Biostatistics 615/815 Lecture 21:
Gibbs Sampling

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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: \( \lambda = (\pi_1, \cdots, \pi_k, \mu_1, \cdots, \mu_k, \sigma^2_1, \cdots, \sigma^2_k) \).
- Sample each \( \lambda_i \) 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 \( z \).
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

```cpp
// 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 = NormMix615::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] * NormMix615::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 $i \in \{1, \cdots, k\}$
  - $n_i = \sum_{j=1}^{n} I(z_j = i)$
  - $\pi_i = n_i / n$
  - $\mu_i = \sum_{j=1}^{n} x_j I(z_j = i) / n_i$
  - $\sigma^2_i = \sum_{j=1}^{n} I(z_j = i)(x_j - \mu_i)^2 / n_i$

- 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 ($O(k)$)?
Constant 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) {
        pis[i] = (double)counts[i]/(double)(numObs);
        means[i] = sums[i]/counts[i];
        sigmas[i] = sqrt((sumsq[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

```cpp
void normMixGibbs::runGibbs() {
    initParams(); // initialize 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

```cpp
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
Minimum = 3043.46, at pi = 0.667271,
between N(-0.0304604,1.00326) and N(5.01226,0.956009)

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

user@host:~/> ./mixSA ./mix.dat
Minimum = 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-likelihood changes
Mixing proportions

![Graph showing mixing proportions over iterations](image-url)
Means
Standard deviations

![Graph showing standard deviations for Component 1 and Component 2 over iterations.](image)
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 irreducibility.

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 $\pi_i$ and $\pi_j$ be the relative probabilities 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 $\pi_j$ and $\pi_i$.
- The equilibrium distribution $\Pr(q_t = i) = \pi_i$ will be reached.
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 $\tau$
- $\pi_i$ 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 temperatures, larger weights are given to high probability states
Summary

Simulated Annealing

- Simulated Annealing
- Markov-Chain Monte-Carlo method
- Searching for global minimum among local minima

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