A Simple Gibbs Sampler

Biostatistics 615/815

Lecture 23

Scheduling

- Practice Exam
- Review session
  - Next Monday, December 6
- Final Assessment
  - Monday, December 13

Optimization Strategies

- Single Variable
  - Golden Search
  - Quadratic Approximations

- Multiple Variables
  - Simplex Method
  - E-M Algorithm
  - Simulated Annealing

Simulated Annealing

- Stochastic Method
- Sometimes takes up-hill steps
  - Avoids local minima
- Solution is gradually *frozen*
  - Values of parameters with largest impact on function values are fixed earlier

Gibbs Sampler

- Another MCMC Method
- Update a single parameter at a time
- Sample from conditional distribution when other parameters are fixed

Gibbs Sampler Algorithm

Consider a particular choice of parameter values $\boldsymbol{\theta}^{(t)}$

Define the next set of parameter values by:

a. Selecting component to update, say i

b. Sample value for $\theta_i^{(t+1)}$ from $p(\theta_i \mid x, \theta_1, \theta_2, \ldots \theta_{i-1}, \theta_{i+1}, \ldots \theta_k)$

Increment t and repeat previous steps.

Alternative Algorithm

Consider a particular choice of parameter values $\boldsymbol{\theta}^{(t)}$

Define the next set of parameter values by:

a. Update each component, 1 .. k, in turn

b. Sample value for $\theta_1^{(t+1)}$ from $p(\theta_1 \mid x, \theta_2, \theta_3, \ldots \theta_k)$

c. Sample value for $\theta_2^{(t+1)}$ from $p(\theta_2 \mid x, \theta_1, \theta_3, \ldots \theta_k)$

...

z. Sample value for $\theta_k^{(t+1)}$ from $p(\theta_k \mid x, \theta_1, \theta_3, \ldots \theta_{k-1})$

Increment t and repeat previous steps.

Key Property: Stationary Distribution

Suppose that $(\theta_1^{(t)}, \theta_2^{(t)}, \ldots, \theta_k^{(t)}) \sim p(\theta_1, \theta_2, \ldots, \theta_k \mid x)$

Then $(\theta_1^{(t+1)}, \theta_2^{(t)}, \ldots, \theta_k^{(t)})$ is distributed as

$$p(\theta_1 \mid \theta_2, \ldots, \theta_k, x) p(\theta_2, \ldots, \theta_k \mid x) = p(\theta_1, \theta_2, \ldots, \theta_k \mid x)$$

In fact...

$$\boldsymbol{\theta}^{(t)} \sim p(\boldsymbol{\theta} \mid x) \Rightarrow \boldsymbol{\theta}^{(t+1)} \sim p(\boldsymbol{\theta} \mid x)$$

Eventually, we expect the Gibbs sampler to sample parameter values from their posterior distribution

Gibbs Sampling for Mixture Distributions

- Sample each of the mixture parameters from conditional distribution
  - Dirichlet, Normal and Gamma distributions are typical

- Simple alternative is to sample the *origin* of each observation
  - Assign observation to specific component

Sampling A Component

$$\Pr(Z_j = i \mid x_j, \boldsymbol{\pi}, \boldsymbol{\varphi}, \eta) = \frac{\pi_i f(x_j \mid \phi_i, \eta)}{\sum_l \pi_l f(x_j \mid \phi_l, \eta)}$$

- Calculate the probability that the observation originated from each component…
- … use random number(s) to assign component membership. How?

C Code: Sampling A Component

```
int sample_group(double x, int k,
                 double * probs, double * mean, double * sigma)
   {
   int group; double p = Random();
   double lk = dmix(x, k, probs, mean, sigma);

   for (group = 0; group < k - 1; group++)
      {
      double pgroup = probs[group] *
                      dnorm(x, mean[group], sigma[group])/lk;

      if (p < pgroup) return group;

      p -= pgroup;
      }

   return k - 1;
   }
```

Calculating Mixture Parameters

$$n_i = \sum_{j:Z_j=i} 1$$

$$p_i = n_i / n$$

$$\bar{x}_i = \sum_{j:Z_j=i} x_j / n_i$$

$$s_i = \left(\sum_{j:Z_j=i} x_j^2 - n_i \bar{x}_i^{\,2} \right) \Big/ n_i$$

- Before sampling a new origin for an observation…
- … update mixture parameters given current assignments
- Could be expensive!

C Code:
Updating Parameters

```
void update_estimates(int k, int n,
              double * prob, double * mean, double * sigma,
              double * counts, double * sum, double * sumsq)
   {
   int i;

   for (i = 0; i < k; i++)
      {
      prob[i] = counts[i]/ n;
      mean[i] = sum[i] / counts[i];
      sigma[i] = sqrt((sumsq[i] - mean[i]*mean[i]*counts[i])
                 / counts[i] + 1e-7);
      }
   }
```

C Code: Updating Mixture Parameters II

```
void remove_observation(double x, int group,
            double * counts, double * sum, double * sumsq)
   {
   counts[group] --;
   sum[group] -= x;
   sumsq[group] -= x * x;
   }

void add_observation(double x, int group,
            double * counts, double * sum, double * sumsq)
   {
   counts[group] ++;
   sum[group] += x;
   sumsq[group] += x * x;
   }
```

