Biostatistics 615/815 Lecture 20: Simulated Annealing Gibbs Sampling

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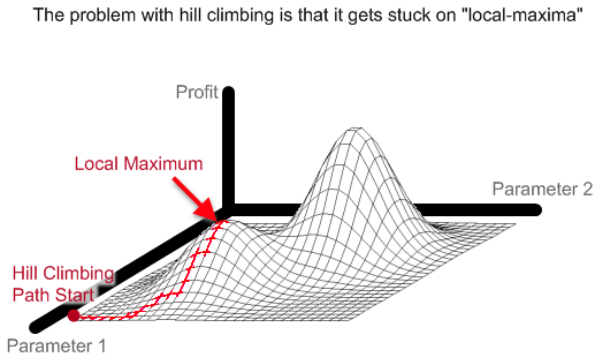
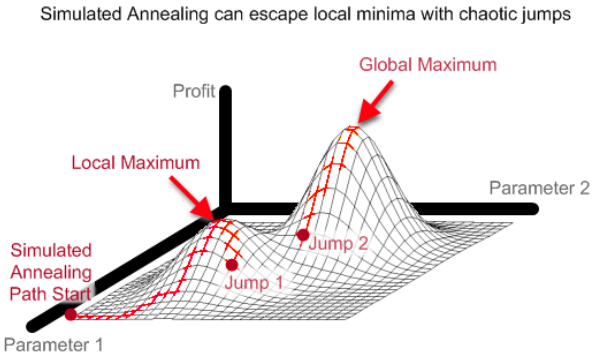
Local minimization methods



Images by Max Dama from

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

Global minimization with Simulated Annealing



Images by Max Dama from

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Example Applications

- The traveling salesman problem (TSP)
  - Salesman must visit every city in a set
  - Given distances between pairs of cities
  - Find the shortest route through the set
- No polynomial time algorithm is known for finding optimal solution
- Simulated annealing or other stochastic optimization methods often provide near-optimal solutions.

Examples of simulated annealing results

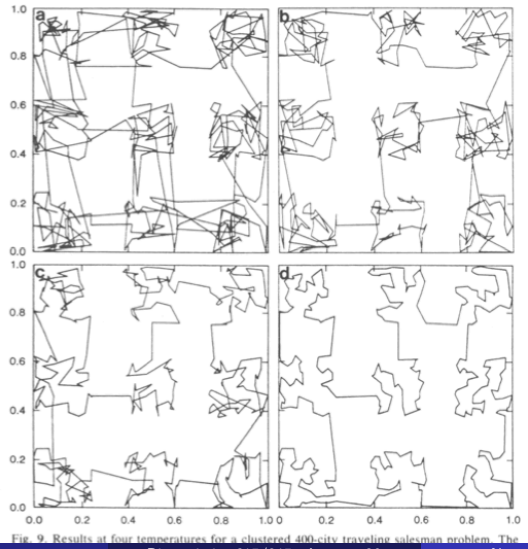

Fig. 9. Results at four temperatures for a clustered 400-city traveling salesman problem. The

Update scheme in Simulated Annealing

- Random walk by Metropolis criterion (1953)
- Given a configuration, assume a probability proportional to the Boltzmann factor

$$P_A = e^{-E_A/T}$$

- Changes from E_0 to E_1 with probability

$$\min\left(1, \frac{P_1}{P_0}\right) = \min\left(1, \exp\left(-\frac{E_1 - E_0}{T}\right)\right)$$

- Given sufficient time, leads to equilibrium state

Using Markov Chains

Markov Chain Revisited

- The Markovian property

$$\Pr(q_t|q_{t-1}, q_{t-2}, \cdots, q_0) = \Pr(q_t|q_{t-1})$$

- Transition probability

$$\theta_{ij} = \Pr(q_t = j|q_{t-1} = i)$$

Simulated Annealing using Markov Chain

- Start with some state q_t.
- Propose a changed q_{t+1} given q_t
- Decide whether to accept change based on $\theta_{q_t q_{t+1}}$
  - Decision is based on relative probabilities of two outcomes

Key requirements

- Irreducibility : it is possible to get any state from any state
  - There exist t where $\Pr(q_t = j|q_o = i) > 0$ for all (i, j).
- Aperiodicity : return to the original state can occur at irregular times

$$\gcd\{t : \Pr(q_t = i|q_0 = i) > 0\} = 1$$

- These two conditions guarantee the existence of a unique equilibrium distribution

