Biostatistics 615/815 Lecture 19: Expectation-Maximization (EM) Algorithm Simulated Annealing

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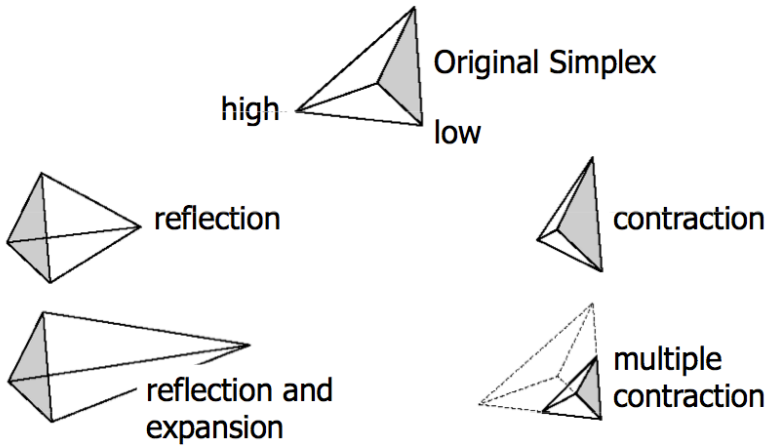
Recap - The Simplex Method

- General method for optimization
  - Makes few assumptions about function
- Crawls towards minimum using simplex
- Some recommendations
  - Multiple starting points
  - Restart maximization at proposed solution

Summary : The Simplex Method



Implementing Gaussian Mixture : `normMix615.h`

```
class NormMix615 {
 public:
  static double dnorm(double x, double mu, double sigma) {
    return 1.0 / (sigma * sqrt(M_PI * 2.0)) *
           exp (-0.5 * (x - mu) * (x-mu) / sigma / sigma);
  }
  static double dmix(double x, std::vector<double>& pis, std::vector<double>& means,
                     std::vector<double>& sigmas) {
    double density = 0;
    for(int i=0; i < (int)pis.size(); ++i)
      density += pis[i] * dnorm(x,means[i],sigmas[i]);
    return density;
  }
  static double mixLLK(std::vector<double>& xs, std::vector<double>& pis,
                       std::vector<double>& means, std::vector<double>& sigmas) {
    int i=0;
    double llk = 0.0;
    for(int i=0; i < xs.size(); ++i)
      llk += log(dmix(xs[i], pis, means, sigmas));
    return llk;
  }
};
```

Gaussian Mixture Function Object

```
class LLKNormMixFunc {
public:     // below are public functions
  LLKNormMixFunc(int k, std::vector<double>& y) :
      numComponents(k), data(y), numFunctionCalls(0) {}
  // core function - called when foo() is used
  // x is the combined list of MLE parameters (pis, means, sigmas)
  double operator() (std::vector<double>& x);
  std::vector<double> data;
  int numComponents;
  int numFunctionCalls;
};
```


Implementing likelihood of data

```
double LLKNormMixFunc::operator() (std::vector<double>& x) {
// x has (3*k-1) dimensions
  std::vector<double> priors;
  std::vector<double> means;
  std::vector<double> sigmas;
  assignPriors(x, priors); // transform (k-1) real numbers to priors
  for(int i=0; i < numComponents; ++i) {
    means.push_back(x[numComponents-1+i]);
    sigmas.push_back(x[2*numComponents-1+i]);
  }
  return 0-NormMix615::mixLLK(data, priors, means, sigmas);
}
```


Transforming between bounded and unbounded space

```
void LLKNormMixFunc::assignPriors(std::vector<double>& x,
                                  std::vector<double>& priors) {
  priors.clear();
  double p = 1.;
  for(int i=0; i < numComponents-1; ++i) {
    double logit = 1./(1.+exp(0-x[i]));
    priors.push_back(p*logit);
    p = p*(1.-logit);
  }
  priors.push_back(p);
}
```


