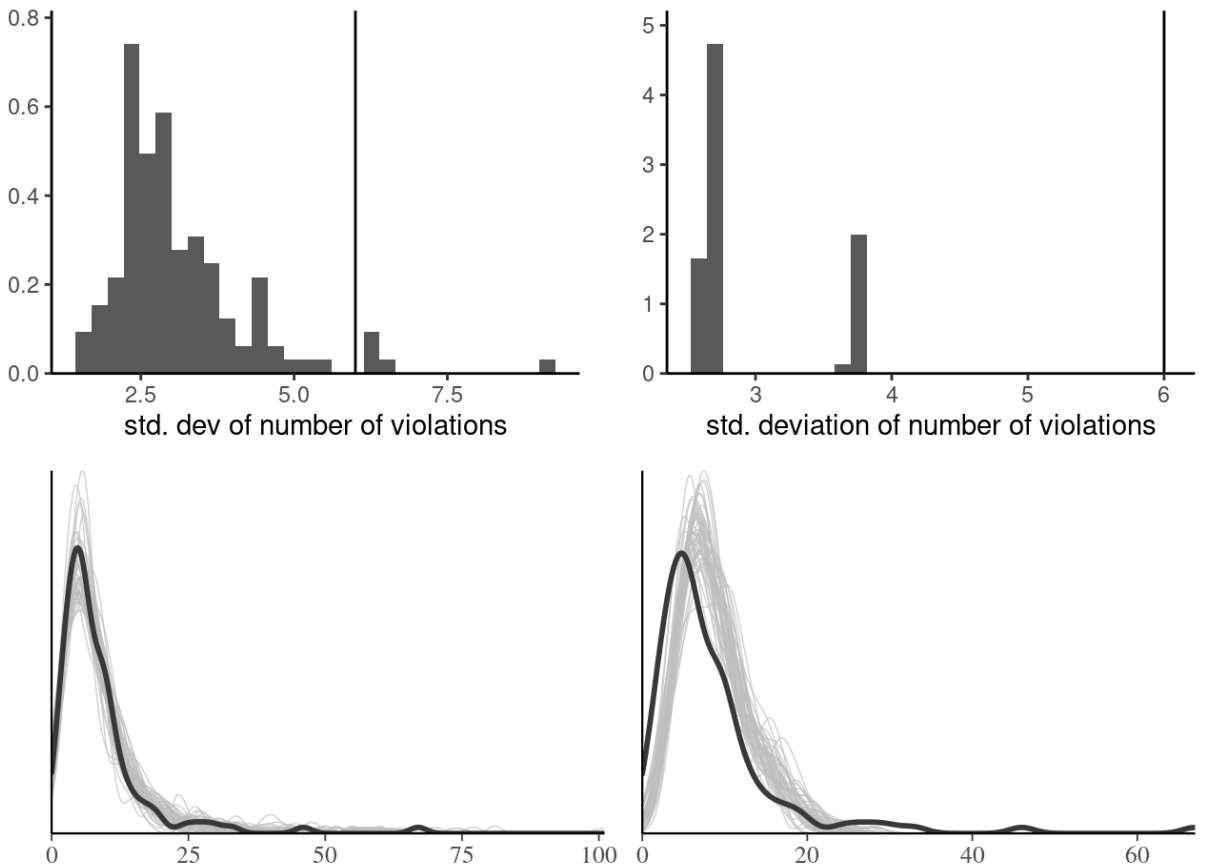


Figure 4: Posterior predictive checks for the standard deviation (top) and density of posterior draws (bottom) for hierarchical Poisson model with individual effects (left) and simpler model with only conditions (right).

Log pointwise predictive density

Consider the expected value of the log observation-wise log density with respect to the posterior distribution $p(\boldsymbol{\theta} \mid \boldsymbol{y})$,

$$\text{LPPD}_i = \text{E}_{\boldsymbol{\theta}|\boldsymbol{y}} \left\{ \log p(y_i \mid \boldsymbol{\theta}) \right\},$$

The higher the value of LPPD_i, the better the fit for that observation.

Widely available information criterion

To build an information criterion, we add a penalization factor that approximates the effective number of parameters in the model, with

$$n\mathsf{WAIC} = -\sum_{i=1}^{n} \mathsf{LPPD}_i + \sum_{i=1}^{n} \mathsf{Va}_{\boldsymbol{\theta}|\boldsymbol{y}}\{\log p(y_i \mid \boldsymbol{\theta})\}$$

where we use again the empirical variance to compute the rightmost term.

Smaller values of WAIC are better.

