Lecture 18: some mcmc practicalities

STAT 545: Intro. to Computational Statistics

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Summary so far...

Independent samples from prob. distrib. p is often difficult.

MCMC addresses this by producing dependent samples.

- Begin with an arbitrary initialization X_0.
- Sequentially produce samples $X_1 \to X_2 \to \ldots \to X_N$.

If the chain is stationary w.r.t. $p(x)$, irreducible and aperiodic:

$$\frac{1}{S}\sum_{i=1}^{S} h(X_i) \to \mathbb{E}_p[h]$$

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In practice, S is finite.
Assessing error is much harder

How well does your chain mix?

Are our MCMC samples representative of the overall posterior?

- Difficult with multimodal distributions.

Do we have enough samples to estimate expectations accurately?

- This is hard with Monte Carlo methods in general
- Trickier with MCMC because of correlation between samples.

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However, it's worthwhile remembering that N MCMC samples correspond to a smaller number of independent samples.

Effective sample size

A good diagnostic is the effective sample size (ESS):

$$N_{ESS} = \frac{N}{1 + 2\sum_{k=1}^{\infty} \rho_k}$$

ρ_k is the auto-correlation between X_i and X_{i+k}:

$$\rho_k = \frac{\mathbb{E}[(X_{i+k} - \mu)(X_i - \mu)]}{\sigma^2}$$

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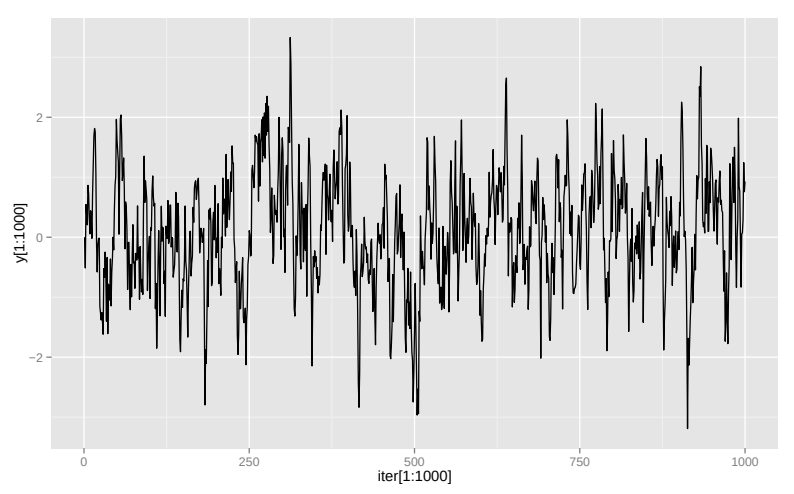
Comes from CLT for Markov chains:

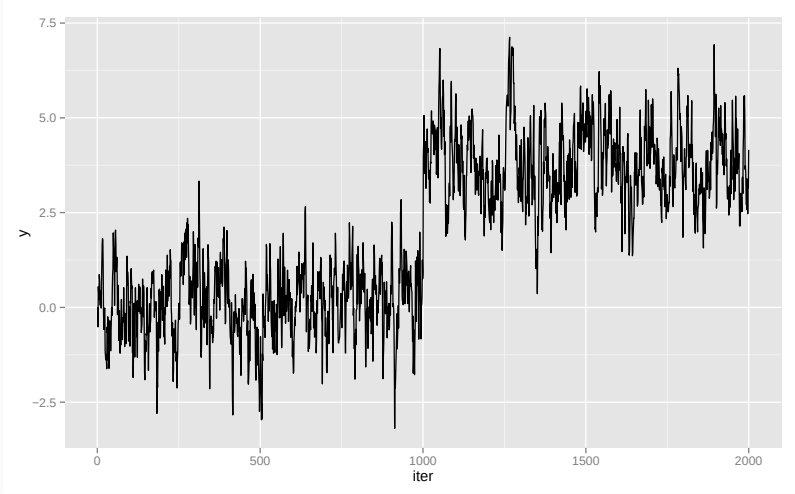
$$\left(\frac{1}{N} \sum_{i=1}^{N} f(X_i) - \mathbb{E}[f(X)] \right) \to \mathcal{N}(0, \sigma^2 / N_{ESS})$$

Effective sample size

The `Coda` package in `R`calculates this and other diagnostics.