Probably a better way of transformation

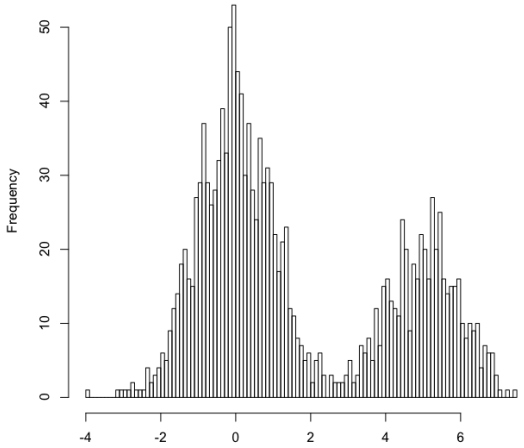
```
void LLKNormMixFunc::assignPriors(std::vector<double>& x,
                                  std::vector<double>& priors) {
  priors.clear();
  double psum = 0, xsum = 0;
  for(int i=0; i < numComponents-1; ++i) {
    double logit = 1./(1.+exp(0-x[i]));
    priors.push_back(logit);
    psum += logit;
    xsum += x[i];
  }
  double pe = 1./(1+exp(xsum));    // probability of last component
  double pec = 1./(1+exp(0-xsum)); // pec = 1-pe

  priors.push_back(pe);
  for(int i=0; i < numComponents-1; ++i)
    priors[i] = priors[i] / psum * pec;
}
```

Simplex Method for Gaussian Mixture

```
#include <iostream>
#include <fstream>
#include "simplex615.h"
#include "normMix615.h"
#include "llkNormMixFunc.h"
#define ZEPS 1e-10
int main(int main, char** argv) {
  double point[5] = {0, -1, 1, 1, 1};   // 50:50 mixture of N(-1,1) and N(1,1)
  simplex615<LLKNormMixFunc> simplex(point, 5);
  std::vector<double> data;                // input data
  std::ifstream file(argv[1]);             // open file
  double tok;                              // temporary variable
  while(file >> tok) data.push_back(tok);  // read data from file
  LLKNormMixFunc foo(2, data);             // 2-dimensional mixture model
  simplex.amoeba(foo, 1e-7);               // run the Simplex Method
  std::cout << "Minimum = " << simplex.ymin() << ", at pi = "
            << (1./(1.+exp(0-simplex.xmin()[0]))) << "," << "between N("
            << simplex.xmin()[1] << "," << simplex.xmin()[3] << ") and N("
            << simplex.xmin()[2] << "," << simplex.xmin()[4] << ")" << std::endl;
  return 0;
}
```


A working example



A working example

Simulation of data

```
> x <- rnorm(1000)
> y <- rnorm(500)+5
> write.table(matrix(c(x,y),1500,1),'mix.dat',row.names=F,col.names=F)
```

or use the program from Problem Set 4-1.

A Running Example

```
Minimum = 3043.46, at pi = 0.667271,
between N(-0.0304604,1.00326) and N(5.01226,0.956009)
(305 function evaluations in total)
```


The E-M algorithm

- General algorithm for missing data problem
- Requires "specialization" to the problem in hand
- Frequently applied to mixture distributions

Some citation records

- The E-M algorithm
  - Dempster, Laird, and Rubin (1977) J Royal Statistical Society (B) 39:1-38
  - Cited in over 19,624 research articles
- The Simplex Method
  - Nelder and Mead (1965) Computer Journal 7:308-313
  - Cited in over 10,727 research articles

The Basic E-M Strategy

- $X = (Y, Z)$
  - Complete data X - what we would like to have
  - Observed data Y - individual observations
  - Missing data Z - hidden / missing variables
- The algorithm
  - Use estimated parameters to infer Z
  - Update estimated parameters using Y
  - Repeat until convergence

The E-M Strategy in Gaussian Mixtures

When are the E-M algorithms useful?