Pseudo-code for WAIC

Evaluate the log likelihood for each posterior draw and each observation.

```
#' WAIC
#' @param loglik_pt B by n matrix of pointwise log likelihood
WAIC <- function(loglik_pt){
  -mean(apply(loglik_pt, 2, mean)) +  mean(apply(loglik_pt, 2, var))
}
```

Bayesian leave-one-out cross validation

In Bayesian setting, we can use the leave-one-out predictive density

$$p(y_i \mid \boldsymbol{y}_{-i})$$

as a measure of predictive accuracy. the

We can use importance sampling to approximate the latter.

Requirement: need to keep track of the log likelihood of each observation for each posterior draw ($B \times n$ values).

LOO-CV diagnostics

We can draw B samples from $p(\tilde{y} \mid \boldsymbol{y}_{-i})$ and compute the rank of y_i.

Under perfect calibration, ranks should be uniform.

Leave-one-out with quantile-quantile plots

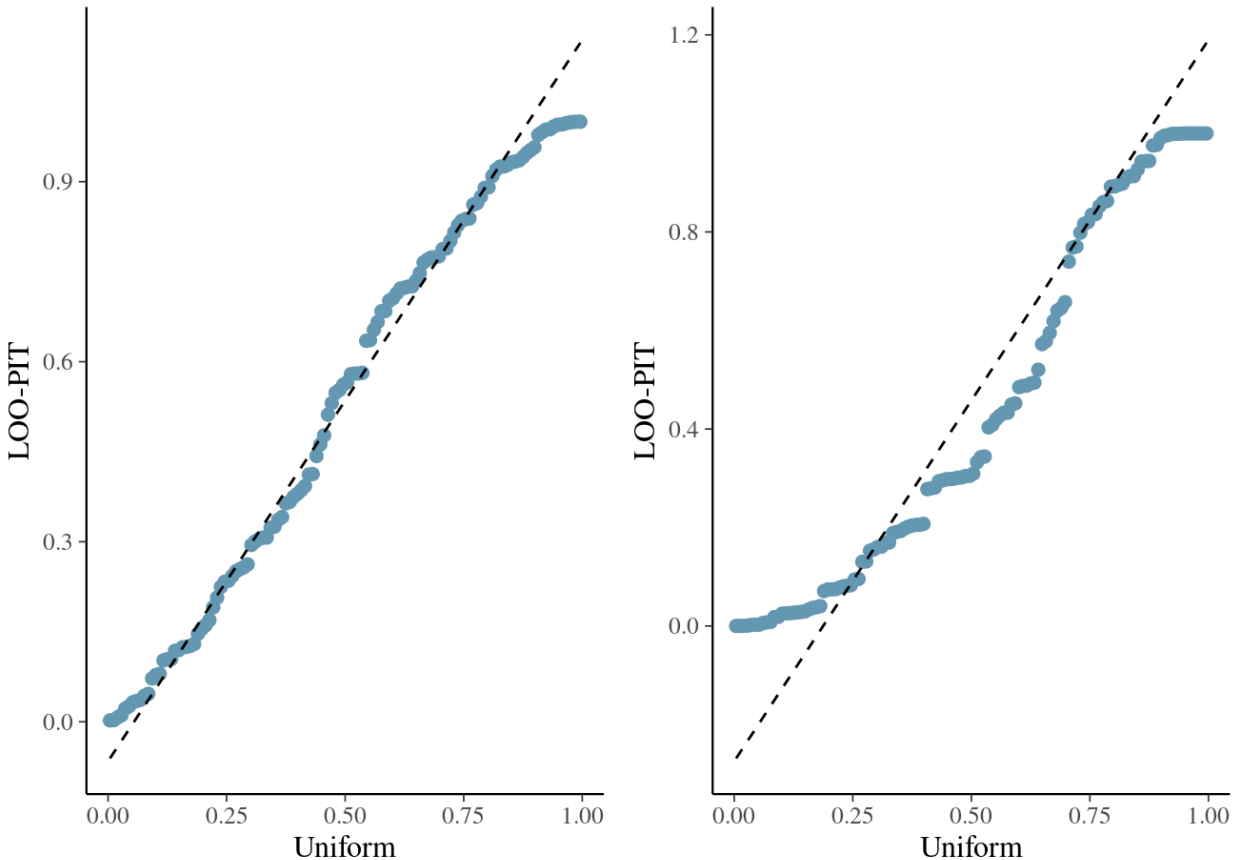


Figure 5: Quantile-quantile plots based on leave-one-out cross validation for model for the hierarchical Poisson model fitted to the Upworthy data with the individual random effects (left) and without (right).

