Biostatistics 615/815 Lecture 19: Multidimensional Optimizations

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Annoucements

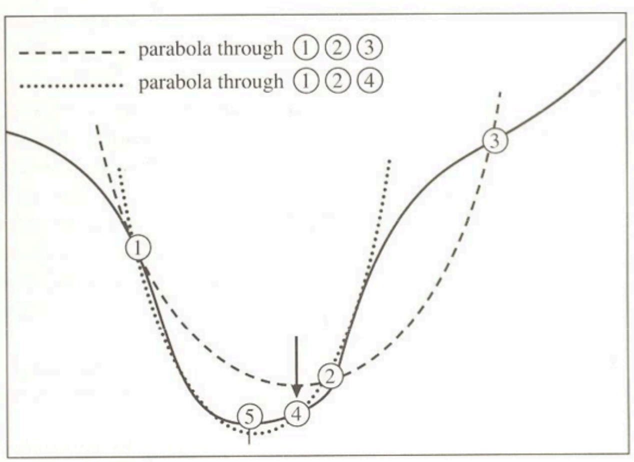
Homework

- Homework #5 due today
- Extension to thursday is allowed

Today's lecture

- The Simplex Method Details
- MLE estimation of mixture of normals

Recap : Single-dimensional minimization using parabola



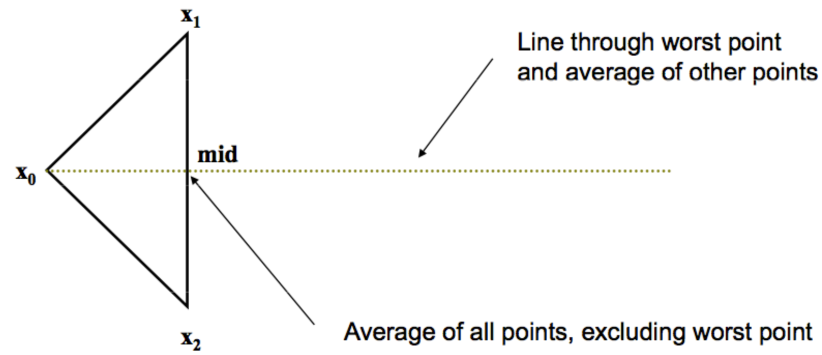
Recap : Adaptive Minimization

- Parabolic interpolation often converges faster
  - The preferred algorithm
- Golden search provides worst-cast performance guarantee
  - A fall-back for uncooperative functions
- Switch algorithms when convergence is slow
- Avoid testing points that are too close

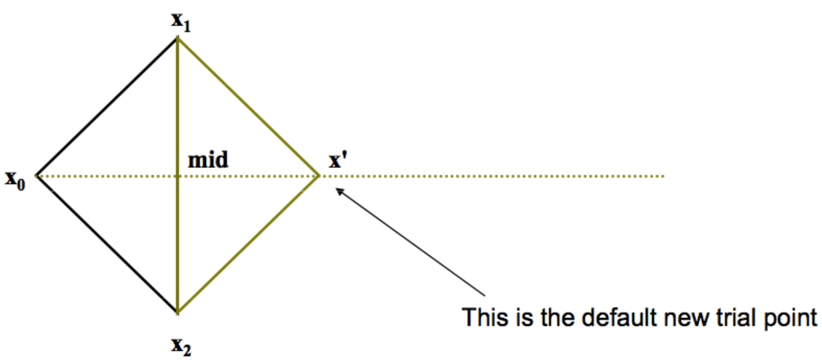
The Simplex Method

- Calculate likelihoods at simplex vetices
  - Geomtric shape with $k+1$ corners
  - A triangle in $k=2$ dimensions
- Simplex *crawls*
  - Towards minimum
  - Away from maximum
- Probably the most widely used optimization method