- Problem is simpler to solve for complete data
  - Maximum likelihood estimates can be calculated using standard methods
- Estimates of mixture parameters would be obtained straightforwardly
  - if the origin of each observation is known

Filling in Missing Data in Gaussian Mixtures

- Missing data is the group assignment of each observation
- Complete data generated by assigning observations to groups 'probabilistically'

E-M formulation of Gaussian Mixture

- Gaussian mixture distribution given $\theta = (\pi, \mu, \sigma)$.

$$p(x_i) = \sum_{k=1}^{K} \pi_K \mathcal{N}(x_i | \mu_k, \sigma_k^2)$$

- Introducing latent variable **z**
  - $z_i \in \{1, \cdots, K\}$ is class assignment
- The marginal likelihood of observed data

$$L(\theta; \mathbf{x}) = p(\mathbf{x}|\theta) = \sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z}|\theta)$$

  is often intractable
- Use complete data likelihood to approximate $L(\theta; \mathbf{x})$

The E-M algorithm

Expectation step (E-step)

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

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

Maximization step (M-step)

- Find the parameter that maximize the expected log-likelihood

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

Implementing Gaussian Mixture E-M

```
class normMixEM {
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
  std::vector<double> probs;  // (n*k) class probability
  normMixEM(std::vector<double>& input, int _k);
  void initParams();
  void updateProbs();         // E-step
  void updatePis();           // M-step (1)
  void updateMeans();         // M-step (2)
  void updateSigmas();        // M-step (3)
  double runEM(double eps);
};
```


Gaussian mixture : The E-step

Key idea

- Estimate the missing data - 'class assignment'
- By conditioning on current parameter values
- Basically, "classify" each observation to the best of current step.

Classification Probabilities

$$\Pr(z_i = j|x_i,\pi,\mu,\sigma) = \frac{\pi_j \mathcal{N}(x_i|\mu_j,\sigma_j^2)}{\sum_k \pi_k \mathcal{N}(x_i|\mu_k,\sigma_k^2)}$$

Implementation of E-step

```
void normMixEM::updateProbs() {
  for(int i=0; i < n; ++i) {
    double cum = 0;
    for(int j=0; j < k; ++j) {
      probs[i*k+j] = pis[j]*NormMix615::dnorm(data[i],means[j],sigmas[j]);
      cum += probs[i*k+j];
    }
    for(int j=0; j < k; ++j) {
      probs[i*k+j] /= cum;
    }
  }
}
```

Mixture of Normals : The M-step

- Update mixture parameters to maximize the likelihood of the data
- Becomes simple when we assume that the current class assignment are correct
- Simply use the same proportions, weighted means and variances to update parameters
- This step is guaranteed never to decrease the likelihood

Updating Mixture Proportions

$$\pi_k = \frac{\sum_{i=1}^{n} \Pr(z_i = k | x_i, \mu, \sigma^2)}{n}$$

- Count the observations assigned to each group

Updating Mixture Proportions - Implementations

```
void normMixEM::updatePis() {
  for(int j=0; j < k; ++j) {
    pis[j] = 0;
    for(int i=0; i < n; ++i) {
      pis[j] += probs[i*k+j];
    }
    pis[j] /= n;
  }
}
```


Updating Component Means

$$\begin{aligned} \hat{\mu}_k &= \frac{\sum_i x_i \Pr(z_i = k | x_i, \mu, \sigma^2)}{\sum_i \Pr(z_i = k | x_i, \mu, \sigma^2)} \\ &= \frac{\sum_i x_i \Pr(z_i = k | x_i, \mu, \sigma^2)}{n\pi_k} \end{aligned}$$

- Calculate weighted mean for group
- Weights are probabilities of group membership

Updating Component Means - Implementations

```
void normMixEM::updateMeans() {
  for(int j=0; j < k; ++j) {
    means[j] = 0;
    for(int i=0; i < n; ++i) {
      means[j] += data[i] * probs[i*k+j];
    }
    means[j] /= (n * pis[j] + TINY);
  }
}
```


Updating Component Variances

$$\sigma_k^2 = \frac{\sum_{i=1}(x_i - \mu_k)^2 \Pr(z_i = k|x_i, \mu, \sigma)}{n\pi_k}$$

- Calculate weighted sum of squared differences
- Weights are probabilities of group membership