Equilibrium distribution

- Starting point does not affect results
- The marginal distribution of resulting state does not change
- Equilibrium distribution π satisfies

$$\begin{aligned} \pi &= \lim_{t\to\infty}\Theta^{t+1} \\ &= (\lim_{t\to\infty}\Theta^{t})\Theta \\ &= \pi\Theta \end{aligned}$$

- In Simulated Annealing, $\Pr(E) \propto e^{-E/T}$

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

Practical issues

- The maximum temperature
- Scheme for decreasing temperature
- Strategy for proposing updates
  - For mixture of normals, suggestion of Brooks and Morgan (1995) works well
  - Select a component to update, and sample from within plausible range

Implementing TSP : `Traverse2D.h`

```
#ifndef __TRAVERSE_2D_H
#define __TRAVERSE_2D_H

#include <vector>
#include <algorithm>
#include <cstdlib>
#include <cmath>

class Traverse2D {
 protected:
  double distance;
  bool stale;

 public:
  std::vector<double> xs;
  std::vector<double> ys;
  std::vector<int> order;
```

Implementing TSP : Traverse2D.h

```
  Traverse2D() : distance(-1), stale(true) {}

  Traverse2D(std::vector<double>& _xs, std::vector<double>& _ys)
            : xs(_xs), ys(_ys), stale(true) {
    int n = (int)xs.size();
    if ( n != ys.size() ) abort();
    for(int i=0; i < n; ++i) {
      order.push_back(i);
    }
  }

  int numPoints() { return (int)order.size(); }

  void addPoint(double x, double y) {
    xs.push_back(x);
    ys.push_back(y);
    order.push_back((int)order.size());
  }
```


Implementing TSP : Traverse2D.h

```
  void initOrder() {
    stale = true;
    std::sort( order.begin(), order.end() );
  }
  bool nextOrder() {
    stale = true;
    return std::next_permutation( order.begin(), order.end() );
  }
  void shuffleOrder() {
    stale = true;
    std::random_shuffle( order.begin(), order.end() );
  }
  void swapOrder(int x, int y) {
    stale = true;
    int tmp = order[x];
    order[x] = order[y];
    order[y] = tmp;
  }
```


Implementing TSP : Traverse2D.h

```
  double getDistance() {
    if ( stale ) {
      int n = (int)order.size();
      distance = 0;
      for(int i=1; i < n; ++i) {
        distance += sqrt(
            (xs[order[i]]-xs[order[i-1]])*(xs[order[i]]-xs[order[i-1]])
            + (ys[order[i]]-ys[order[i-1]])*(ys[order[i]]-ys[order[i-1]]) );
      }
      stale = false;
    }
    return distance;
  }
};

#endif // __TRAVERSE_2D_H
```


Implementing TSP : main()

```
int main(int argc, char** argv) {
  if ( argc != 2 ) {
    std::cerr << "Usage: TSP [infile]" << std::endl;
    return -1;
  }

  Matrix615<double> xy(argv[1]);
  int n = xy.rowNums();
  if ( xy.colNums() != 2 ) {
    std::cerr << "Input matrix does not have exactly two columns" << std::endl;
    return -1;
  }

  // build graph from file
  Traverse2D graph;
  for(int i=0; i < n; ++i) {
    graph.addPoint(xy.data[i][0], xy.data[i][1]);
  }
```

Implementing TSP : main()

```
int start = 0, finish = 0, nperm = 0;
double duration = 0, minDist = DBL_MAX, maxDist = 0, sumDist = 0;
std::vector<int> minOrder;
start = clock();
graph.initOrder();  // initialize order
do {
  double d = graph.getDistance();
  sumDist += d; ++nperm;
  if ( d > maxDist ) maxDist = d;
  if ( d < minDist ) {
    minDist = d;
    minOrder = graph.order;
  }
} while ( graph.nextOrder() );
finish = clock();
duration = (double)(finish-start)/CLOCKS_PER_SEC;
```


Implementing TSP : main()

```
  std::cout << "-------------------------------------------------" << std::endl;
  std::cout << "Minimum distance = " << minDist << std::endl;
  std::cout << "Maximum distance = " << maxDist << std::endl;
  std::cout << "Mean distance = " << sumDist/nperm << std::endl;
  std::cout << "Exhaustive search duration = " << duration << " seconds"
            << std::endl;
  std::cout << "-------------------------------------------------" << std::endl;

  start = clock();
  runTSPSA(graph, 1e-6); // run Simulated Annealing
  finish = clock();
  duration = (double)(finish-start)/CLOCKS_PER_SEC;
  std::cout << "SA distance = " << graph.getDistance() << std::endl;
  std::cout << "SA search Duration = " << duration << " seconds" << std::endl;
  std::cout << "-------------------------------------------------" << std::endl;

  return 0;
}
```