Selecting a Starting State

- Must start with an assignment of observations to groupings

- Many alternatives are possible, I chose to perform random assignments with equal probabilities…

C Code: Starting State

```
void initial_state(int k, int * group,
             double * counts, double * sum, double * sumsq)
   {
   int i;

   for (i = 0; i < k; i++)
      counts[i] = sum[i] = sumsq[i] = 0.0;

   for (i = 0; i < n; i++)
      {
      group[i] = Random() * k;

      counts[group[i]] ++;
      sum[group[i]] += data[i];
      sumsq[group[i]] += data[i] * data[i];
      }
   }
```

The Gibbs Sampler

- Select initial state
- Repeat a large number of times:
  - Select an element
  - Update conditional on other elements
- If appropriate, output summary for each run…

C Code:
Core of The Gibbs Sampler

```
initial_state(k, probs, mean, sigma, group, counts, sum, sumsq);
for (i = 0; i < 10000000; i++)
   {
   int id = rand() % n;

   if (counts[group[id]] < MIN_GROUP) continue;

   remove_observation(data[id], group[id], counts, sum, sumsq);
   update_estimates(k, n - 1, probs, mean, sigma,
                              counts, sum, sumsq);
   group[id] = sample_group(data[id], k, probs, mean, sigma);
   add_observation(data[id], group[id], counts, sum, sumsq);

   if ((i > BURN_IN) && (i % THIN_INTERVAL == 0))
      /* Collect statistics */
   }
```

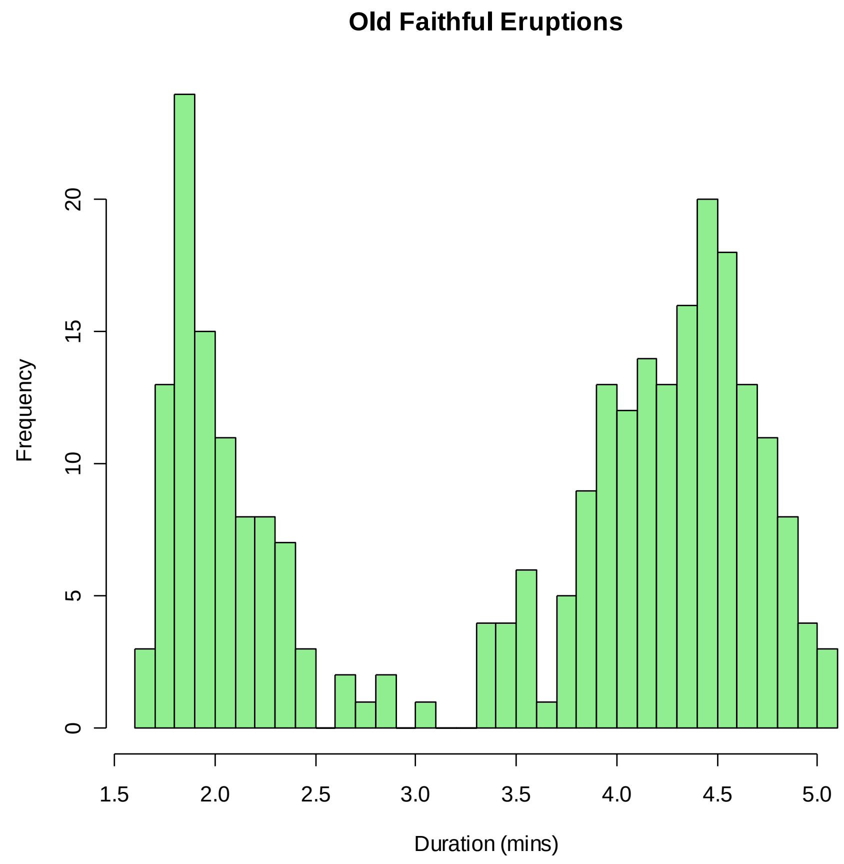
Gibbs Sampler: Memory Allocation and Freeing

```
void gibbs(int k, double * probs, double * mean, double * sigma)
   {
   int i, * group = (int *) malloc(sizeof(int) * n);
   double * sum = alloc_vector(k);
   double * sumsq = alloc_vector(k);
   double * counts = alloc_vector(k);

   /* Core of the Gibbs Sampler goes here */

   free_vector(sum, k);
   free_vector(sumsq, k);
   free_vector(counts, k);
   free(group);
   }
```

Example Application
Old Faithful Eruptions (n = 272)