Updating Component Variances - Implementations

```
void normMixEM::updateSigmas() {
  for(int j=0; j < k; ++j) {
    sigmas[j] = 0;
    for(int i=0; i < n; ++i) {
      sigmas[j] += (data[i]-means[j])*(data[i]-means[j])*probs[i*k+j];
    }
    sigmas[j] = sqrt(sigmas[j] / (n * pis[j] + TINY));
  }
}
```


E-M Algorithm for Mixtures

1. Guesstimate starting parameters
2. Use Bayes' theorem to calculate group assignment probabilities
3. Update parameters using estimated assignments
4. Repeat steps 2 and 3 until likelihood is stable

Implementation of E-M algorithm - putting things together

```
double normMixEM::runEM(double eps) {
  double llk = 0, prevLLK = 0;
  initParams();
  while( ( llk == 0 ) || ( check_tol(llk, prevLLK, eps) == 0 ) ) {
    updateProbs();
    updatePis();
    updateMeans();
    updateSigmas();
    prevLLK = llk;
    llk = NormMix615::mixLLK(data, pis, means, sigmas);
  }
  return llk;
}
```


Constructing normMixEM object

```
normMixEM::normMixEM(std::vector<double>& input, int _k) {
  data = input;
  k = _k;
  n = (int)data.size();
  pis.resize(k);
  means.resize(k);
  sigmas.resize(k);
  probs.resize(k * data.size());
}
```


Initializing the parameters

```
void normMixEM::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
  }
}
```


A working example

main() function

```
int main(int main, char** argv) {
  std::vector<double> data;
  std::ifstream file(argv[1]);
  double tok;
  while(file >> tok) data.push_back(tok);
  normMixEM em(data,2);
  double minLLK = em.runEM(1e-6);
  std::cout << "Minimum = " << minLLK << ", at pi = " << em.pis[0] << ","
            << "between N(" << em.means[0] << "," << em.sigmas[0]<< "^2) and N("
            << em.means[1] << "," << em.sigmas[1] << "^2)" << std::endl;
  return 0;
}
```

Running example

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

Summary : The E-M Algorithm

- Iterative procedure to find maximum likelihood estimate
  - E-step : Calculate the distribution of latent variables and the expected log-likelihood of the parameters given current set of parameters
  - M-step : Update the parameters based on the expected log-likelihood function
- The iteration does not decrease the marginal likelihood function
- But no guarantee that it will converge to the MLE
- Particularly useful when the likelihood is an exponential family
  - The E-step becomes the sum of expectations of sufficient statistics
  - The M-step involves maximizing a linear function, where closed form solution can often be found

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Local and global optimization methods

Local optimization methods

- "Greedy" optimization methods
  - Can get trapped at local minima
  - Outcome might depend on starting point
- Examples
  - Golden Search
  - Nelder-Mead Simplex Method
  - E-M algorithm

Next

- Simulated Annealing
- Markov-Chain Monte-Carlo Method
- Designed to search for global minimum among many local minima

Local minimization methods

The problem

- Most minimization strategies find the *nearest* local minimum from the starting point
- Standard strategy
  - Generate trial point based on current estimates
  - Evaluate function at proposed location
  - Accept new value if it improves solution

The solution

- We need a strategy to find other minima
- To do so, we sometimes need to select new points that does not improve solution
- How?

Simulated Annealing

Annealing

- One manner in which crystals are formed
- Gradual cooling of liquid
  - At high temperatures, molecules move freely
  - At low temperatures, molecules are "stuck"
- If cooling is slow
  - Low energy, organized crystal lattice formed

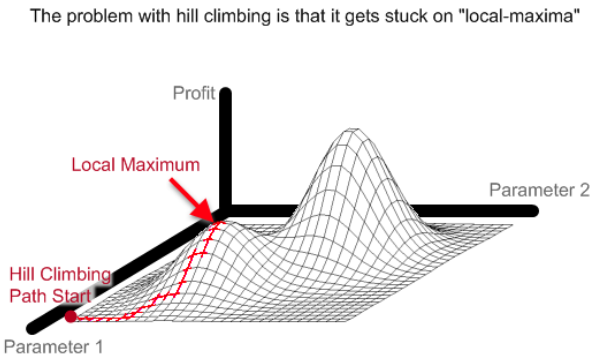
Simulated Annealing

- Analogy with thermodynamics
- Incorporate a temperature parameter into the minimization procedure
- At high temperatures, explore parameter space
- At lower temperatures, restrict exploration

