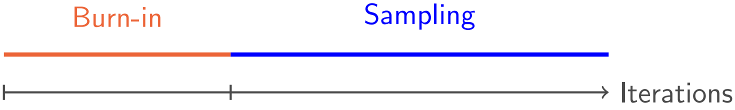
The Convergence Challenge in MCMC

- **Ideal goal**: Assess whether MCMC chains have converged
- **Fundamental problem**:
  - In general, impossible to know for sure that there is no problem
  - But we can sometimes know for sure that there *is* a problem
- **Two phases of MCMC**:
  - Transient phase (burn-in): mixing time
  - Stationary phase: Monte Carlo estimation

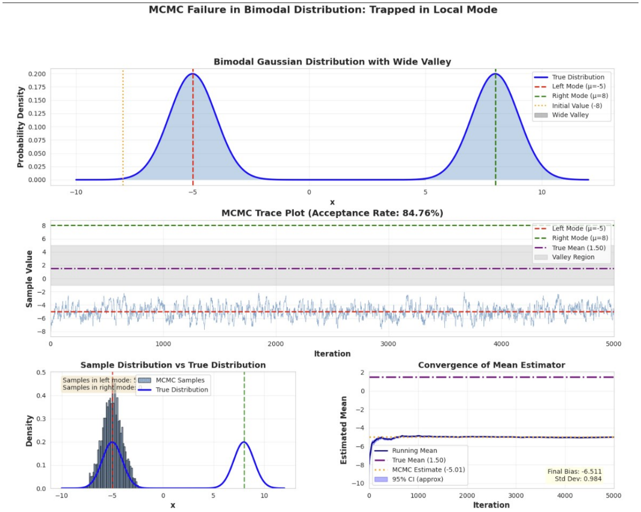


Why Convergence Matters

Non-converged chains:

- Biased estimates
- Incorrect uncertainty quantification
- Missing important modes
- Unreliable inference

Motivating example



The Intuition Behind Gelman-Rubin

Core Idea

If MCMC chains have converged to the target distribution, then:

- Multiple chains started from different points should look similar
- Within-chain variance ≈ Between-chain variance

Compare two sources of variance:

1. Within-chain variance (W)
   How much each chain varies
2. Between-chain variance (B)
   How different chains are from each other

Within-chain variance - W

Run M chains. The sample mean of M sample variances

$$W = \frac{1}{M}\sum_{m=1}^{M}\left[\frac{1}{T-1}\sum_{t=1}^{T}(X_{m,t} - \bar{X}_{m,\cdot})^2\right]$$

We have that the expected sample variance for one chain is

$$\mathbb{E}\left[\frac{1}{T-1}\sum_{t=1}^{T}(X_{m,t} - \bar{X}_{m,\cdot})^2\right] = \frac{T}{T-1}\Big(\sigma^2 - Var(\bar{X}_{m,\cdot})\Big) < \sigma^2$$

[1] making the estimator unbiased only in the case $Var(\bar{X}_{m,.}) = \sigma^2/T$ (iid samples). For MCMC samples, $Var(\bar{X}_{m,.})$ is typically larger than σ^2/T due to autocorrelation, so W underestimates σ^2.

[1] when $Var(\bar{X}_{m,\cdot}) > \sigma^2/T$

Between-chain variance - B

For the M chains, we compute the variance of the chain means:

$$B = \frac{1}{M-1} \sum_{m=1}^{M} (\bar{X}_{m,\cdot} - \bar{X}_{\cdot,\cdot})^2$$

where $\bar{X}_{\cdot,\cdot}$ is the mean across all chains. We have that

$$\mathbb{E}[B] = Var(\bar{X}_{m,\cdot})$$

Formula for V

Let $S_m = \frac{1}{T-1}\sum_{t=1}^{T}(X_{m,t} - \bar{X}_{m,\cdot})^2$ be the sample variance of chain m. On slide 5 we saw that the expected sample variance for one chain is

$$\mathbb{E}[S_m] = \frac{T}{T-1}\Big(\sigma^2 - Var(\bar{X}_{m,\cdot})\Big)$$

Rearranging gives:

$$\sigma^2 = \frac{T-1}{T}\mathbb{E}[S_m] + Var(\bar{X}_{m,\cdot})$$

We can estimate $\mathbb{E}[S_m]$ with W and $Var(\bar{X}_{m,\cdot})$ with B, yielding:

$$V = \frac{T-1}{T}W + B$$

Intuition: Gelman-Rubin corrects for the downward bias in W by adding back an estimate of the between-chain variance B, which captures the additional variability due to correlation in the Markov chains.

Estimators for Target Variance

We have 2 estimators for the target variance σ^2:

$$W = \frac{1}{M} \sum_{m=1}^{M} \left[\frac{1}{T-1} \sum_{t=1}^{T} (X_{m,t} - \bar{X}_m)^2 \right]$$

and

$$V = \frac{T-1}{T} W + B = \left(1 - \frac{1}{T}\right) W + B$$

V weights the within-chain variance W heavily when you have many samples, but adds between-chain variance B to account for the fact that chains might not be fully mixed yet.

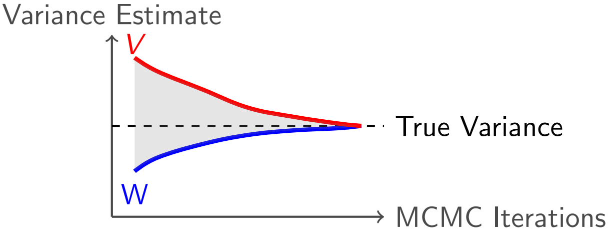
In case we start the chains from overdispersed initial values, we expect B to be large, since chain means $\bar{X}_{m,.}$ are more spread out than they should be. Thus: B overestimates $Var(\bar{X}_{m,.})$. This makes V overestimate σ^2.

The Gelman-Rubin Statistic

Definition

$$\hat{R} = \sqrt{\frac{V}{W}}$$

- Original recommendation: $\hat{R} < 1.1$ for convergence.
- More recent advice: $\hat{R} < 1.01$ (Vehtari et al., 2021)
- But what does $\hat{R}$ really mean?



Connection to Effective Sample Size

Key Approximation (Vats & Knudson, 2021)

$$\hat{R} \approx \sqrt{1 + \frac{M}{\text{ESS}}}$$

Where:

- M = number of chains
- ESS = number of independent samples with the same standard error as a correlated sample.

Implications:

- $\hat{R} = 1.1 \Rightarrow \text{ESS} \approx 5M$ (5 independent samples per chain)
- $\hat{R} = 1.01 \Rightarrow \text{ESS} \approx 50M$ (50 independent samples per chain)

5 effective samples per chain is too small for reliable inference!

Weaknesses of Gelman-Rubin

1. **Only detects lack of convergence**
2. $\hat{R} \approx 1$ does not guarantee convergence
    - Chains might agree but still be wrong
3. **Cannot detect if all modes are found**
    - Only checks if chains agree with each other
    - All chains might miss the same modes
4. **Sensitive to initialization**
    - Chains starting in the same wrong place

Convergence Assessment

Use Multiple Diagnostics

1. **Gelman-Rubin statistic**: $\hat{R} < 1.01$
2. **Effective Sample Size**
3. **Trace plots**: Visual inspection
4. **Autocorrelation**: Check mixing quality

Best Practices:

- Use at least 4 chains (preferably more)
- Initialize chains from overdispersed starting points
- Run chains longer than you think necessary