Deviance information criterion

The **deviance** information criterion of Spiegelhalter et al. (2002) is

$$\text{DIC} = -2\ell(\tilde{\boldsymbol{\theta}}) + 2p_D$$

where p_D is the posterior expectation of the deviance relative to the point estimator of the parameter $\tilde{\boldsymbol{\theta}}$ (e.g., the maximum a posteriori or the posterior mean)

$$p_D = \mathsf{E}\{D(\boldsymbol{\theta}, \tilde{\boldsymbol{\theta}}) \mid \boldsymbol{y}\} = \int 2\{\ell(\tilde{\boldsymbol{\theta}}) - \ell(\boldsymbol{\theta})\} f(\boldsymbol{\theta} \mid \boldsymbol{y} \mathrm{d}\boldsymbol{\theta}$$

Criticism of DIC

- The DIC can be easily evaluated by keeping track of the log likelihood evaluated at each posterior draw from a Markov chain Monte Carlo algorithm.
- The penalty term p_D is however not invariant to reparametrizations.
- A Gaussian approximation to the MLE under suitable regularity conditions shows that the DIC is equivalent in large samples to AIC.

Computational strategies

Sources of poor mixing

Slow mixing can be due to the following:

- poor proposals
- strong correlation between posterior parameters
- overparametrization and lack of identifiability

Computational strategies

These problems can be addressed using one of the following:

- removing redundant parameters or pinning some using sharp priors
- reparametrization
- clever proposals (adaptive MCMC), see Andrieu & Thoms (2008) and Rosenthal (2011).
- marginalization
- blocking

Removing redundant parameters

Consider a one-way ANOVA with K categories, with observation i from group k having

$$Y_{i,k} \sim \textsf{Gauss}(\mu + \alpha_k, \sigma_y^2)$$
$$\alpha_k \sim \textsf{Gauss}(0, \sigma_\alpha^2)$$

and an improper prior for the mean $p(\mu) \propto 1$.

There are $K + 1$ mean parameters for the groups, so we can enforce a sum-to-zero constraint for $\sum_{k=1}^{K} \alpha_k = 0$ and sample $K - 1$ parameters for the difference to the global mean.

Parameter expansion

Add redundant parameter to improve mixing by decorrelating (Liu et al., 1998)

$$Y_{i,k} \sim \text{Gauss}(\mu + \xi\eta_k, \sigma_y^2)$$
$$\eta_k \sim \text{Gauss}(0, \sigma_\eta^2)$$

so that $\sigma_\alpha = |\xi|\sigma_\eta$.

Marginalization

Given a model $p(\boldsymbol{\theta}, \boldsymbol{Z})$, reduce the dependance by sampling from the marginal

$$p(\boldsymbol{\theta}) = \int p(\boldsymbol{\theta}, \boldsymbol{z}) \mathrm{d}\boldsymbol{z}.$$

This happens for data augmentation, etc., and reduces dependency between parameters, but typically the likelihood becomes more expensive to compute

Gaussian model with random effects

Consider a hierarchical Gaussian model of the form

$$\boldsymbol{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{B} + \boldsymbol{\varepsilon}$$

where

- $\mathbf{X}$ is an $n \times p$ design matrix with centered inputs,
- $\boldsymbol{\beta} \sim \text{Gauss}(\mathbf{0}_p, \sigma^2\mathbf{I}_p)$,
- $\boldsymbol{B} \sim \text{Gauss}_q(\mathbf{0}_q, \boldsymbol{\Omega})$ are random effects and
- $\boldsymbol{\varepsilon} \sim \text{Gauss}_n(\mathbf{0}_n, \kappa^2\mathbf{I}_n)$ are independent white noise.

Marginalization of Gaussian models

We can write

$$\begin{aligned}\boldsymbol{Y} \mid \beta, \boldsymbol{B} &\sim \textsf{Gauss}_n(\mathbf{X}\beta + \mathbf{Z}\boldsymbol{B}, \sigma^2\mathbf{I}_p) \\ \boldsymbol{Y} \mid \beta &\sim \textsf{Gauss}_n(\mathbf{X}\beta, \mathbf{Q}^{-1}),\end{aligned}$$

where the second line corresponds to marginalizing out the random effects $\boldsymbol{B}$.