Simulated Annealing Strategy

- Consider decreasing series of temperatures
- For each temperature, iterate these step
  - Propose an update and evaluation function
  - Accept updates that improve solution
  - Accept some updates that don't improve solution
    - Acceptance probability depends on "temperature" parameter
- If cooling is sufficiently slow, the global minimum will be reached

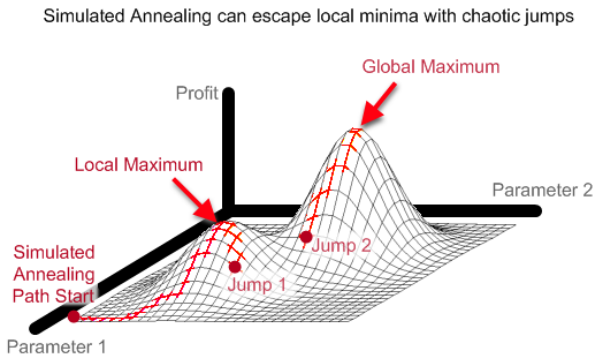
Local minimization methods



Images by Max Dama from

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

Global minimization with Simulated Annealing



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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.

Simulated Annealing TSP : Update Scheme

- A good scheme should be able to
  - Connect any two possible paths
  - Propose improvements to good solutions
- Some possible update schemes
  - Swap a pair of cities in current path
  - Invert a segment in current path

Examples of simulated annealing results

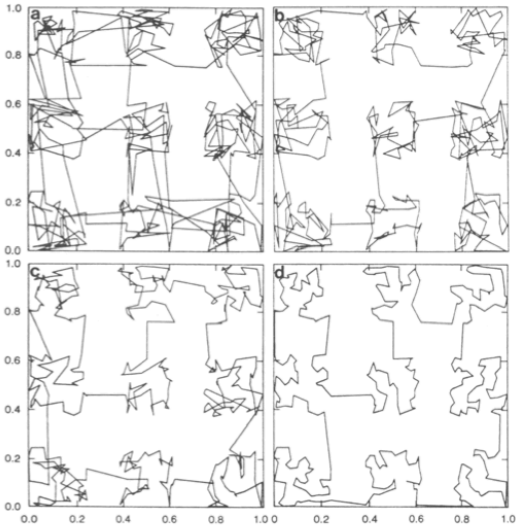

Fig. 9. Results at four temperatures for a clustered 400-city traveling salesman problem. The

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 += ( (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]]) );
      }
      distance = sqrt(distance);
      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 = 3.45434
Maximum distance = 8.00868
Mean distance = 6.053
Exhaustive search duration = 9.69001 seconds
-------------------------------------------
SA distance = 3.50017
SA search Duration = 0.456339 seconds
-------------------------------------------

$ ./TSP tsp.10.in.txt
-------------------------------------------
Minimum distance = 3.45434
Maximum distance = 8.00868
Mean distance = 6.053
Exhaustive search duration = 9.72787 seconds
-------------------------------------------
SA distance = 3.45434
SA search Duration = 0.457726 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 = 3.50014
Maximum distance = 9.53825
Mean distance = 7.28444
Exhaustive search duration = 115.615 seconds
---------------------------------------------
SA distance = 3.52509
SA search Duration = 0.514433 seconds
---------------------------------------------

$ ./TSP tsp.11.in.txt
---------------------------------------------
Minimum distance = 3.50014
Maximum distance = 9.53825
Mean distance = 7.28444
Exhaustive search duration = 116.613 seconds
---------------------------------------------
SA distance = 3.50014
SA search Duration = 0.507408 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;
}
```



```
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.

Summary

Simulated Annealing

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

Next lecture

- More on MCMC Method
- A simple Gibbs Sampler