Implementing TSP : runTSPSA()

```
#define MAX_TEMP 1000
#define N_ITER 1000

double runTSPSA(Traverse2D& graph, double eps) {
  srand(std::time(0));
  graph.shuffleOrder();

  double temperature = MAX_TEMP;
  double prevDist = graph.getDistance();
  int n = graph.numPoints();
  while( temperature > eps ) {
    for(int i=0; i < N_ITER; ++i) {
      int i1 = (int)floor( rand()/(RAND_MAX+1.) * n);
      int i2 = (int)floor( rand()/(RAND_MAX+1.) * n);
      graph.swapOrder(i1,i2);
      double newDist = graph.getDistance();
      double diffDist = newDist-prevDist;
```


Implementing TSP : runTSPSA()

```
      if ( diffDist < 0 ) {
        prevDist = newDist;
      }
      else {
        double p = rand()/(RAND_MAX+1.);
        if ( p < exp(0-diffDist/temperature) ) {
          prevDist = newDist;
        }
        else {
          graph.swapOrder(i1,i2);
        }
      }
    }
    temperature *= 0.90;
  }
}
```

TSP : Working examples

```
$ cat tsp.10.in.txt
-2.30963348991357 0.0773267767084084
-1.13260001198939 0.194723763831079
-0.47887704546568 -1.49043206086804
-1.14183413926286 -0.386463669289195
-0.0684871826034848 0.362329163828058
-1.28322395967065 -0.173892955683618
-0.684913927794102 0.0967915142130205
1.87577059887638 -0.229129514295367
-0.796217725319515 1.77563911372358
0.936967861258253 -0.103803298997143
```


TSP : Working examples

```
$ ./TSP tsp.10.in.txt
-----------------------------------------------
Minimum distance = 9.43062
Maximum distance = 22.4157
Mean distance = 16.3802
Exhaustive search duration = 15.85 seconds
-----------------------------------------------
SA distance = 9.56846
SA search Duration = 1.51 seconds
-----------------------------------------------
```


TSP : Working examples

```
$ cat tsp.11.in.txt
-0.636066544886696 2.25053338615707
0.0860940972604061 0.231139523090642
0.219459494449743 -0.518180472158068
0.0566391380933713 -1.10184323809265
-0.300676076997908 -0.765625163407885
2.64204087640419 1.29479579271570
0.152911487506204 0.228909136397270
-0.933319389247532 -0.846940788411644
-0.447908403019059 -1.16451734926683
1.61047052169711 1.66393401261582
-1.16737084487488 1.04729096252209
```


TSP : Working examples

```
$ ./TSP tsp.11.in.txt
-----------------------------------------------
Minimum distance = 9.14731
Maximum distance = 28.1806
Mean distance = 20.3772
Exhaustive search duration = 192.85 seconds
-----------------------------------------------------------
SA distance = 9.14731
SA search Duration = 1.78 seconds
-----------------------------------------------
SA distance = 3.52509
SA search Duration = 0.514433 seconds
-----------------------------------------------
```

Simulated Annealing for Gaussian Mixtures

```
class normMixSA {
public:
  int k;                      // # of components
  int n;                      // # of data
  std::vector<double> data;   // observed data
  std::vector<double> pis;    // pis
  std::vector<double> means;  // means
  std::vector<double> sigmas; // sds
  double llk;                 // current likelihood
  normMixSA(std::vector<double>& _data, int _k);  // constructor
  void initParams();                              // initialize parameters
  double updatePis(double temperature);
  double updateMeans(double temperature, double lo, double hi);
  double updateSigmas(double temperature, double sdlo, double sdhi);
  double runSA(double eps);                       // run Simulated Annealing
  static int acceptProposal(double current, double proposal, double temperature);
};
```


Evaluating Proposals in Simulated Annealing

```
int normMixSA::acceptProposal(double current, double proposal,
                              double temperature) {
  if ( proposal < current )  return 1;  // return 1 if likelihood decreased
  if ( temperature == 0.0 )  return 0;  // return 0 if frozen
  double prob = exp(0-(proposal-current)/temperature);
  return (randu(0.,1.) < prob); // otherwise, probabilistically accept proposal
}
```


Updating Means and Variances

- Select component to update at random
- Sample a new mean (or variance) within plausible range for parameter
- Decide whether to accept proposal or not