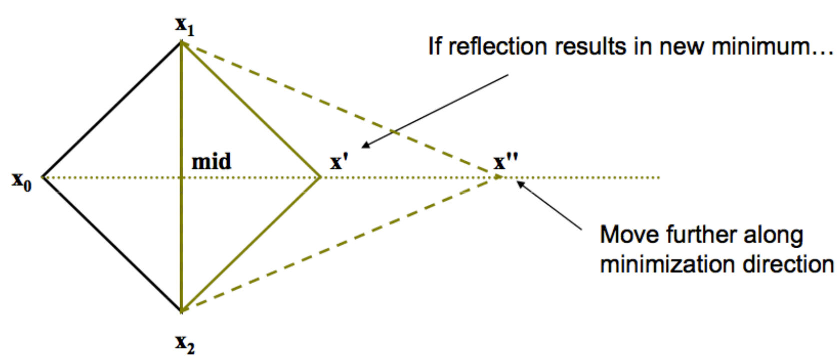
Direction for Optimization



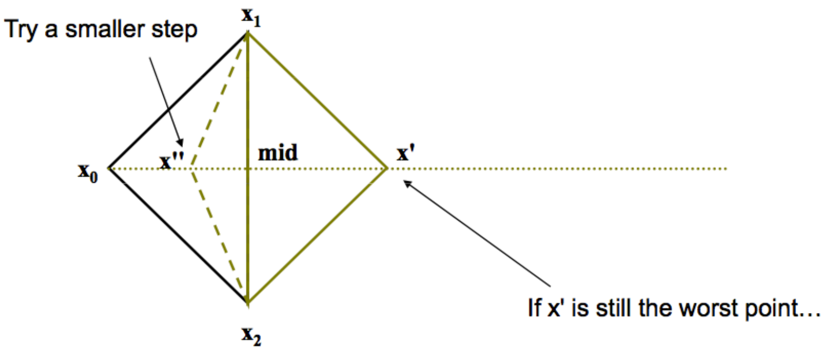
Reflection



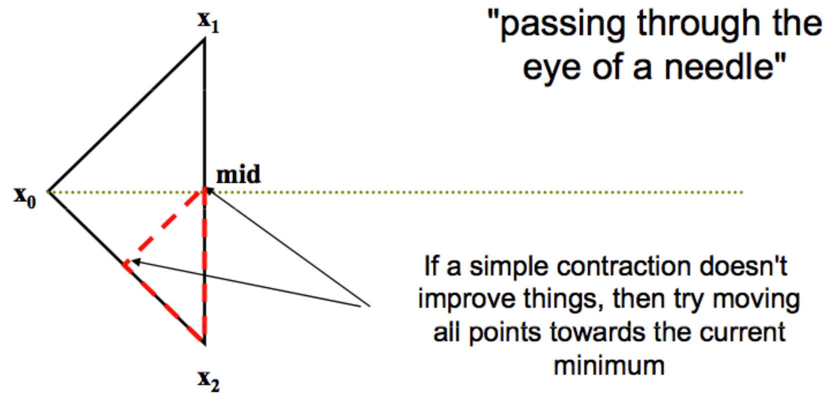
Reflection and Expansion



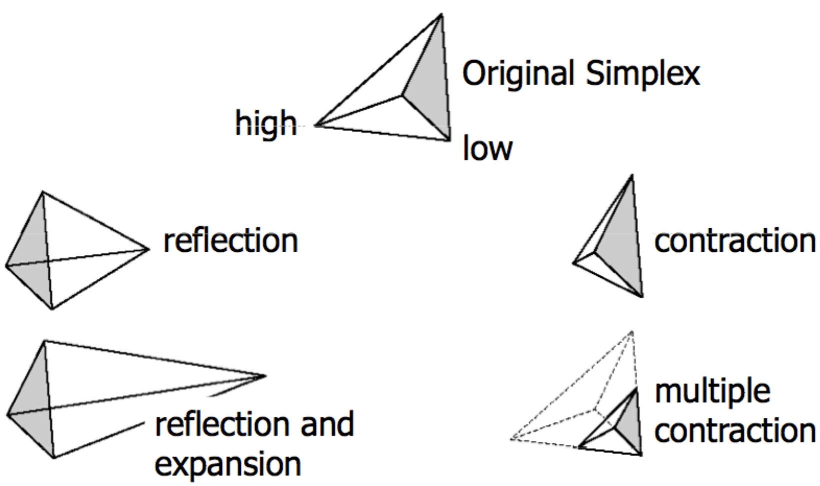
Contraction (1-dimension)