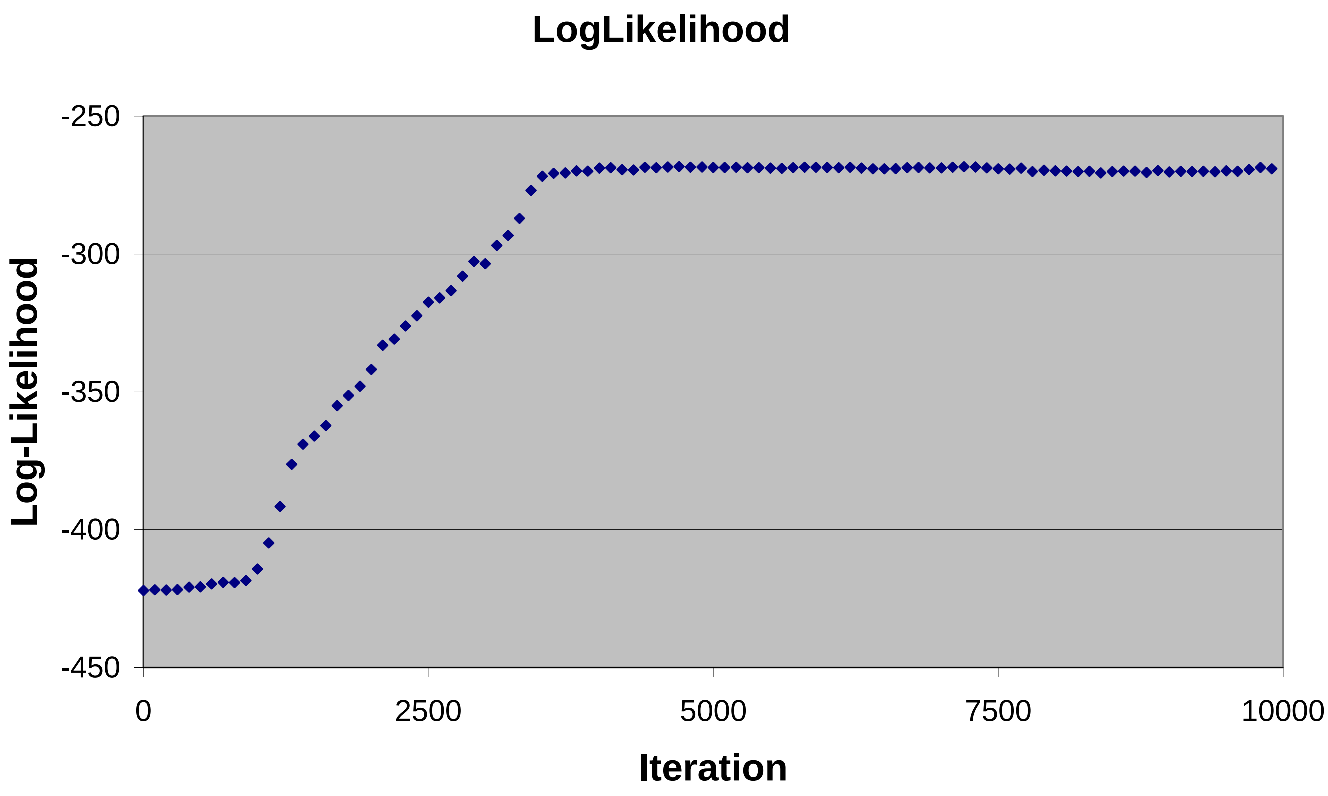


Notes ...

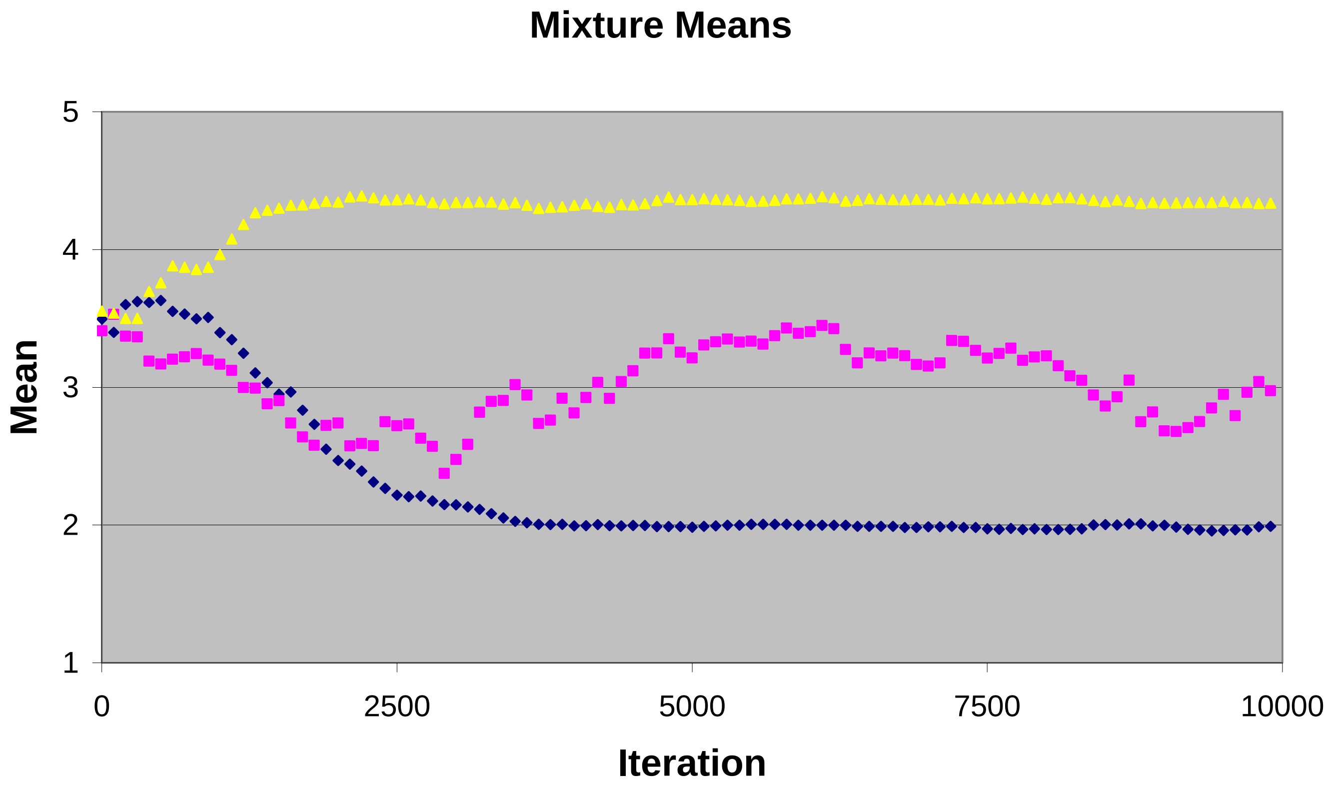
- My first few runs found excellent solutions by fitting components accounting for very few observations but with variance near 0

