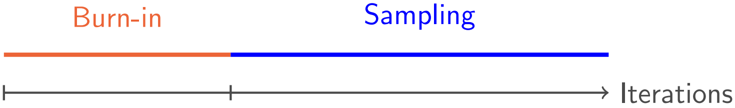
The Convergence Challenge in MCMC

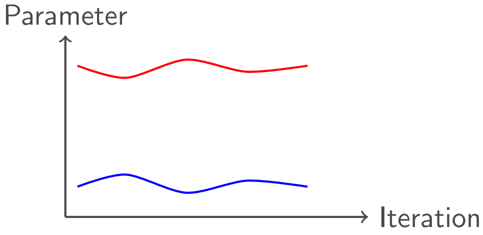
- **Ideal goal**: Assess whether MCMC chains have converged
- **Fundamental problem**:
  - In general, impossible to know for sure that there is no problem
  - But we can sometimes know for sure that there *is* a problem
- **Two phases of MCMC** [2]:
  - Transient phase (burn-in): mixing time
  - Stationary phase: Monte Carlo estimation



Why Convergence Matters

Non-converged chains:

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



Chains in different regions

Key Question

How can we diagnose whether our MCMC chains have converged to the target distribution?

The Intuition Behind Gelman-Rubin

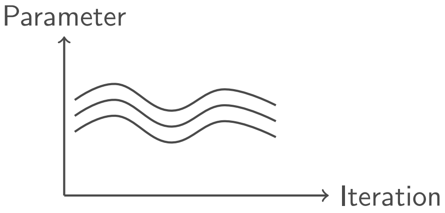
Core Idea

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

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



Converged chains overlap

Mathematical Foundation

Consider M chains, each of length T:

Variance Decomposition

Total sum of squares = Inter-group + Intra-group

$$\sum_{m=1}^{M}\sum_{t=1}^{T}(X_{m,t}-\bar{X}_{..})^2 = \sum_{m=1}^{M}\sum_{t=1}^{T}(\bar{X}_m-\bar{X}_{..})^2 + \sum_{m=1}^{M}\sum_{t=1}^{T}(X_{m,t}-\bar{X}_m)^2$$

- Intra-group = Within-chain variance (W)
- Inter-group = Between-chain variance (B)

Key insight: After convergence, both estimate the same target variance!

The Gelman-Rubin Statistic

Definition

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

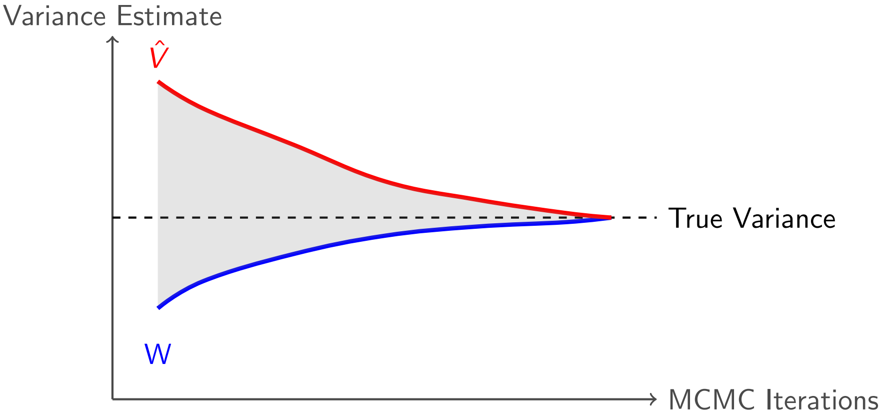
Where:

$$W = \frac{1}{M} \sum_{m=1}^{M} s_m^2 \quad \text{(average within-chain variance)}$$

$$B = \frac{T}{M-1} \sum_{m=1}^{M} (\bar{X}_m - \bar{X}_{..})^2 \quad \text{(between-chain variance)}$$

$$\hat{V} = \frac{T-1}{T} W + \frac{1}{T} B \quad \text{(pooled variance estimate)}$$

Why It Works: The Variance Sandwich



- Initially: $W <$ True Variance $< \hat{V}$
- As chains converge: Both W and $\hat{V} \rightarrow$ True Variance
- Therefore: $\hat{R} = \sqrt{\hat{V}/W} \rightarrow 1$

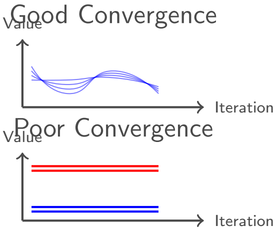
Example: Detecting Convergence Issues

Good convergence:

```
# Chains sampling from same distribution
chains_good = np.random.normal(0, 1, (4, 1000))
R_good = gelman_rubin(chains_good)
print(f"R-hat␣=␣{R_good:.3f}")
# Output: R-hat = 1.002
```

Poor convergence:

```
# Chains stuck in different modes
chains_bad = np.array([
    np.random.normal(-5, 0.5, 1000),
    np.random.normal(-5, 0.5, 1000),
    np.random.normal(5, 0.5, 1000),
    np.random.normal(5, 0.5, 1000)
])
R_bad = gelman_rubin(chains_bad)
print(f"R-hat␣=␣{R_bad:.3f}")
# Output: R-hat = 3.764
```



Evolution of Convergence Thresholds

Historical Development

- **1992**: Gelman & Rubin propose the diagnostic
- **2004**: Gelman recommends $\hat{R} < 1.1$
- **2021**: Vehtari et al. recommend $\hat{R} < 1.01$

Why the stricter threshold?