Efficient calculations for Gaussian models

If, as is often the case, $\boldsymbol{\Omega}^{-1}$ and $\mathbf{Z}$ are sparse matrices, the full precision matrix can be efficiently computed using Shermann–Morisson–Woodbury identity as

$$\begin{aligned}\mathbf{Q}^{-1} &= \mathbf{Z}\boldsymbol{\Omega}^{-1}\mathbf{Z}^\top + \kappa^2\mathbf{I}_n, \\ \kappa^2\mathbf{Q} &= \mathbf{I}_n - \mathbf{Z}\boldsymbol{G}^{-1}\mathbf{Z}^\top, \\ \boldsymbol{G} &= \mathbf{Z}^\top\mathbf{Z} + \kappa^2\boldsymbol{\Omega}^{-1}\end{aligned}$$

Section 3.1 of Nychka et al. (2015) details efficient ways of calculating the quadratic form involving $\mathbf{Q}$ and it's determinant.

Blocking

Identify groups of strongly correlated parameters and propose a joint update for these.

- The more parameters we propose at the same time, the lower the chance of acceptance
- Often ways to sample these efficiently

Tokyo rainfall

We consider data from Kitagawa (1987) that provide a binomial time series giving the number of days in years 1983 and 1984 (a leap year) in which there was more than 1mm of rain in Tokyo; see section 4.3.4 of Rue & Held (2005).

We have $T = 366$ days and $n_t \in \{1, 2\}$ $(t = 1, \ldots, T)$ the number of observations in day t and $y_t = \{0, \ldots, n_t\}$ the number of days with rain.

Smoothing probabilities

The objective is to obtain a smoothed probability of rain. The underlying probit model considered takes $Y_t \mid n_t, p_t \sim \textsf{binom}(n_t, p_t)$ and $p_t = \Phi(\beta_t)$.

We specify the random effects $\boldsymbol{\beta} \sim \textsf{Gauss}_T(\mathbf{0}, \tau^{-1}\mathbf{Q})$, where $\mathbf{Q}$ is a $T \times T$ precision matrix that encodes the local dependence.

A circular random walk structure of order 2 is used to model the smooth curves by smoothing over neighbors, and enforces small second derivative. This is a suitable prior because it enforces no constraint on the mean structure.

Random walk prior

This amounts to specifying the process with for $t \in \mathbb{N} \mod 366 + 1$ *[Math Processing Error]*

Circulant precision matrix

This yields an intrinsic Gaussian Markov random field with a circulant precision matrix $\tau\mathbf{Q}$ of rank $T-1$, where *[Math Processing Error]* Because of the linear dependency, the determinant of $\mathbf{Q}$ is zero.