- Why?
  - Repeated values due to rounding
  - To avoid this, set MIN_GROUP to 13 (5%)

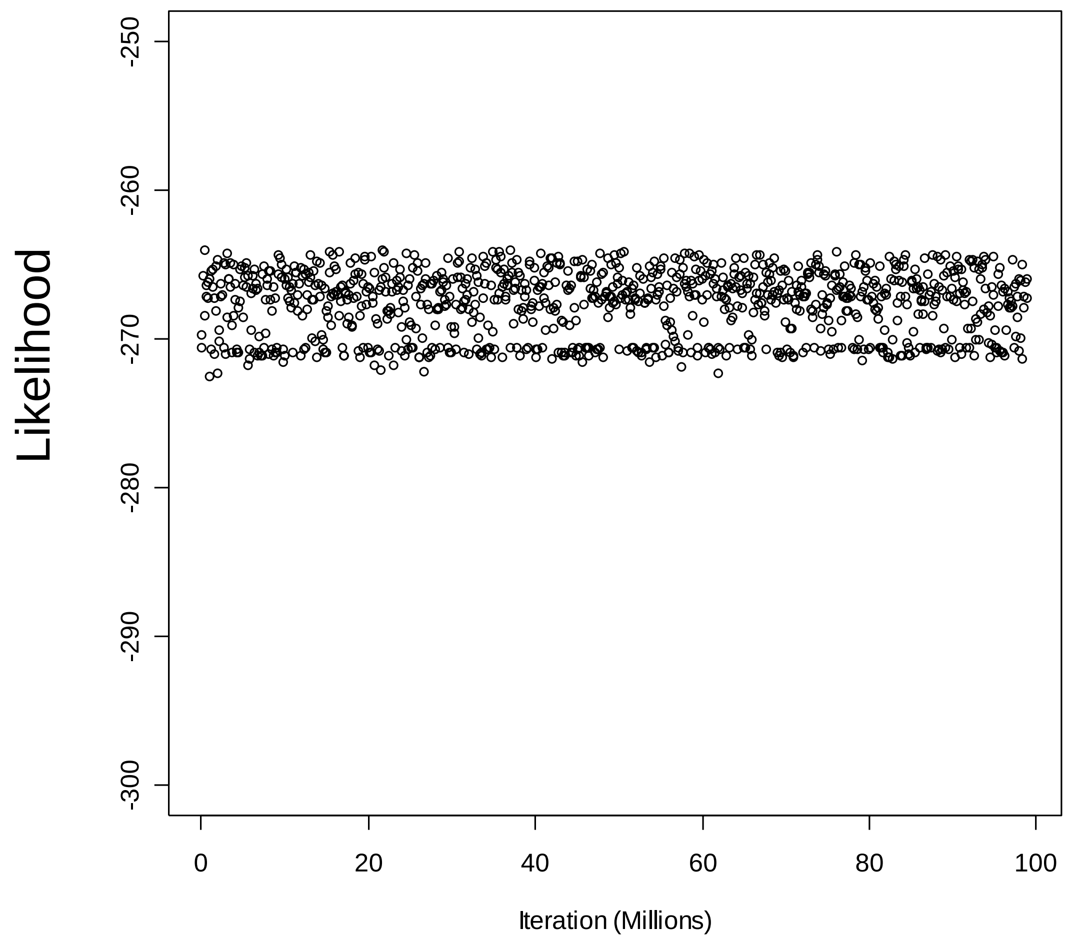
Gibbs Sampler Burn-In



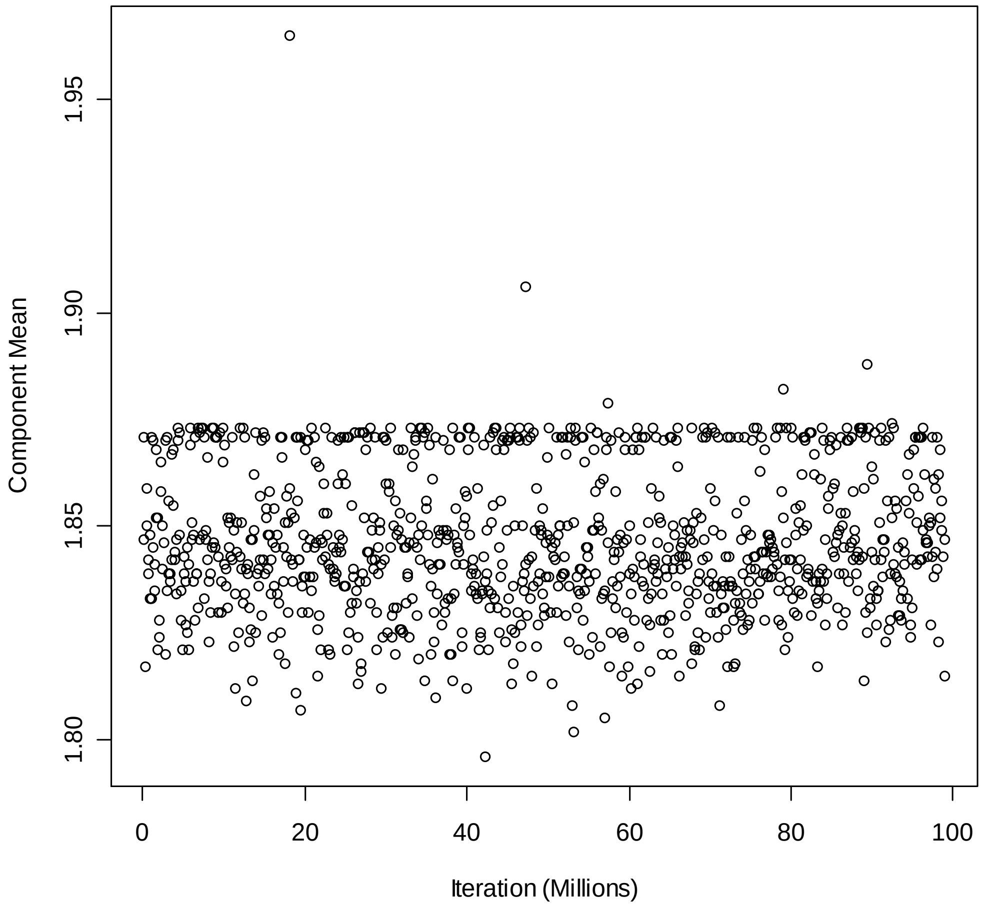