Contraction



Summary : The Simplex Method



Implementing the Simplex Method

```
class simplex615 { // contains (dim+1) points of size (dim)
 protected:
  std::vector<std::vector<double> > X; // (dim+1)*dim matrix
  std::vector<double> Y;               // (dim+1) vector
  std::vector<double> midPoint;        // variables for update
  std::vector<double> thruLine;        // variables for update
  int dim, idxLo, idxHi, idxNextHi;    // dimension, min, max, 2ndmax values
  void evaluateFunction(optFunc& foo); // evaluate function value at each point
  void evaluateExtremes();             // determine the min, max, 2ndmax
  void prepareUpdate();                // calculate midPoint, thruLine
  bool updateSimplex(optFunc& foo, double scale);  // for reflection/expansion..
  void contractSimplex(optFunc& foo);  // for multiple contraction
  static int check_tol(double fmax, double fmin, double ftol); // check tolerance
 public:
  simplex615(double* p, int d);          // constructor with initial points
  void amoeba(optFunc& foo, double tol); // main function for optimization
  std::vector<double>& xmin();           // optimal x value
  double ymin();                         // optimal y value
};
```

Implementation overview

- Data representation
  - Each `X[i]` is point of the simplex
  - `Y[i]` corresponds to $f(X[i])$
  - `midPoint` is the average of all points (except for the worst point)
  - `thruLine` is vector from the worse point to the `midPoint`
- Reflection, Expansion and Contraction
  After calculating `midPoint` and `thruLine`
  - Reflection: Call `updateSimplex(foo, -1.0)`
  - Expansion: Call `updateSimplex(foo, -2.0)`
  - Contraction: Call `updateSimplex(foo, 0.5)`

Initializing a Simplex

```
// constructor of simplex615 class : initial point is given
simplex615::simplex615(double* p, int d) : dim(d) { // set dimension
  // Determine the space required
  X.resize(dim+1);      // X is vector-of-vector, like 2-D array
  Y.resize(dim+1);      // Y is function value at each simplex point
  midPoint.resize(dim);
  thruLine.resize(dim);
  for(int i=0; i < dim+1; ++i) {
    X[i].resize(dim);  // allocate the size of content in the 2-D array
  }
  // Initially, make every point in the simplex identical
  for(int i=0; i < dim+1; ++i)
    for(int j=0; j < dim; ++j)
      X[i][j] = p[j];  // set each simple point to the starting point
  // then increase each dimension by one unit except for the last point
  for(int i=0; i < dim; ++i)
    X[i][i] += 1.;     // this will generate a simplex
}
```