Prior draws

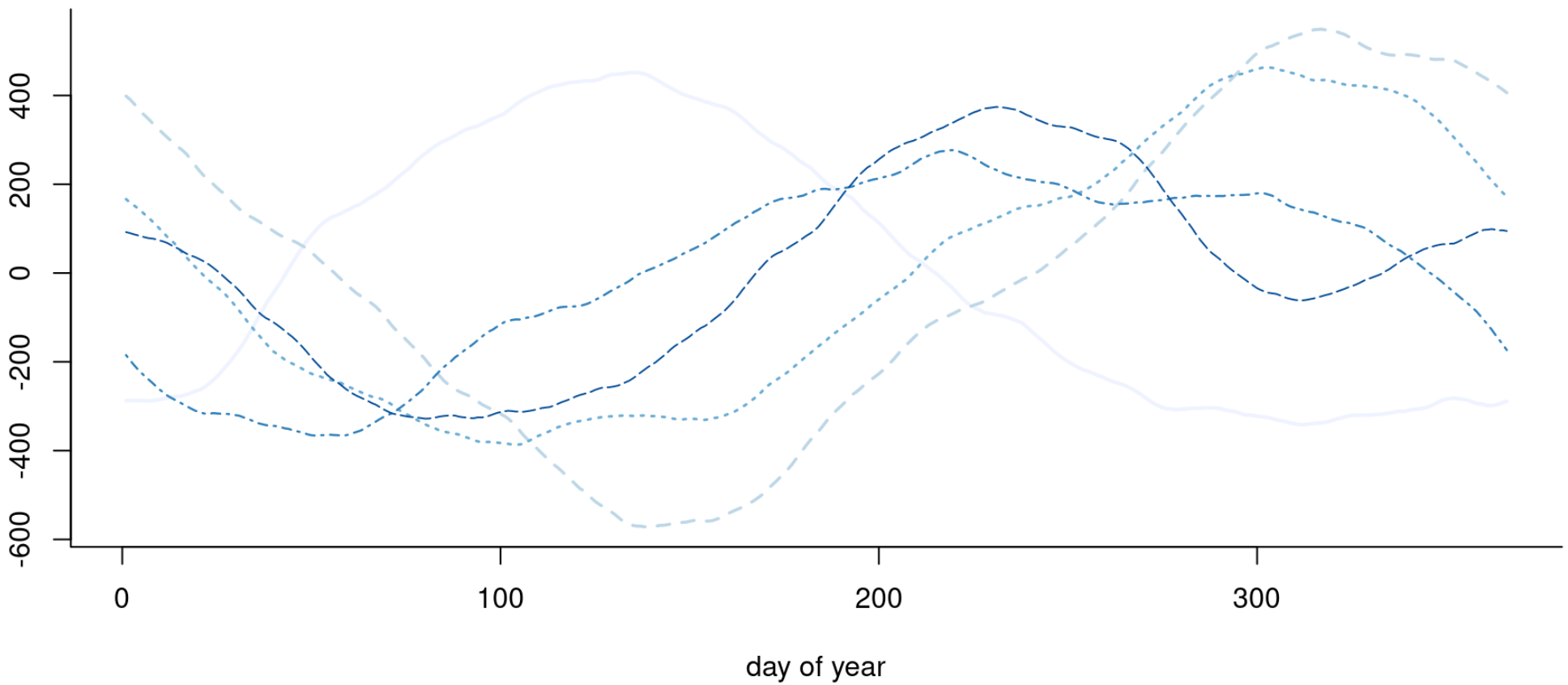


Figure 6: Five realizations from the cyclical random walk Gaussian prior of order 2.

Gibbs sampling for Tokyo data

We can perform data augmentation by imputing Gaussian variables, say $\{z_{t,i}\}$ from truncated Gaussian, where $z_{t,i} = \beta_t + \varepsilon_{t,i}$ and $\varepsilon_{t,i} \sim \textbf{Gauss}(0,1)$ are independent standard Gaussian and *[Math Processing Error]*

