Biostatistics 615/815 Lecture 22: Gibbs Sampling

Hyun Min Kang

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Recap: The E-M algorithm

Expectation step (E-step)

- Given the current estimates of parameters $\lambda^{(t)}$, calculate the conditional distribution of latent variable $\mathbf{z}$.
- Then the expected log-likelihood of data given the conditional distribution of $\mathbf{z}$ can be obtained

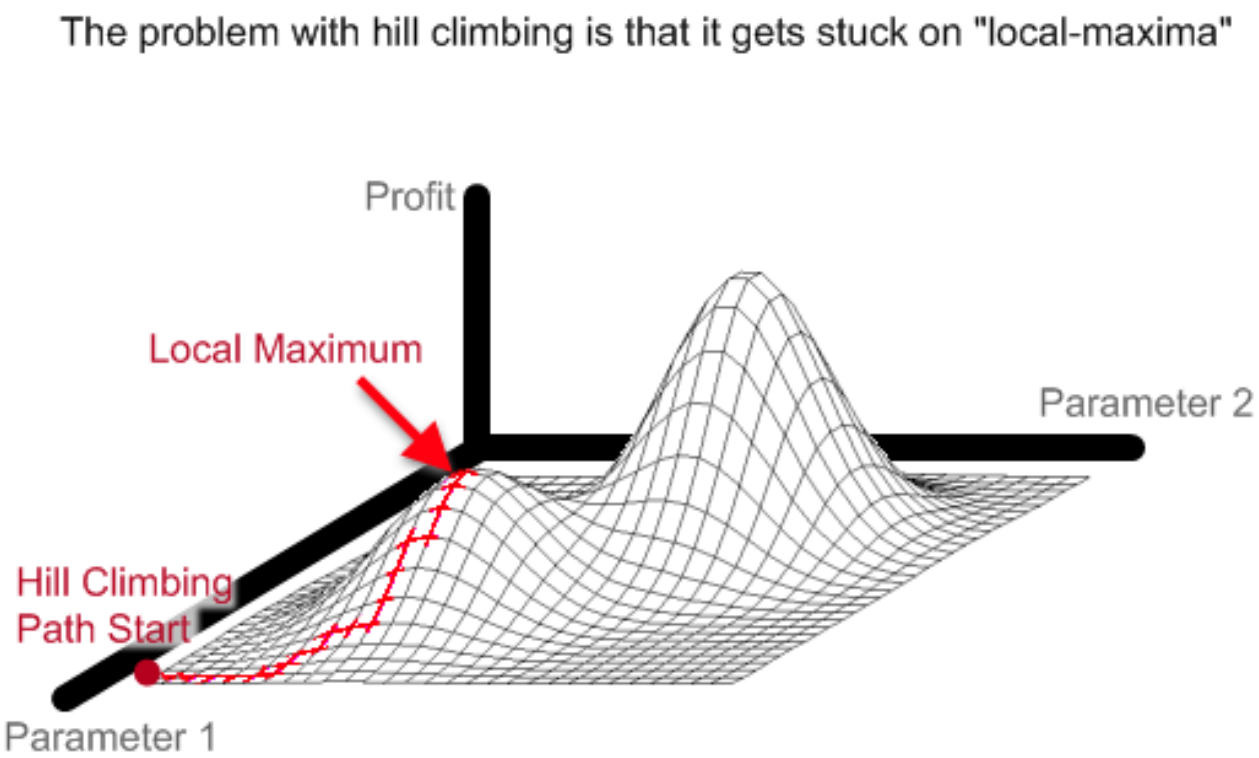
$$Q(\lambda|\lambda^{(t)}) = \mathbf{E}_{\mathbf{z}|\mathbf{x},\lambda^{(t)}}\left[\log p(\mathbf{x},\mathbf{z}|\lambda)\right]$$

Maximization step (M-step)