Updating Means

```
double normMixSA::updateMeans(double temperature, double min, double max) {
  int c = randn(0,k)          // select a random integer between 0..(k-1)
  double old = means[c];      // save the old mean for recovery
  means[c] = randu(min, max); // update mean and evaluate the likelihood
  double proposal = 0-NormMix615::mixLLK(data, pis, means, sigmas);
  if ( acceptProposal(llk, proposal, temperature) ) {
    llk = proposal;           // if accepted, keep the changes
  }
  else {
    means[c] = old;           // if rejected, rollback the changes
  }
  return llk;
}
```

Updating Component Variances

```
double normMixSA::updateSigmas(double temperature, double min, double max) {
  int c = randn(0,k)           // select a random integer between 0..(k-1)
  double old = sigmas[c];      // save the old mean for recovery
  sigmas[c] = randu(min, max); // update a component and evaluate the likelihood
  double proposal = 0-NormMix615::mixLLK(data, pis, means, sigmas);
  if ( acceptProposal(llk, proposal, temperature) ) {
    llk = proposal;            // if accepted, keep the changes
  }
  else {
    sigmas[c] = old;           // if rejected, rollback the changes
  }
  return llk;
}
```


Updating Mixture Proportions

- Mixture proportions must sum to 1.0
- When updating one proportion, must take others into account
- Select a component at random
  - Increase or decrease probability by up to 25%
  - Rescale all proportions so they sum to 1.0

Updating Mixture Proportions

```
double normMixSA::updatePis(double temperature) {
  std::vector<double> pisCopy = pis; // make a copy of pi
  int c = randn(0,k);              // select a component to update
  pisCopy[c] *= randu(0.8,1.25);  // update the component
  // normalize pis
  double sum = 0.0;
  for(int i=0; i < k; ++i)
    sum += pisCopy[i];
  for(int i=0; i < k; ++i)
    pisCopy[i] /= sum;
  double proposal = 0-NormMix615::mixLLK(data, pisCopy, means, sigmas);
  if ( acceptProposal(llk, proposal, temperature) ) {
    llk = proposal;
    pis = pisCopy;   // if accepted, update pis to pisCopy
  }
  return llk;
}
```


Initializing parameters

```
void normMixSA::initParams() {
  double sum = 0, sqsum = 0;
  for(int i=0; i < n; ++i) {
    sum += data[i];
    sqsum += (data[i]*data[i]);
  }
  double mean = sum/n;
  double sigma = sqrt(sqsum/n - sum*sum/n/n);
  for(int i=0; i < k; ++i) {
    pis[i] = 1./k;                // uniform priors
    means[i] = data[rand() % n]; // pick random data points
    sigmas[i] = sigma;            // pick uniform variance
  }
}
```

Putting things together

```
double normMixSA::runSA(double eps) {
  initParams();                          // initialize parameter
  llk = 0-NormMix615::mixLLK(data, pis, means, sigmas); // initial likelihood
  double temperature = MAX_TEMP;         // initialize temperature
  double lo = min(data), hi = max(data); // min(), max() can be implemented
  double sd = stdev(data);               // stdev() can also be implemented
  double sdhi = 10.0 * sd, sdlo = 0.1 * sd;
  while( temperature > eps ) {
    for(int i=0; i < 1000; ++i) {
      switch( randn(0,3) ) {  // generate a random number between 0 and 2
      case 0:                 // update one of the 3*k components
        llk = updatePis(temperature);  break;
      case 1:
        llk = updateMeans(temperature, lo, hi); break;
      case 2:
        llk = updateSigmas(temperature, sdlo, sdhi); break;
      }
    }
    temperature *= 0.90;      // cool down slowly
  }
  return llk;
}
```


Running examples

```
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)
```


Comparisons

2-component Gaussian mixtures

- Simplex Method : 306 Evaluations
- E-M Algorithm : 12 Evaluations
- Simulated Annealing : $\sim 100,000$ Evaluations

For higher dimensional problems

- Simplex Method may not converge, or converge very slowly
- E-M Algorithm may stuck at local maxima when likelihood function is multimodal
- Simulated Annealing scale robustly with the number of dimensions.

Optimization Strategies

- 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 $p(\lambda_i|x, \lambda_1^{(t)}, \cdots, \lambda_{i-1}^{(t)}, \lambda_{i+1}^{(t)}, \cdots, \lambda_k^{(t)})$.
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 $p(\lambda_2|x, \lambda_1, \lambda_3, \cdots, \lambda_k)$.
   - $\cdots$
   - 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