Gibbs Sampler Burn-In



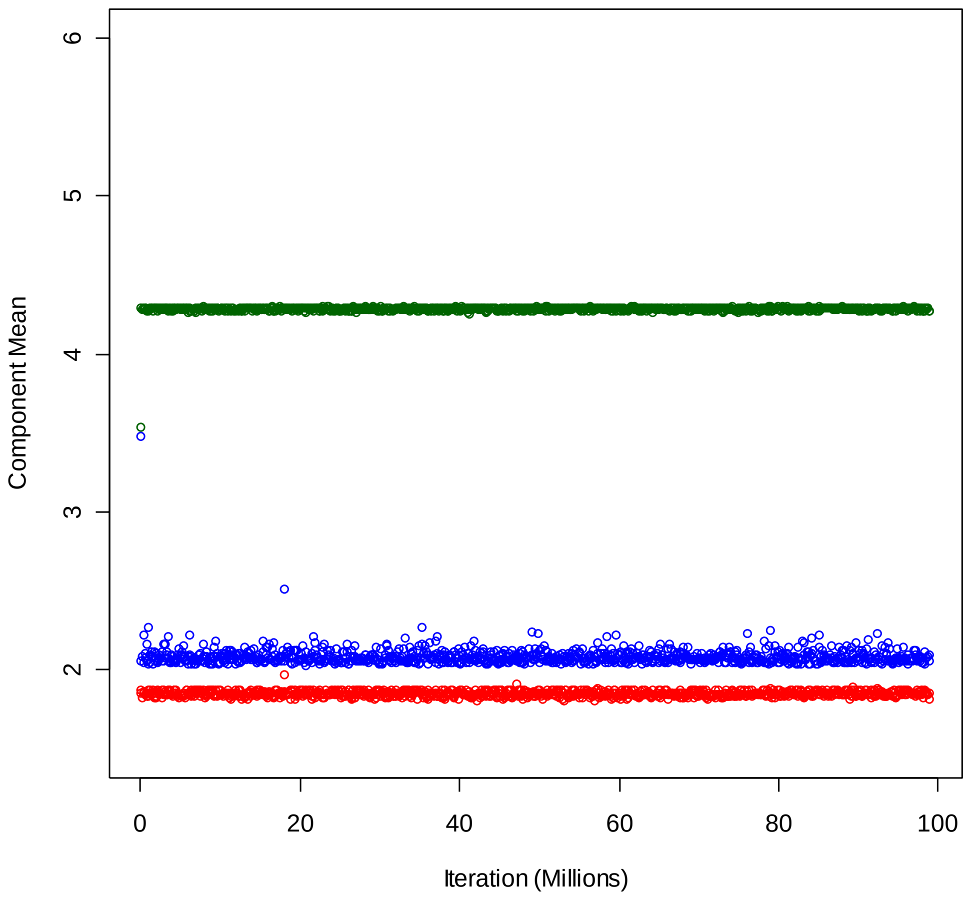
Gibbs Sampler After Burn-In Likelihood



Gibbs Sampler After Burn-In Mean for First Component



Gibbs Sampler After Burn-In