- Find the parameter that maximize the expected log-likelihood

$$\lambda^{(t+1)} = \arg\max_{\lambda} Q(\lambda|\lambda^{t})$$

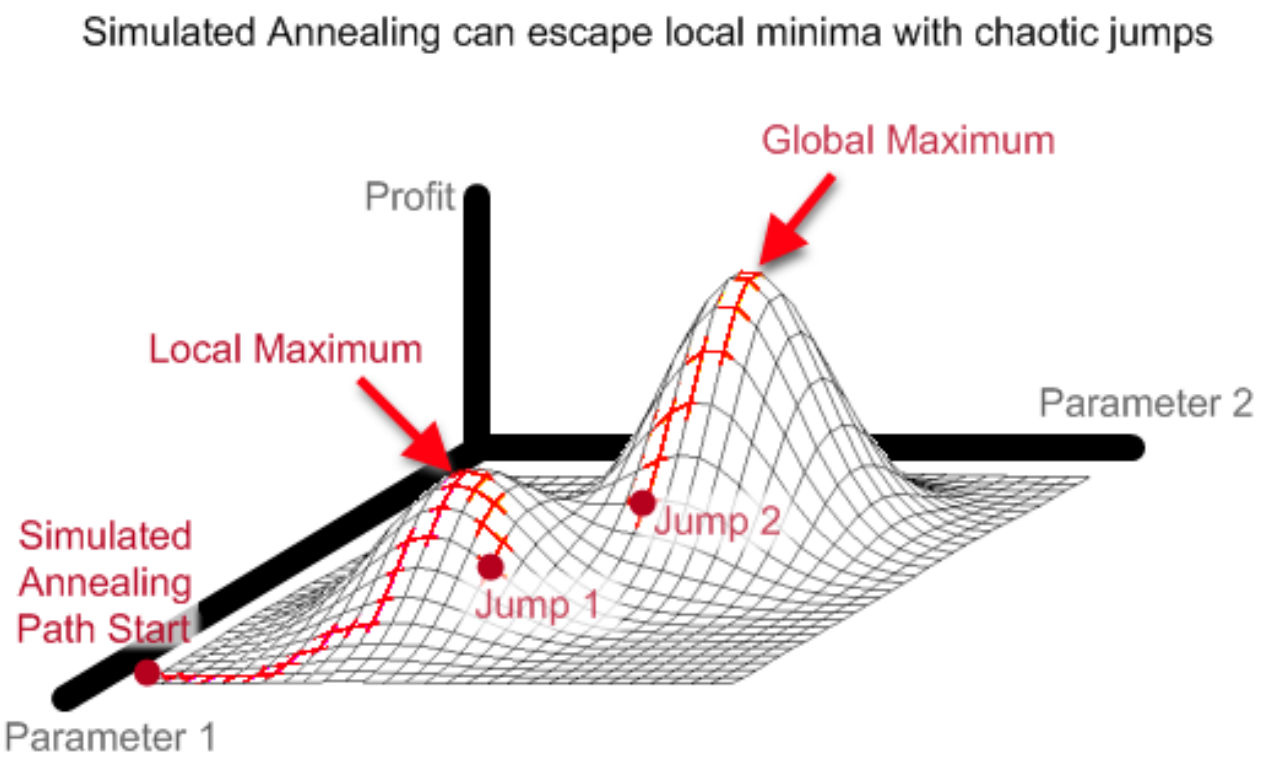
Recap - Local minimization methods



Images by Max Dama from

http://maxdama.blogspot.com/2008/07/trading-optimization-simulated.html

Recap - Global minimization with Simulated Annealing



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Recap - Simulated Annealing Recipes

1. Select starting temperature and initial parameter values
2. Randomly select a new point in the neighborhood of the original
3. Compare the two points using the *Metropolis criterion*
4. Repeat steps 2 and 3 until system reaches equilibrium state
   - In practice, repeat the process N times for large N.
5. Decrease temperature and repeat the above steps, stop when system reaches frozen state

Optimization Streategies

- Single Dimension
  - Golden Search
  - Parabolic Approximations
- Multiple Dimensions
  - Simplex Method
  - E-M Algorithm
  - Simulated Annealing

Optimization Streategies

- Single Dimension
  - Golden Search
  - Parabolic Approximations
- Multiple Dimensions
  - Simplex Method
  - E-M Algorithm
  - Simulated Annealing
  - Gibbs Sampling

Gibbs Sampler

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

Gibbs Sampler Algorithm

1. Consider a particular choice of parameter values $\lambda^{(t)}$.
2. Define the next set of parameter values by
   - Selecting a component to update, say i.
   - Sample value for $\lambda_i^{(t+1)}$, from $p(\lambda_i | x, \lambda_1, \cdots, \lambda_{i-1}, \lambda_{i+1}, \cdots, \lambda_k)$.
3. Increment t and repeat the previous steps.