Posterior for Tokyo data

The posterior is proportional to *[Math Processing Error]*

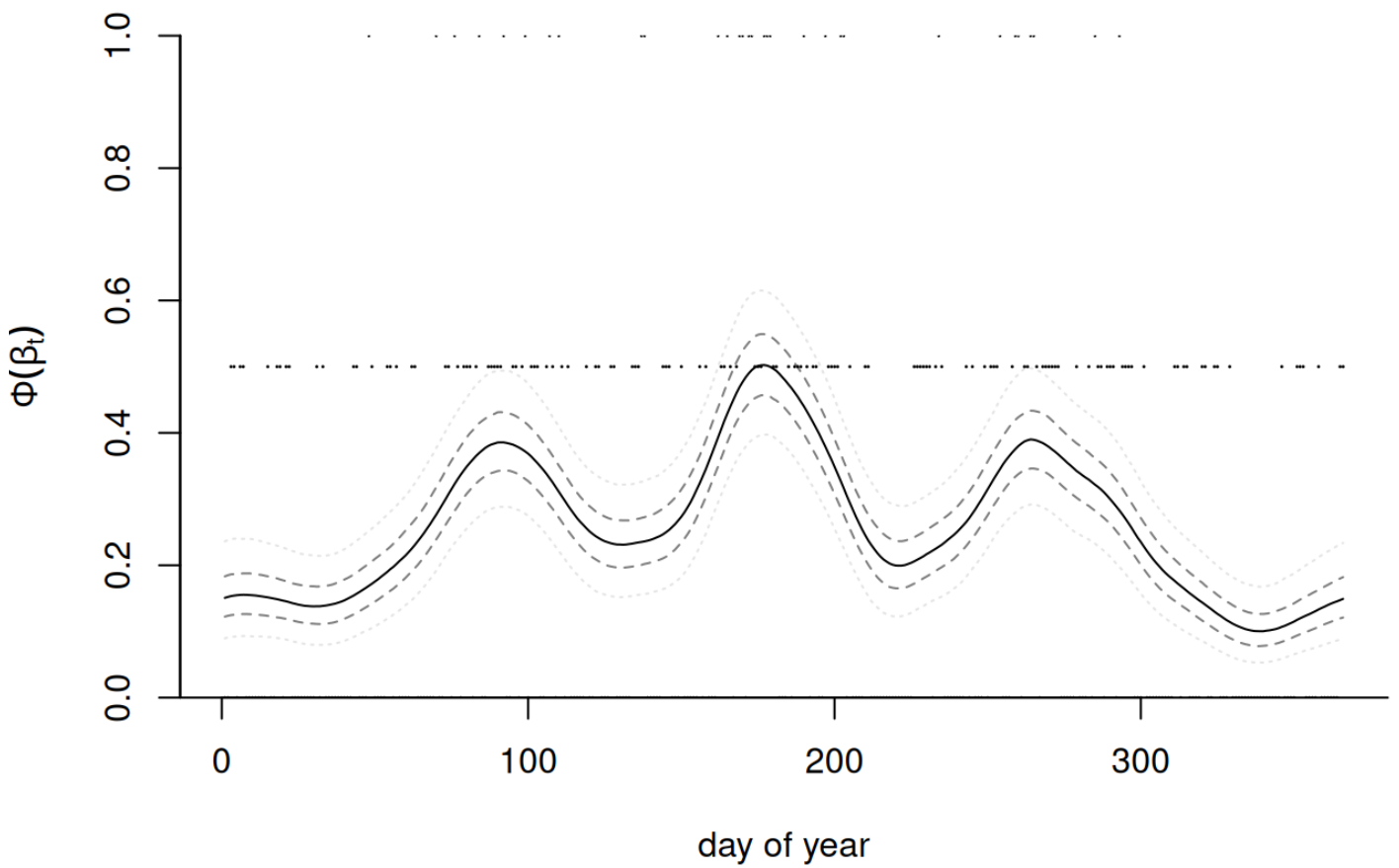
Data augmentation for Tokyo data

Once we have imputed the Gaussian latent vectors, we can work directly with the values of $z_t = \sum_{i=1}^{n_t} z_{i,t}$. The posterior is *[Math Processing Error]* where $\boldsymbol{z} = (z_1, \ldots, z_T)$.

Gibbs for Tokyo data - conditionals

Completing the quadratic form shows that *[Math Processing Error]*

Posterior prediction for probability of rainfall



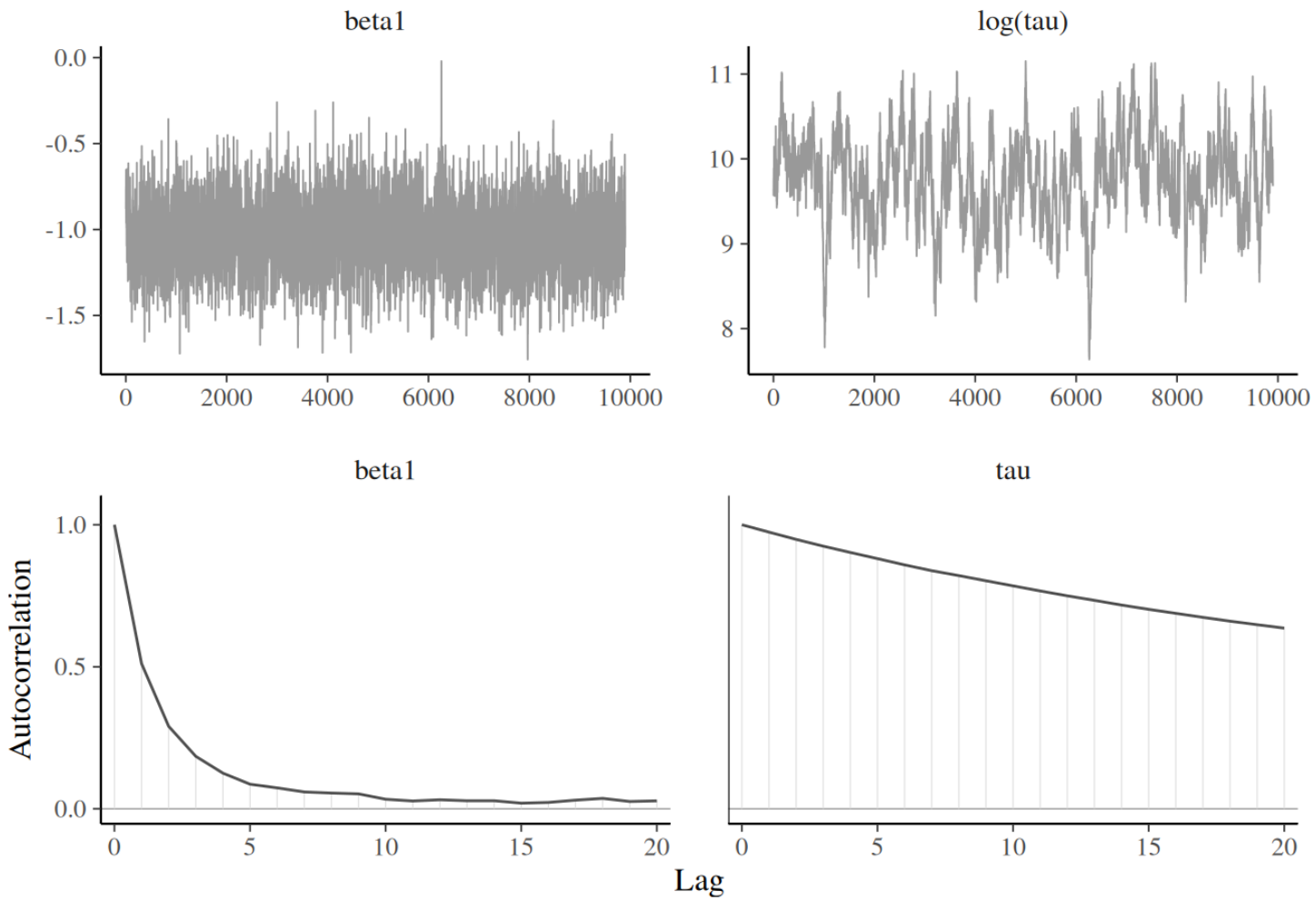
Posterior prediction for probability of rainfall