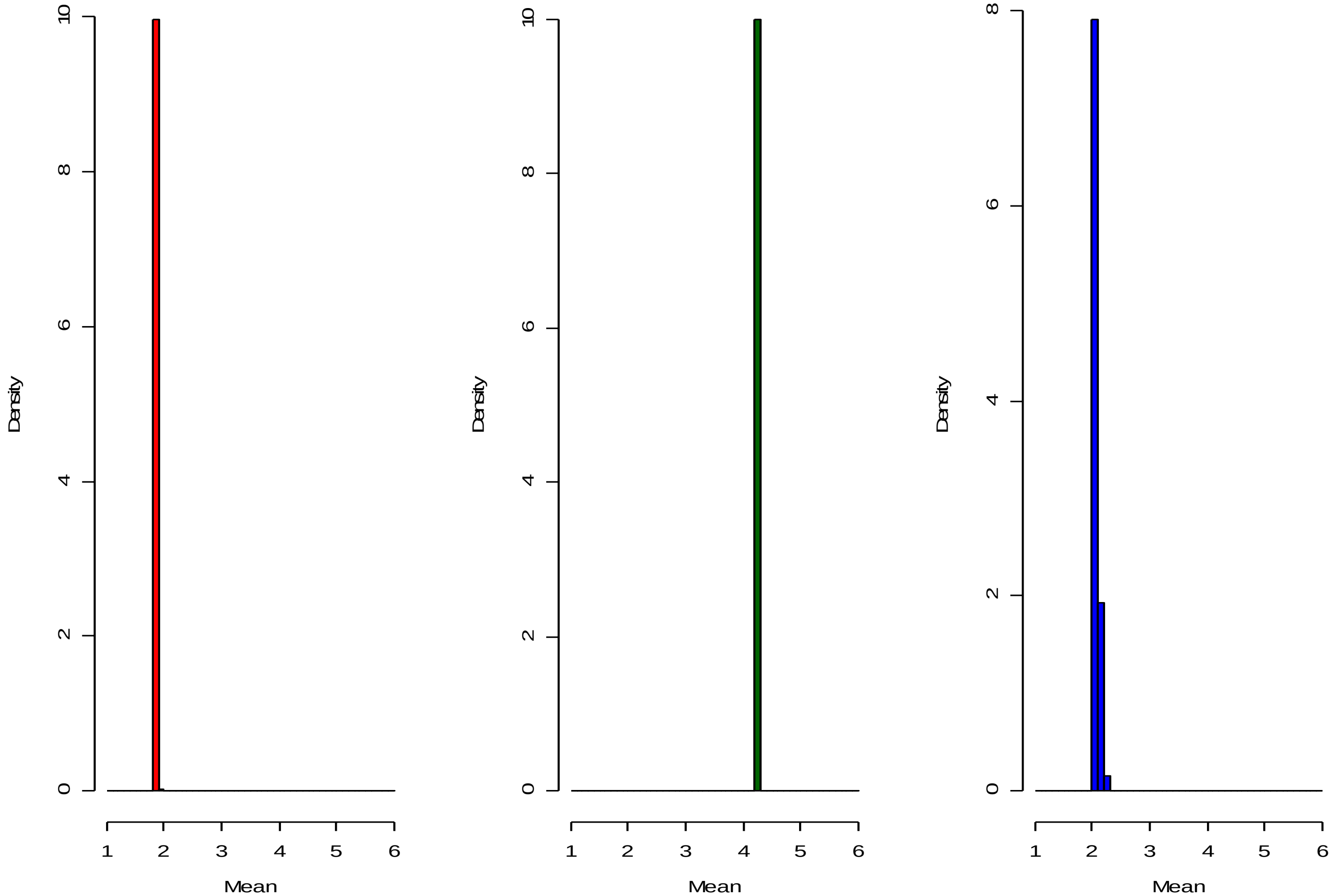
Notes on Gibbs Sampler

- Previous optimizers settled on a minimum eventually
- The Gibbs sampler continues wandering through the stationary distribution…
- Forever!