An alternative Gibbs Sampler Algorithm

1. Consider a particular choice of parameter values $\lambda^{(t)}$.
2. Define the next set of parameter values by
   - Sample value for $\lambda_1^{(t+1)}$, from $p(\lambda_1|x, \lambda_2, \lambda_3, \cdots, \lambda_k)$.
   - Sample value for $\lambda_2^{(t+1)}$, from $p(\lambda_1|x, \lambda_1, \lambda_3, \cdots, \lambda_k)$.
   - $\cdots$
   - Sample value for $\lambda_k^{(t+1)}$, from $p(\lambda_k|x, \lambda_1, \lambda_2, \cdots, \lambda_{k-1})$.
3. Increment t and repeat the previous steps.

Gibbs Sampling for Gaussian Mixture

Using conditional distributions

- Observed data : $\mathbf{x} = (x_1, \cdots, x_n)$
- Parameters : $\lambda = (\pi_1, \cdots, \pi_k, \mu_1, \cdots, \mu_k, \sigma_1^2, \cdots, \sigma_k^2)$.
- Sample each λ_i from conditional distribution - not very straightforward

Using source of each observations

- Observed data : $\mathbf{x} = (x_1, \cdots, x_n)$
- Parameters : $\mathbf{z} = (z_1, \cdots, z_n)$ where $z_i \in \{1, \cdots, k\}$.
- Sample each z_i conditioned by all the other $\mathbf{z}$.

Update procedure in Gibbs sampler

$$\Pr(z_j = i | x_j, \lambda) = \frac{\pi_i \mathcal{N}(x_j | \mu_i, \sigma_i^2)}{\sum_l \pi_l \mathcal{N}(x_j | \mu_l, \sigma_l^2)}$$

- Calculate the probability that the observation is originated from a specific component
- For a random $j \in \{1, \cdots, n\}$, sample z_j based on the current estimates of mixture parameters.

Initialization

- Must start with an initial assignment of component labels for each observed data point
- A simple choice is to start with random assignment with equal probabilities

The Gibbs Sampler

- Select initial parameters
- Repeat a large number of times
  - Select an element
  - Update conditional on other elements

Implementing Gaussian Mixture Gibbs Sampler

```
class normMixGibbs {
public:
  int k;                        // # of components
  int n;                        // # of data
  std::vector<double> data;     // size n : observed data
  std::vector<double> labels;   // size n : label assignment for each observations
  std::vector<double> pis;      // size k : pis
  std::vector<double> means;    // size k : means
  std::vector<double> sigmas;   // size k : sds
  std::vector<int>    counts;   // size k : # of elements in each labels
  std::vector<double> sums;     // size k : sum across each label
  std::vector<double> sumsqs;   // size k : squared sum across each label
  normMixGibbs(std::vector<double>& _data, int _k); // constructor
  void initParams();                // initialize parameters
  void updateParams(int numObs); // update parameters
  void remove(int i);               // remove elements
  void add(int i, int label);       // add an element with new label
  int sampleLabel(double x);        // sample the label of an element
  void runGibbs();                  // run Gibbs sampler
};
```

Update procedure in Gibbs sampler

$$\Pr(z_j = i | x_j, \pi, \lambda) = \frac{\pi_i \mathcal{N}(x_j | \mu_i, \sigma_i^2)}{\sum_l \pi_l \mathcal{N}(x_j | \mu_l, \sigma_l^2)}$$

- Calculate the probability that the observation is originated from a specific component
- For a random $j \in \{1, \cdots, n\}$, sample z_j based on the current estimates of mixture parameters.