Blocking vs joint update

Compare the following two stategies

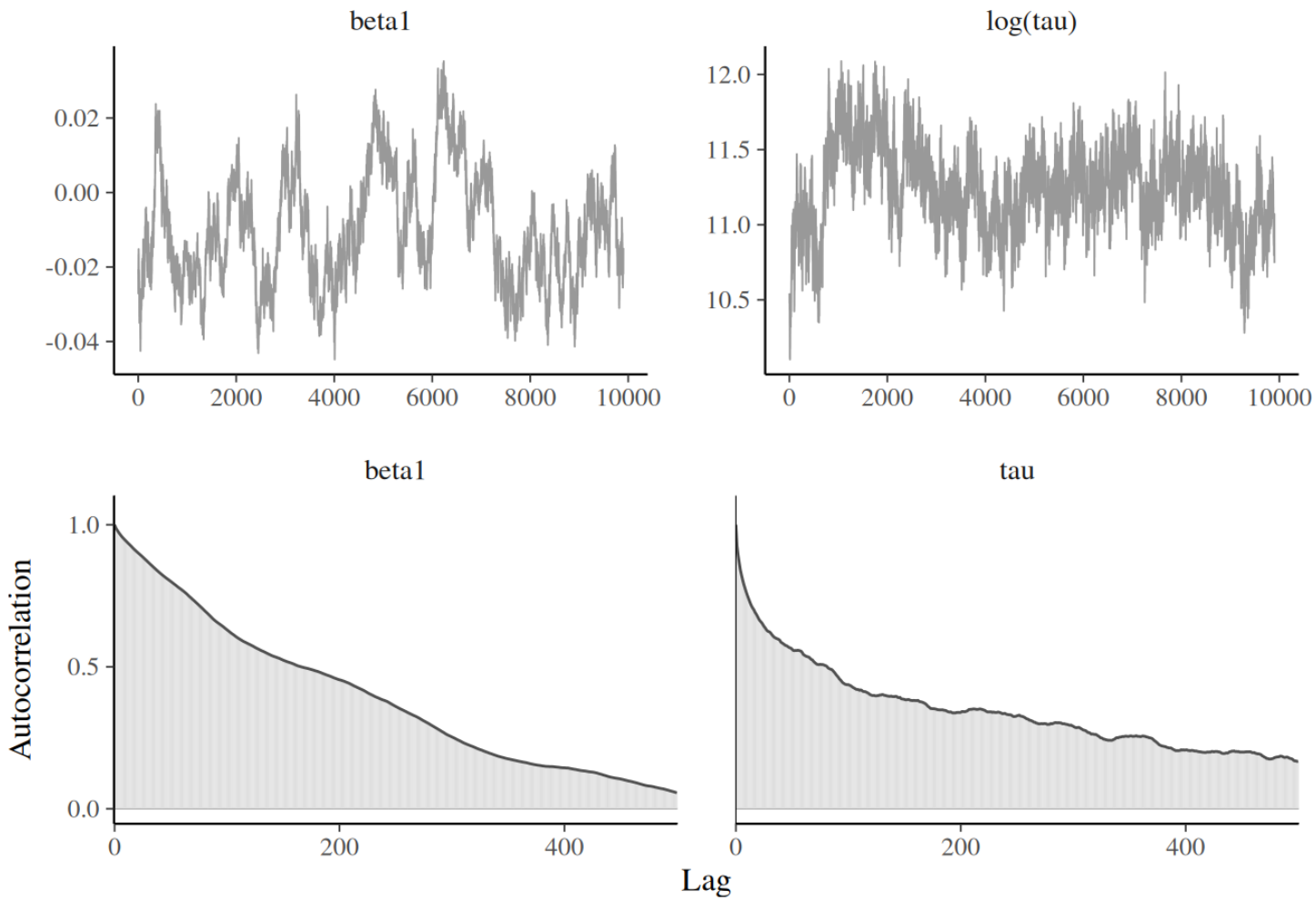
- joint update: given $\boldsymbol{z}$ and τ, simulate $\boldsymbol{\beta}$ jointly
- one-parameter at a time: starting from $i \sim \textsf{unif}(\{1, \ldots, 366\})$, get index $t = i \mod 366 + 1$ and simulate $\beta_i \mid \boldsymbol{\beta}_{-i}, \boldsymbol{z}, \tau$ one at a time.