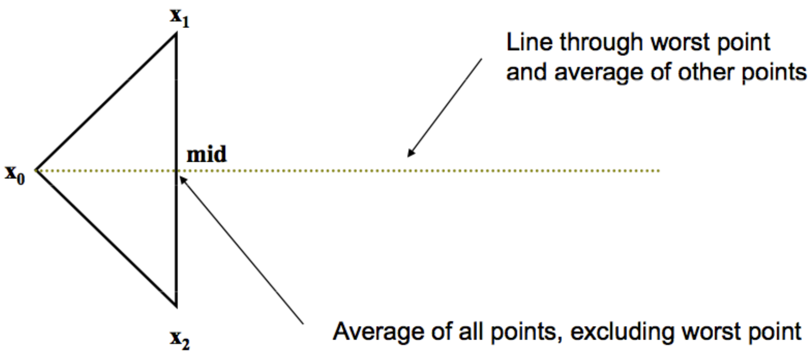

Evaluating function values at each simplex point

```
// simple function for evaluating the function value at each simple point
// after calling this function Y[i] = foo(X[i]) should hold
void simplex615::evaluateFunction(optFunc& foo) {
  for(int i=0; i < dim+1; ++i) {
    Y[i] = foo(X[i]);  // foo is a function object, which will be visited later
  }
}
```


Determine the best, worst, and the second-worst points

```
void simplex615::evaluateExtremes() {
  if ( Y[0] > Y[1] ) {  // compare the first two points
    idxHi = 0; idxLo = idxNextHi = 1;
  }
  else {
    idxHi = 1; idxLo = idxNextHi = 0;
  }
  // for each of the next points
  for(int i=2; i < dim+1; ++i) {
    if ( Y[i] <= Y[idxLo] )           // update the best point if lower
      idxLo = i;
    else if ( Y[i] > Y[idxHi] ) {     // update the worst point if higher
      idxNextHi = idxHi; idxHi = i;
    }
    else if ( Y[i] > Y[idxNextHi] ) { // update also if it is the 2nd-worst point
      idxNextHi = i;
    }
  }
}
```

Direction for Optimization



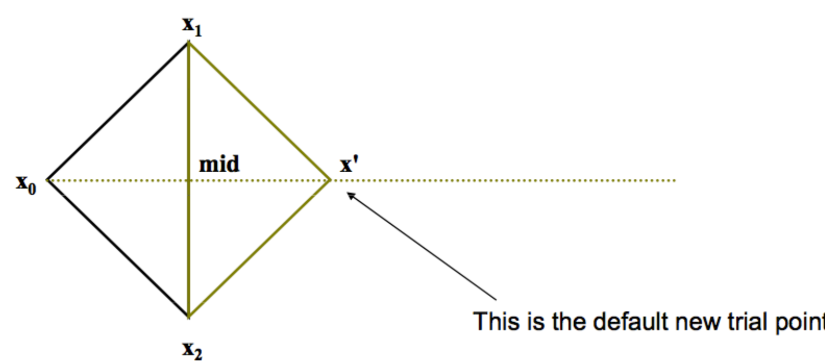
Determining the direction for optimization

```
void simplex615::prepareUpdate() {
  for(int j=0; j < dim; ++j) {
    midPoint[j] = 0;        // average of all points but the worst point
  }
  for(int i=0; i < dim+1; ++i) {
    if ( i != idxHi ) {     // exclude the worst point
      for(int j=0; j < dim; ++j) {
midPoint[j] += X[i][j];
      }
    }
  }
  for(int j=0; j < dim; ++j) {
    midPoint[j] /= dim;     // take average
    thruLine[j] = X[idxHi][j] - midPoint[j]; // direction for optimization
  }
}
```