Sampling label of selected value

```
// x is the data needs a new label assignment
int normMixGibbs::sampleLabel(double x) {
  double p = randu(0,1);  // generate a random probability
  // evaluate the likelihood of the observations given parameters
  double lk = mixLLKFunc::dmix(x, pis, means, sigmas);
  // use randomized values to randomly assign labels
  // based on the likelihood contributed by each component,
  for(int i=0; i < k-1; ++i) {
    double pl = pis[i] * mixLLKFunc::dnorm(x,means[i],sigmas[i])/lk;
    if ( p < pl ) return i;
    p -= pl;
  }
  // evaluate only k-1 components and assign to the last one if not found
  return k-1;
}
```

Calculating the parameters at each update

- For each $i \in \{1, \cdots, k\}$
  - $n_i = \sum_{j=1}^{n} I(z_j = i)$
  - $\pi_i = n_i / n$
  - $\mu_i = \sum_{j=1}^{n} x_j I(z_j = i)$
  - $\sigma_i^2 = \sum_{j=1}^{n} I(z_j = i)(x_j - \mu_i)^2 / n_i$
- This procedure takes $O(n)$, which is quite expensive to run over a large number of iterations.
- Is it possible to reduce the time complexity to constant ($O(k)$)?

Contant time update of parameters

```
// update parameters for each components
// having counts, sums, sumsqs allows to reduce time complexity
void normMixGibbs::updateParams(int numObs) {
  for(int i=0; i < k; ++i) { // This takes O(k) complexity
    pis[i] = (double)counts[i]/(double)(numObs);
    means[i] = sums[i]/counts[i];
    sigmas[i] = sqrt((sumsqs[i]/counts[i] - means[i]*means[i])+1e-7);
  }
}
```

Removing and adding elements

```
// We want to remove object to calculate the conditional distribution
// excluding one component's label information
void normMixGibbs::remove(int i) {
  int l = labels[i];
  --counts[l];
  sums[l] -= data[i];
  sumsqs[l] -= (data[i]*data[i]);
}
// Adding the removed object with newer label assignment
void normMixGibbs::add(int i, int label) {
  labels[i] = label;
  ++counts[label];
  sums[label] += data[i];
  sumsqs[label] += (data[i]*data[i]);
}
```

The Gibbs Sampler

```
void normMixGibbs::runGibbs() {
  initParams();  // initialze label assignments
  for(int i=0; i < 10000000; ++i) { // repeat a large number of times
    int id = randn(0,n);           // select a label to update
    if ( counts[labels[id]] < MIN_COUNTS ) continue; // avoid boundary conditions
    remove(id);                    // remove the elements
    updateParams(n-1);             // update pis, means, sigmas
    int label = sampleLabel(data[id]); // sample new label conditionally
    add(id, label);                // add the element back with new label

    if ( ( i > BURN_IN ) && ( i % THIN_INTERVAL == 0 ) ) {
      // report intermediate results if needed
      // calculate summary statistics of the parameters to estimate
    }
  }
}
```

Initialization

```
void normMixGibbs::initParams() {
  // set everything to zero
  for(int i=0; i < k; ++i) {
    counts[i] = 0;
    sums[i] = sumsqs[i] = 0;
  }

  int r;
  for(int i=0; i < n; ++i) {
    r = randn(0, k);
    labels[i] = r;   // assign random labels at the beginning
    ++counts[r];     // update counts, sums, sumsqs accordingly
    sums[r] += data[i];
    sumsqs[r] += (data[i]*data[i]);
  }
}
```

A running example

```
user@host:~/> ./mixSimplex ./mix.dat
Minimim = 3043.46, at pi = 0.667271,
between N(-0.0304604,1.00326) and N(5.01226,0.956009)

user@host:~/> ./mixEM ./mix.dat
Minimim = 3043.46, at pi = 0.667842,
between N(-0.0299457,1.00791) and N(5.0128,0.913825)

user@host:~/> ./mixSA ./mix.dat
Minimim = 3043.46, at pi = 0.667793,
between N(-0.030148,1.00478) and N(5.01245,0.91296)

user@host:~/> ./mixGibbs ./mix.dat
Minimum = 3043.46, pi = 0.667772,
between N(-0.0301499,1.00764) and N(5.01214,0.915481)
```