Blocking strategy



Trace plots for Tokyo with blocking of random effects

Individual update strategy



Trace plots for Tokyo with random scan Gibbs for random effects

Lessons from the Tokyo example

What happened?

- there is lower autocorrelation with the joint update (also faster here!) for the $\boldsymbol{\beta}$
- in both cases, $\tau \mid \cdot$ mixes poorly because the values of $\boldsymbol{\beta}$ were sampled conditional on the previous value.

A better avenue would be to use a Metropolis random walk for $\tau^\star$, simulate $\boldsymbol{\beta} \mid \tau^\star$ and propose the joint vector $(\tau^\star, \boldsymbol{\beta}^\star)$ simultaneously.

One step further

We could also remove the data augmentation step and propose from a Gaussian approximation of the log likelihood, using a Taylor series expansion of the log likelihood about $\boldsymbol{\beta}_{t-1}$ *[Math Processing Error]* and the y_t are conditionally independent in the likelihood. Refer to Section 4.4.1 of Rue & Held (2005) for more details.

Technical aside: in sparsity we trust!

It is crucial to exploit the sparsity structure of $\mathbf{Q}$ for efficient calculations of the likelihood

- typically requires re-ordering elements to get a banded precision matrix
- precompute the sparse Cholesky
- compute inverse by solving systems of linear equations; there are dedicated algorithms

References

Andrieu, C., & Thoms, J. (2008). A tutorial on adaptive MCMC. *Statistics and Computing*, *18*(4), 343–373. https://doi.org/10.1007/s11222-008-9110-y

Kitagawa, G. (1987). Non-Gaussian state–space modeling of nonstationary time series. *Journal of the American Statistical Association*, *82*(400), 1032–1041. https://doi.org/10.1080/01621459.1987.10478534

Liu, C., Rubin, D. B., & Wu, Y. N. (1998). Parameter expansion to accelerate EM: The PX-EM algorithm. *Biometrika*, *85*(4), 755–770. https://doi.org/10.1093/biomet/85.4.755

Nychka, D., Bandyopadhyay, S., Hammerling, D., Lindgren, F., & Sain, S. (2015). A multiresolution Gaussian process model for the analysis of large spatial datasets. *Journal of Computational and Graphical Statistics*, *24*(2), 579–599.

Rosenthal, J. (2011). Optimal proposal distributions and adaptive MCMC. In S. Brooks, A. Gelman, G. Jones, & X. L. Meng (Eds.), *Handbook of Markov chain Monte Carlo* (pp. 93–112). CRC Press. https://doi.org/10.1201/b10905-5

Rue, H., & Held, L. (2005). *Gaussian Markov random fields: Theory and applications* (p. 280). CRC Press.

Säilynoja, T., Bürkner, P.-C., & Vehtari, A. (2022). Graphical test for discrete

uniformity and its applications in goodness-of-fit evaluation and multiple sample comparison. *Statistics and Computing*, *32*(2), 32. https://doi.org/10.1007/s11222-022-10090-6

Spiegelhalter, D. J., Best, N. G., Carlin, B. P., & Van Der Linde, A. (2002). Bayesian measures of model complexity and fit. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, *64*(4), 583–639. https://doi.org/10.1111/1467-9868.00353

Talts, S., Betancourt, M., Simpson, D., Vehtari, A., & Gelman, A. (2020). *Validating Bayesian inference algorithms with simulation-based calibration*. https://doi.org/10.48550/arXiv.1804.06788