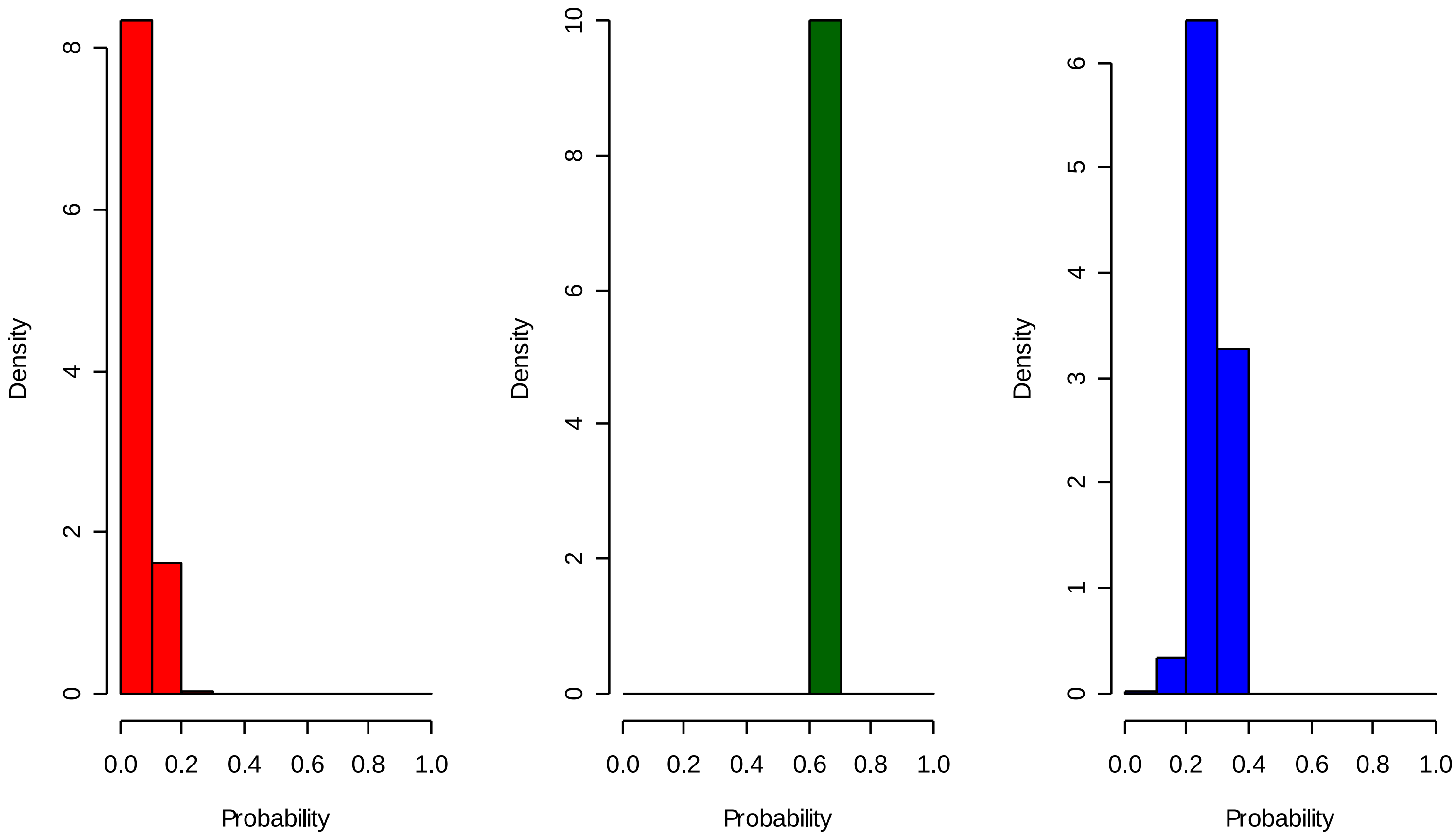
Drawing Inferences...

- To draw inferences, summarize parameter values from stationary distribution
- For example, might calculate the mean, median, etc.