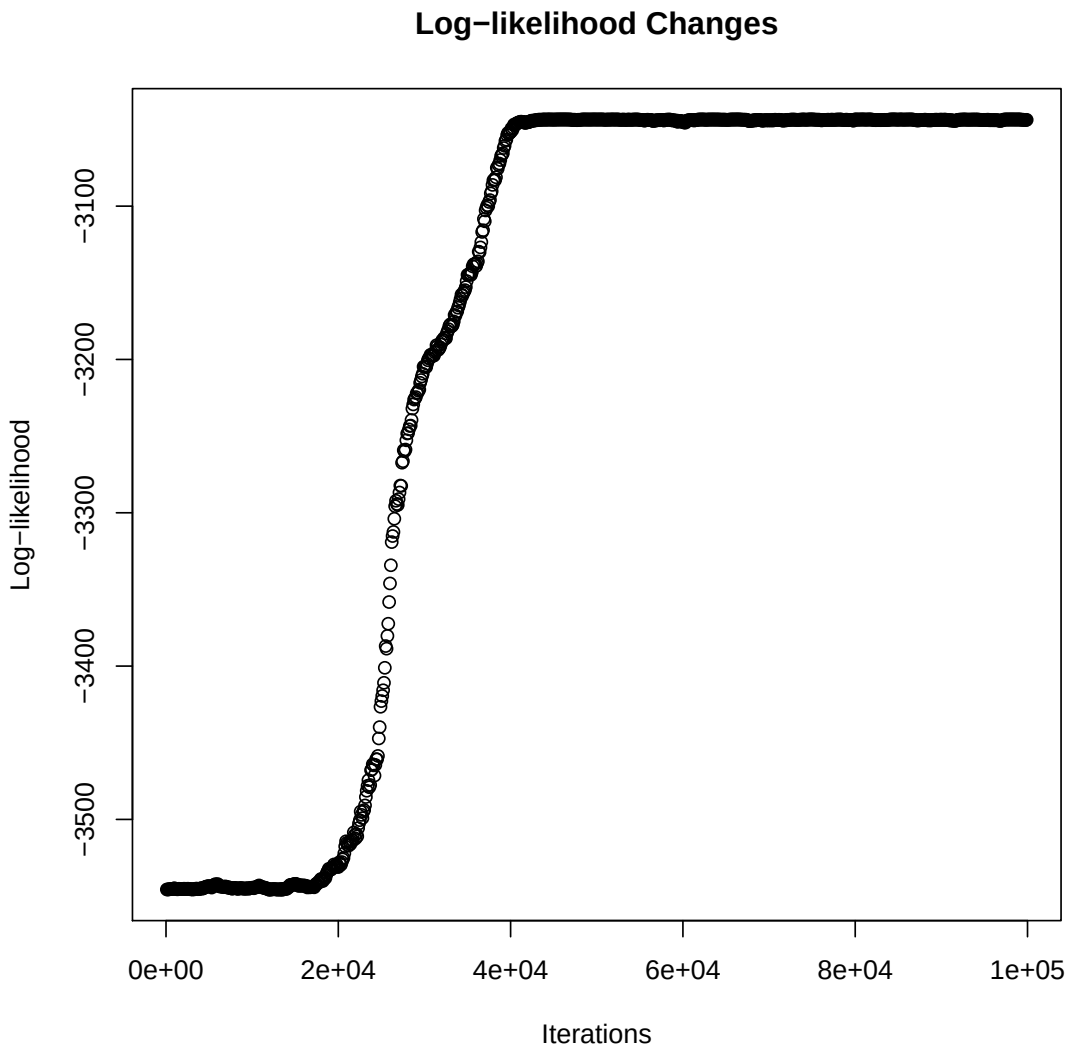
Notes on Gibbs Sampler

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

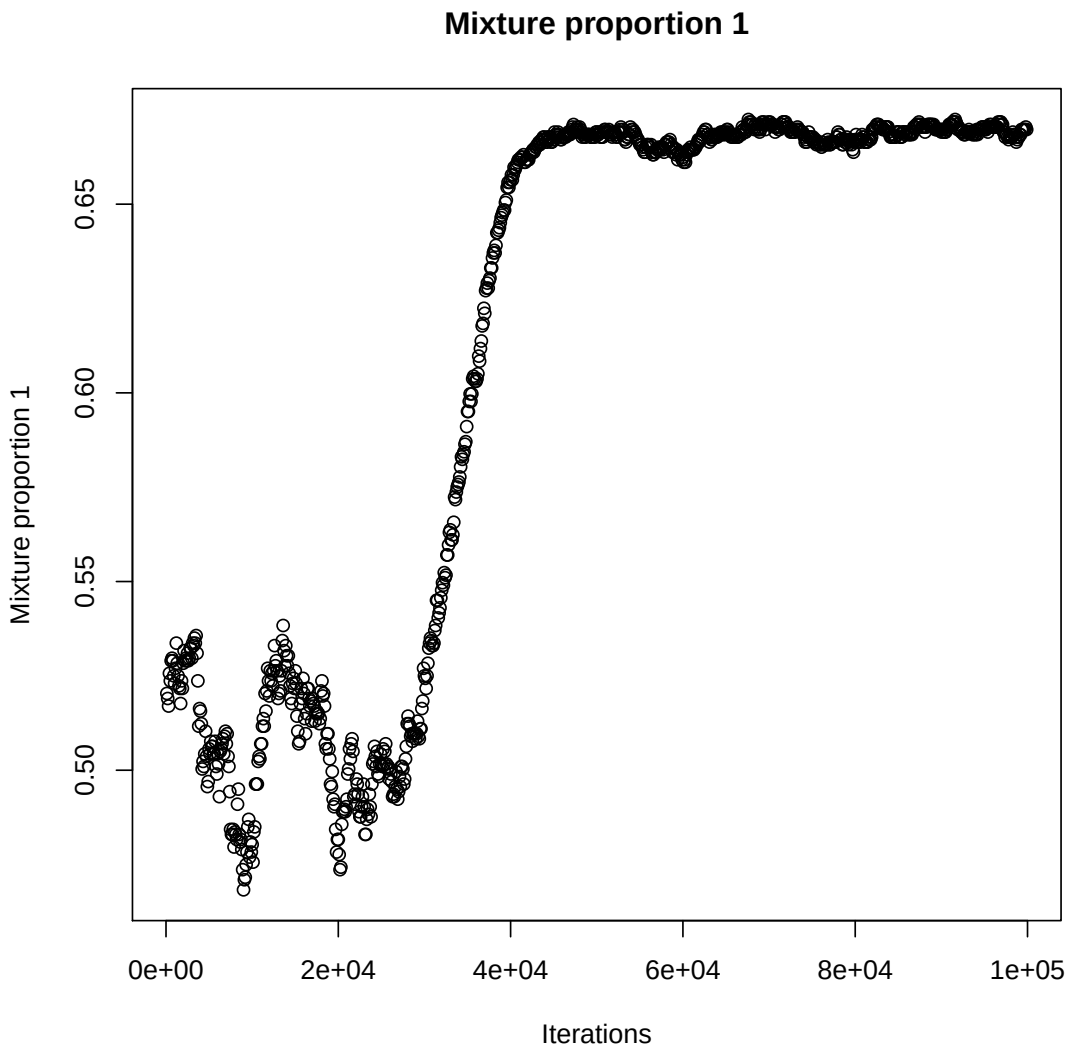
Drawing Inferences

- To draw inferences, summarize parameter values from stationary distribution
- For example, calculate the means or medians.
- Burn-in time required to converge to a reasonable solution before start collecting the estimated parameter values