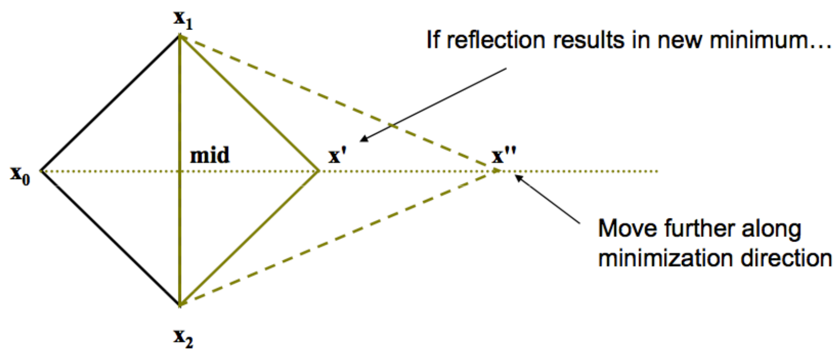

Updating simplex along the line

```
// scale determines which point to evaluate along the line
// scale = 1 : worse point, scale = 0 : midPoint
bool simplex615::updateSimplex(optFunc& foo, double scale) {
  std::vector<double> nextPoint;   // next point to evaluate
  nextPoint.resize(dim);
  for(int i=0; i < dim; ++i) {
    nextPoint[i] = midPoint[i] + scale * thruLine[i];
  }
  double fNext = foo(nextPoint);
  if ( fNext < Y[idxHi] ) {        // update only maximum values (if possible)
    for(int i=0; i < dim; ++i) {   //   because the order can be changed with
      X[idxHi][i] = nextPoint[i];  //   evaluateExtremes() later
    }
    Y[idxHi] = fNext;
    return true;
  }
  else {
    return false;                  // never mind if worse than the worst
  }
}
```

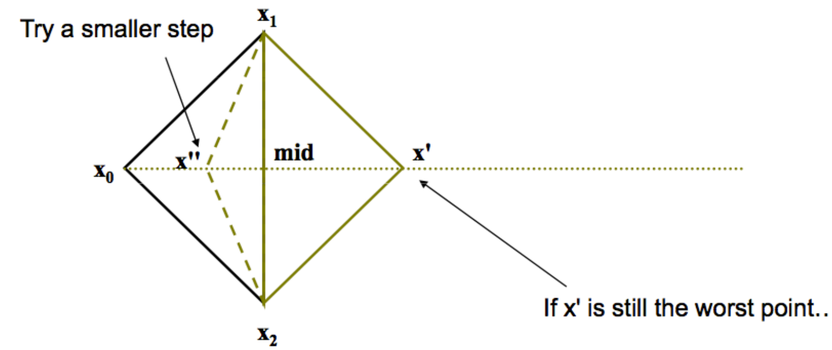

Reflection



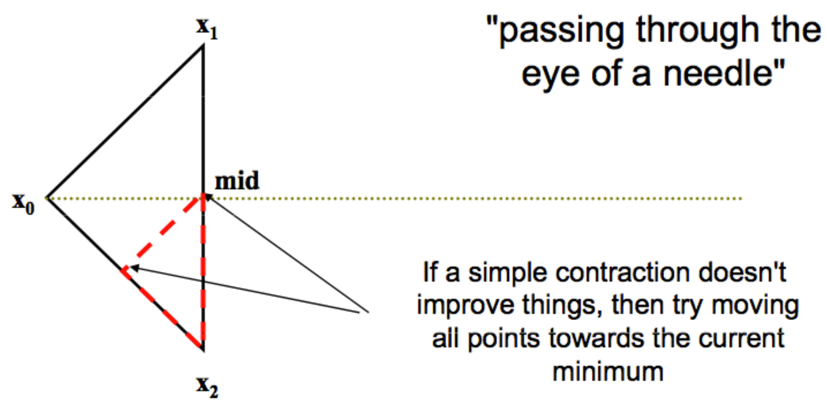
Reflection and Expansion



Contraction (1-dimension)



Multiple Contraction



Updating simplex along the line

```
// if none of the tried points make things better
//   reduce the search space towards the minimum point
void simplex615::contractSimplex(optFunc& foo) {
  for(int i=0; i < dim+1; ++i) {
    if ( i != idxLo ) {    // except for the minimum point
      for(int j=0; j < dim; ++j) {
X[i][j] = 0.5*( X[idxLo][j] + X[i][j] ); // move the point towards minimum
Y[i] = foo(X[i]);                        // re-evaluate the function
      }
    }
  }
}
```