Component Means



Component Probabilities



Overall Parameter Estimates

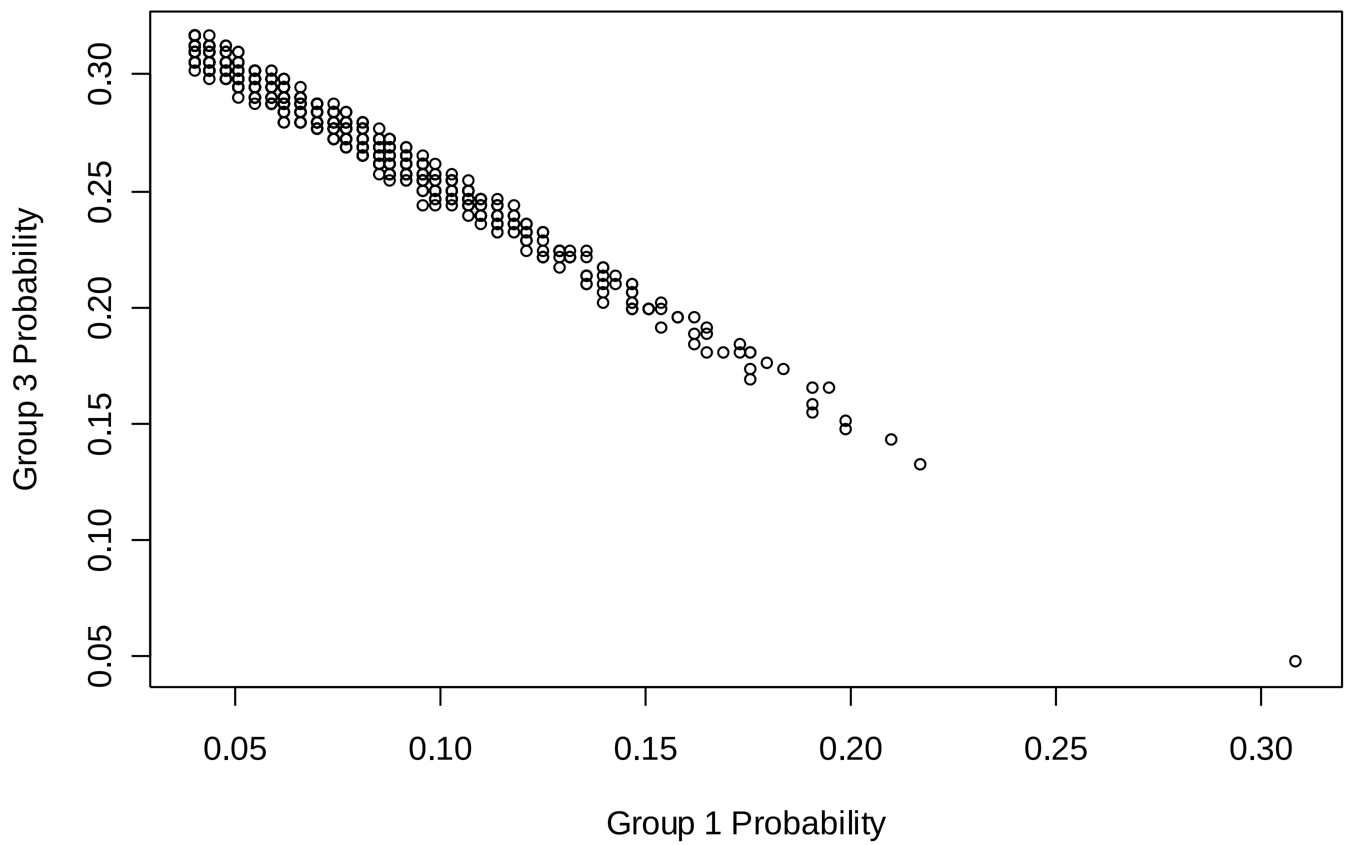
- The means of the posterior distributions for the three components were:
  - Frequencies of 0.073, 0.278 and 0.648
  - Means of 1.85, 2.08 and 4.28
  - Variances of 0.001, 0.065 and 0.182

- Our previous estimates were:
  - Components contributing .160, 0.195 and 0.644
  - Component means are 1.856, 2.182 and 4.289
  - Variances are 0.00766, 0.0709 and 0.172

Joint Distributions

- Gibbs Sampler provides other interesting information and insights
- For example, we can evaluate joint distribution of two parameters…

Component Probabilites



Today …

- Introduction to Gibbs sampling
- Generates posterior distributions of parameters conditional on data
- Provides insight into joint distributions

A little bit of theory

- Highlight connection between Simulated Annealing and the Gibbs sampler …

- Fill in some details of the Metropolis algorithm

Both Methods Are Markov Chains

- The probability of any state being chosen depends only on the previous state

$$\Pr(S_n = i_n \mid S_{n-1} = i_{n-1}, \ldots, S_0 = i_0) = \Pr(S_n = i_n \mid S_{n-1} = i_{n-1})$$

- States are updated according to transition matrix with elements p_{ij}. This matrix defines important properties, including **periodicity** and **irreducibility.**

Metropolis-Hastings Acceptance Probability

Let $q_{ij} = q(\text{propose } S_{n+1} = j \mid S_n = i)$

Let π_i and π_j be the relative probabilities of each state

The Metropolis-Hastings acceptance probability is:

$$a_{ij} = \min\left(1, \frac{\pi_j q_{ji}}{\pi_i q_{ij}}\right) \quad \text{or} \quad a_{ij} = \min\left(1, \frac{\pi_j}{\pi_i}\right) \text{if } q_{ij} = q_{ji}$$

Only the ratio $\frac{\pi_j}{\pi_i}$ must be known, not the actual values of π

Metropolis-Hastings Equilibrium

If we use the Metropolis - Hastings algorithm to update a Markov Chain, it will reach an equilibrium distribution where $\Pr(S = i) = \pi_i$

For this to happen, the proposal density must allow all states to communicate.

Gibbs Sampler

The Gibbs sampler ensures that $\pi_i q_{ij} = \pi_j q_{ji}$

As a consequence, $a_{ij} = \min\left(1, \dfrac{\pi_j q_{ji}}{\pi_i q_{ij}}\right) = 1$

Simulated Annealing

Given a temperature parameter τ,

replace π_i with $\pi_i^{(\tau)} = \dfrac{\pi_i^{\frac{1}{\tau}}}{\sum_j \pi_j^{\frac{1}{\tau}}}$

At high temperatures, the probability distribution is flattened

At low temperatures, larger weights are given to high probability states

Additional Reading

- If you need a refresher on Gibbs sampling
  - Bayesian Methods for Mixture Distributions
    M. Stephens (1997)
    http://www.stat.washington.edu/stephens/
- Numerical Analysis for Statisticians
  - Kenneth Lange (1999)
  - Chapter 24