- More computing power available
- Better understanding of convergence
- Need for more reliable inference
- Connection to effective sample size

$\hat{R}$ threshold	ESS per chain
1.1	≈ 5
1.05	≈ 20
1.01	≈ 50

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 = effective sample size (accounting for autocorrelation)

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!

Major Weaknesses of Gelman-Rubin

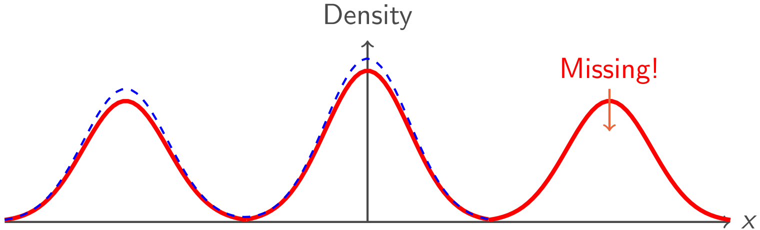
1. **Cannot detect if all modes are found**
   - Only checks if chains agree with each other
   - All chains might miss the same modes
2. **Sensitive to initialization**
   - Chains starting in the same wrong place
3. **Struggles with metastable states**
   - Chains get stuck but occasionally jump
   - Similar statistics but poor mixing
4. **Poor for heavy-tailed distributions**
   - Variance might not exist or be unstable

Remember

$\hat{R} < 1.01$ is necessary but not sufficient for convergence!

Example: Missing Modes

True distribution: Mixture of 3 Gaussians



Chains sample only 2 modes

Result: $\hat{R} < 1.01$ but completely wrong posterior!
All chains agree because they all miss the same mode.

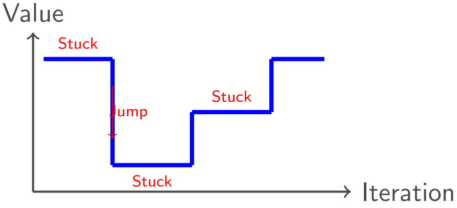
Example: Metastable States

Pathological behavior:

- Chains get "stuck" for long periods
- Occasionally jump to other regions
- All chains show same behavior
- $\hat{R} \approx 1$ despite poor mixing!

Detection:

- Very high autocorrelation
- Low effective sample size
- Visual inspection of trace plots



Despite poor mixing:

- Similar means across chains
- Similar variances
- $\hat{R} \approx 1$

Comprehensive Convergence Assessment

Use Multiple Diagnostics

1. **Gelman-Rubin statistic**: $\hat{R} < 1.01$
2. **Effective Sample Size**: ESS $>$ 400 (minimum)
3. **Trace plots**: Visual inspection
4. **Autocorrelation**: Check mixing quality
5. **Geweke test**: Compare chain beginning and end

Best Practices:

- Use at least 4 chains (preferably more)
- Initialize chains from overdispersed starting points
- Run chains longer than you think necessary
- Use rank-normalized $\hat{R}$ (more robust)
- Check both bulk and tail $\hat{R}$

Modern Extensions

Rank-Normalized $\hat{R}$ (Vehtari et al., 2021)

- Transform samples to ranks (more robust to outliers)
- Split chains in half (detect within-chain problems)
- Separate bulk and tail diagnostics

Bulk-$\hat{R}$:

- Convergence of center
- Mean, median
- Usually converges faster

Tail-$\hat{R}$:

- Convergence of extremes
- 5%, 95% quantiles
- Needs more samples

Modern tools (Stan, ArviZ) implement these improvements

Summary Checklist

MCMC Convergence Checklist

1. Run at least 4 chains with dispersed starts
2. Check $\hat{R} < 1.01$ for all parameters
3. Verify ESS > 400 (bulk and tail)
4. Examine trace plots visually
5. Check autocorrelation is low
6. Run sensitivity analysis with different seeds
7. Compare results from different samplers if possible

Remember:

No single diagnostic is perfect

Key Takeaways

1. **Gelman-Rubin compares within vs between chain variance**
    - Elegant idea: converged chains should agree
2. **Modern threshold is** $\hat{R} < 1.01$
    - Old threshold (1.1) gives only 5 effective samples
    - New threshold ensures 50 effective samples
3. $\hat{R}$ **has important limitations**
    - Can miss modes
    - Fooled by metastable states
    - Necessary but not sufficient
4. **Always use multiple diagnostics**
    - ESS, trace plots, autocorrelation
    - Visual inspection remains crucial

Good MCMC diagnostics = Reliable scientific inference

References

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Thank You!

Questions?