Putting things together

```
void simplex615::amoeba(optFunc& foo, double tol) {
  evaluateFunction(foo);  // evaluate the function at the initial points
  while(true) {
    evaluateExtremes();   // determine three important points
    prepareUpdate();      // determine direction for optmization

    if ( check_tol(Y[idxHi],Y[idxLo],tol) ) break; // check convergence
    updateSimplex(foo, -1.0);     // reflection
    if ( Y[idxHi] < Y[idxLo] ) {
      updateSimplex(foo, -2.0);   // expansion
    }
    else if ( Y[idxHi] >= Y[idxNextHi] ) {
      if ( !updateSimplex(foo, 0.5) ) {  // 1-d contraction
         contractSimplex(foo);   // multiple contractions
      }
    }
  }
}
```


amoeba() function

- A general purpose minimization routine
  - Works in multiple dimensions
  - Uses only function evaluations
  - Does not require derivatives

Checking convergence

```
// Note that the function is declared as "static" function as
//
// static int check_tol(double fmax, double fmin, double ftol);
//
//   because it does not use any member variables
int simplex615::check_tol(double fmax, double fmin, double ftol) {
  // calculate the difference
  double delta = fabs(fmax - fmin);
  // calculate the relative tolerance
  double accuracy = (fabs(fmax) + fabs(fmin)) * ftol;
  // check if difference is within tolerance
  return (delta < (accuracy + ZEPS));
}
```


Using the Simplex Method Implementation

```
#include <vector>
#include <cmath>
#include <iostream>
#include "simplex615.h"
#define ZEPS 1e-10

int main(int main, char** argv) {
  double point[2] = {-1.2, 1};  // initial point to start

  arbitraryOptFunc foo;         // WILL BE DISCUSSED LATER
  simplex615 simplex(point, 2); // create a simplex
  simplex.amoeba(foo, 1e-7);    // optimize for a function
  // print outputs
  std::cout << "Minimim = " << simplex.ymin() << ", at ("
            << simplex.xmin()[0] << ", " << simplex.xmin()[1]
            << ")" << std::endl;
  return 0;
}
```

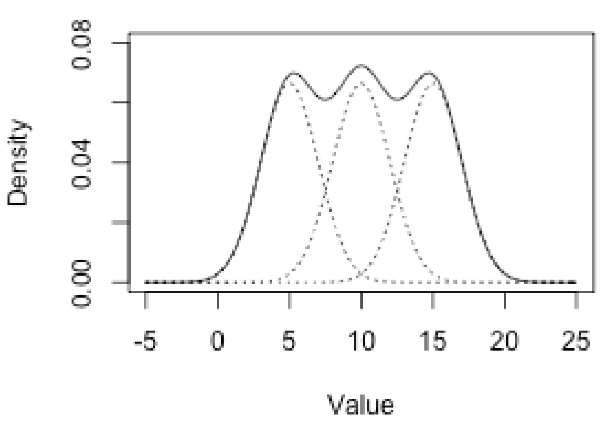
Defining a function using inheritance

```
// this is an abstract base class, which CAN NOT be used as class instance
class optFunc {
 public:
  // 'virtual' means inherited method can be used when
  // optFunc class is used via pointer or reference
  virtual double operator() (std::vector<double>& x) = 0; // function disabled
};
// Define a function inherits the function
// when foo() is called at the simplex, this function is actually called
class arbitraryOptFunc : public optFunc {
 public:
  virtual double operator() (std::vector<double>& x) {
    // 100*(x1-x0^2)^2 + (1-x0)^2
    return 100*(x[1]-x[0]*x[0])*(x[1]-x[0]*x[0])+(1-x[0])*(1-x[0]);
  }
};
```


A working example

```
Minimim = 1.35567e-11, at (0.999999, 0.999997)
```


Recap : A mixture distribution



Recap : MLE in Gaussian mixture

Parameter estimation in Gaussian mixture

- No analytical solution
- Numerical optimization required
- Multi-dimensional optimization problem
  - $\mu_1, \mu_2, \cdots, \mu_k$
  - $\sigma_1^2, \sigma_2^2, \cdots, \sigma_k^2$