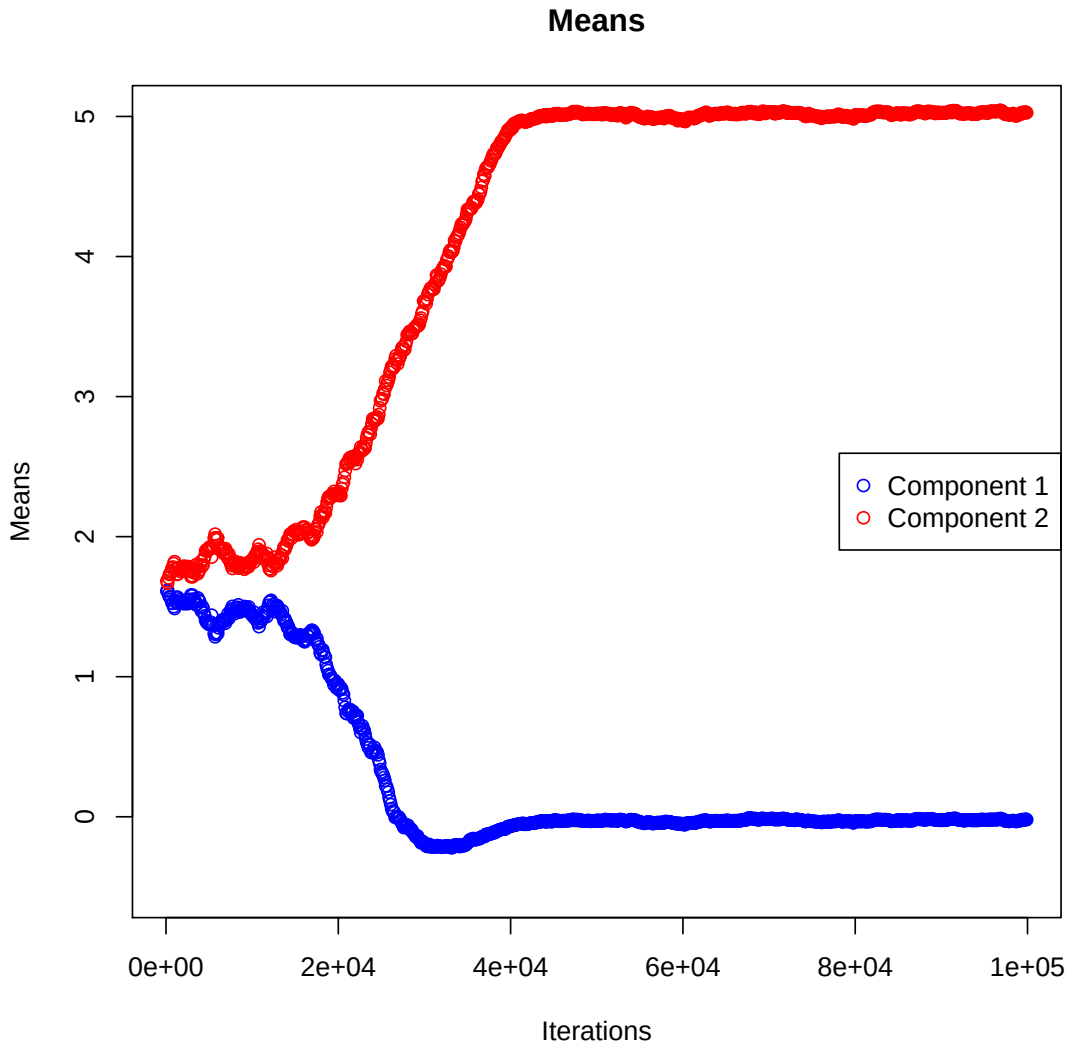
Log-likelihoods changes



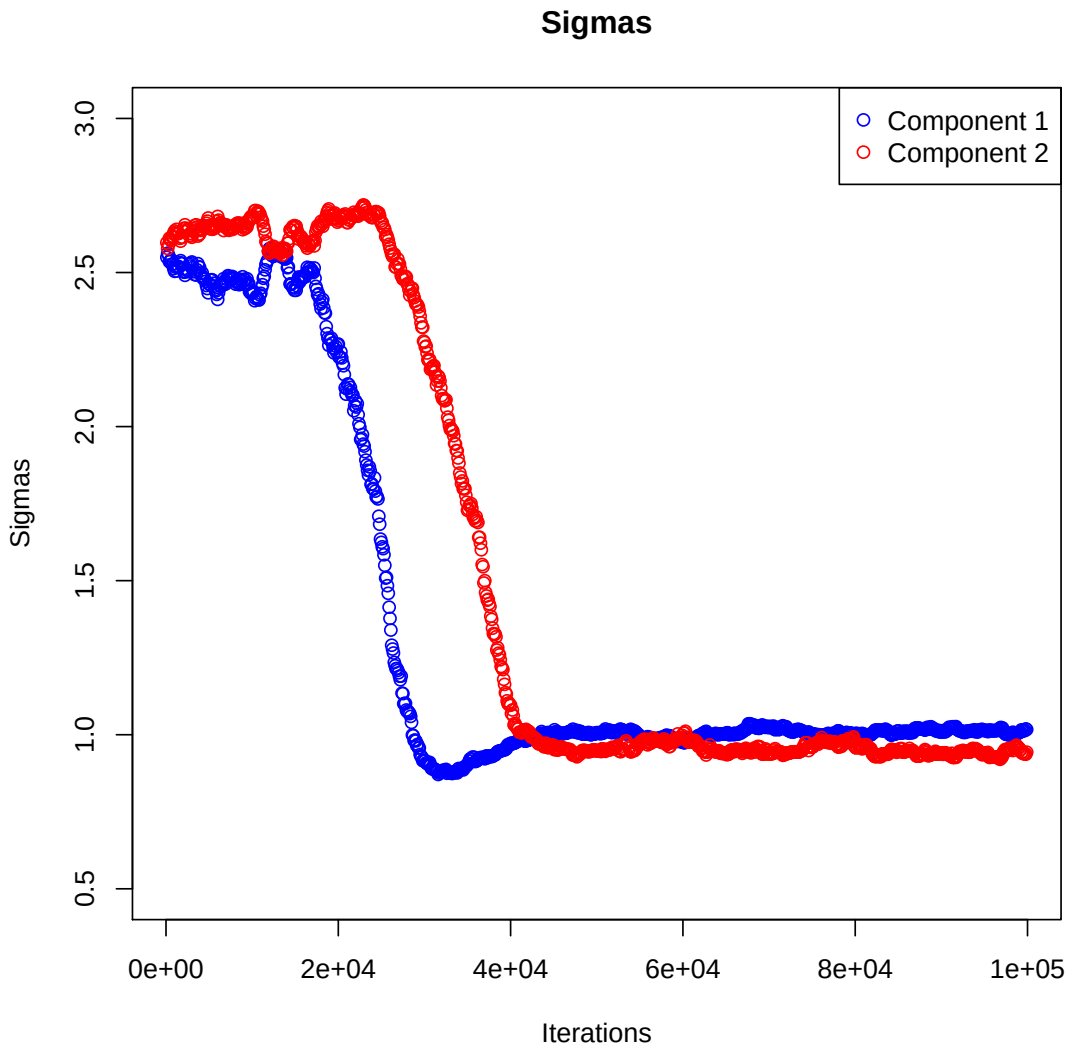
Mixing proportions



Means


Means
Means
Iterations
Component 1
Component 2
0
1
2
3
4
5
0e+00
2e+04
4e+04
6e+04
8e+04
1e+05

Standard deviations



Advantages of Gibbs Samplers

- Gibbs sampler allows to obtain posterior distribution of parameters, conditioned on the observed data.
- Joint distribution between parameters can also be obtained

Connecting Simulated Annealing and Gibbs Sampler

Both Methods are Markov Chains

- The distribution of $\lambda^{(t)}$ only depends on $\lambda^{(t-1)}$
- Update rule defines the transition probabilities between two states, requiring aperiodicity and irreducbility.

Both Methods are Metropolis-Hastings Algorithms

- Acceptance of proposed update is probabilistically determined by relative probabilities between the original and proposed states

Metropolis-Hastings Acceptance Probability

- Let $\theta_{ij} = \Pr(q_t = j | q_{t-1} = i)$
- Let π_i and π_j be the relative proabilities of each state
- The Metropolis-Hasting acceptance probability is

$$a_{ij} = \min\left(1, \frac{\pi_j \theta_{ji}}{\pi_i \theta_{ij}}\right)$$

- We need to know relative ratio between π_j and π_i.
- The equilibrium distribution $\Pr(q_t = i) = \pi_i$ will be reached.

Gibbs Sampler

- The Gibbs sampler ensures that $\pi_i \theta_{ij} = \pi_j \theta_{ji}$
- As a consequence,

$$a_{ij} = \min\left(1, \frac{\pi_j \theta_{ji}}{\pi_i \theta_{ij}}\right) = 1$$

Simulated Annealing

- Given a temperature parameter τ
- π_i are replaced with

$$\pi_i^{(\tau)} = \frac{\pi_i^{1/\tau}}{\sum_j \pi_j^{1/\tau}}$$

- At high temperatures, the probability distribution between the states are flattened.
- At low tempearatures, larger weights are given to high probability states

Summary

Today - Gibbs Sampler

- MCMC + Metropolis-Hasting Method
- Proposed updates per each parameter based on conditional distribution
- Effective way to obtain joint distribution between the parameters empirically

Next lecture

- Further applications of multidimensional optimization methods