ESS: 130.4

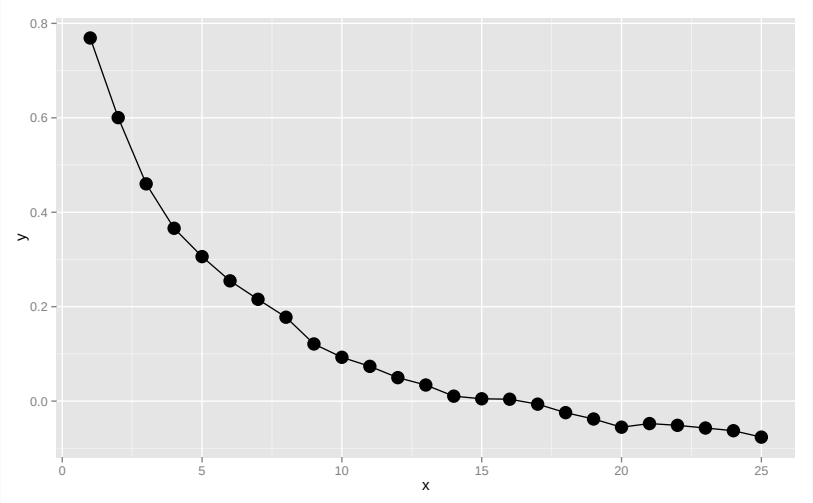


ESS: 9.21

```
> effectiveSize(data.frame(half=z[1:1000],full=z))
      half       full
260.997261   9.216991
```

Note: always useful to visualize traceplots.

Other diagnostics

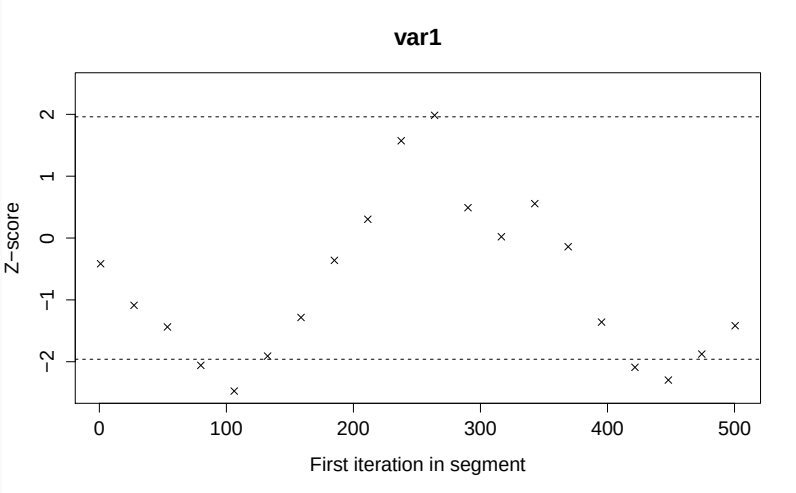


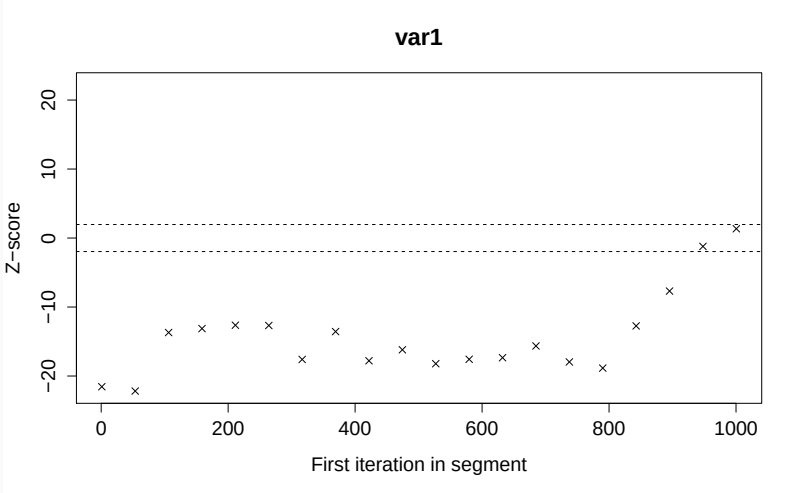
Correlation vs lag

```
> acf <- autocorr(mcmc(z[1:1000]),c(1:25))
```

Other diagnostics

Geweke diagnostic:





Compare 2 non-overlapping parts of the chain (in R CODA is the first 10% and last 50%, and test if their means come from the same distribution.

Can repeat, successively discarding initial parts.

```
> geweke.plot(mcmc(z[1:1000]))
> geweke.plot(mcmc(z))
```

Other diagnostics

Gelman-Rubin diagnostic: Run $m \geq 2$ independent chains with overdispersed starting points (e.g. sampled from the prior)

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- Calculate within-chain variance and between-chain variance.
- Former typically underestimates variance (bad mixing), and latter overestimates it (overdispersed initialization).
- If latter is much larger than former, run chain longer

```
> gelman.diag
```

One long chain vs many shorter chains?

M short chain of length N vs 1 chain of length MN:

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Cons:

- Each chain still has a burn-in period B. Must discard MB samples vs B for a single chain.

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Can you analytically calculate the posterior for 1 observation or 2 states or 2 time-periods?

Using MCMC samples:

Consider a Markov chain on (x, y, z) with stationary distrib. $P()$.
We obtain samples $(x_1, y_1, z_1), (x_2, y_2, z_2), (x_3, y_3, z_3), \ldots$

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Can we do better? E.g. what if x is continuous and we want the density $p(x = 1)$?

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Typically, this estimate will have lower variance.