Possible approaches

- Simplex Method
- Expectation Maximization
- Markov-Chain Monte Carlo

Normal Density

Normal density function

$$f(x|\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right]$$

Implementation

```
class mixLLKFunc : public optFunc {
protected:
  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);
  }
  ...
}
```


Gaussian mixture distribution

Density function

$$p(x|k,\pi,\mu,\sigma) = \sum_{i=1}^{k} \pi_i f(x|\mu_i,\sigma_i)$$

Implementation

```
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;
}
```


Likelihood of multiple observations

Calculating in log-space

$$L = \prod_i p(x_i|\pi,\pi,\mu,\sigma)$$

$$l = \sum_i \log p(x_i|\pi,\mu,\sigma)$$

Implementation

```
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 mixLLKFunc : public optFunc {
protected:  // these are internal function
  static double dnorm(double x, double mu, double sigma);
  static double dmix(...);
  static double mixLLK(...);
public:     // below are public functions
  mixLLKFunc(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)
  virtual double operator() (std::vector<double>& x);
  std::vector<double> data;
  int numComponents;
  int numFunctionCalls;
};
```

Avoiding boundary conditions

Problem

- The simplex algorithm do not know that $0 \leq \pi_i \leq 1$, and $\sum_{i=1}^n \pi_i = 1$
- During the iteration of simplex algorithm, it is possible that π_i goes out of bound

Possible solutions

- Modify simplex algorithm to avoid boundary conditions
- Transform the parameter space to infinite ranges

Transforming the parameter space

Contraints

- $0 \leq \pi_i \leq 1$
- $\sum_{i=1}^n \pi_i = 1$

Mapping between the space

- Given $x \in \mathbb{R}^{n-1}$, for $i = 1, \cdots, n-1$
- $\pi_i = \frac{1}{1+e^{-x_i}}(1 - \sum_{j=1}^{i-1} \pi_j)$
- $\pi_n = 1 - \sum_{i=1}^{n-1} \pi_i$.

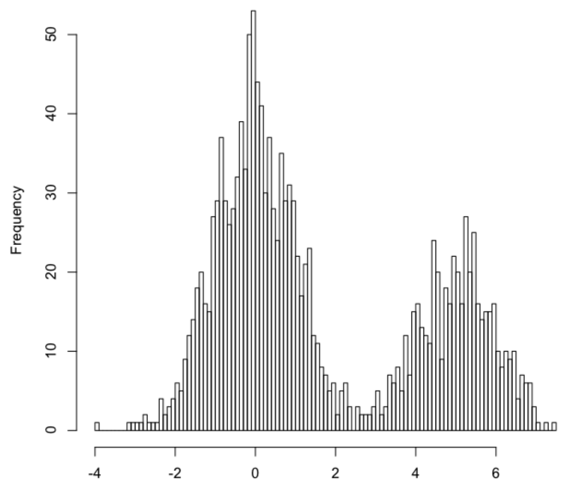
Implementing likelihood of data

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


Simplex Method for Gaussian Mixture

```
#include <iostream>
#include <fstream>
#include "simplex615.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 simplex(point, 5);
  std::vector<double> data;               // input data
  std::ifstream file(argv[1]);            // open file
  double tok;                             // temporaru variable
  while(file >> tok) data.push_back(tok); // read data from file
  mixLLKFunc foo(2, data);                // 2-dimensional mixture model
  simplex.amoeba(foo, 1e-7);              // run the Simplex Method
  std::cout << "Minimim = " << 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)
```

A Running Example

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


Summary

Today

- Implementation of the Simplex Method
- Application to mixture of normal distributions

Recommended Readings

- Numerical recipes 10.5 - clear description of simplex method
- Subsequent sections contains more sophisticated multivariate normal distribution

Next Lecture

- The Expectation-Maximization Algorithm