Multidimensional Optimization: The Simplex Method

Lecture 17

Biostatistics 615/815

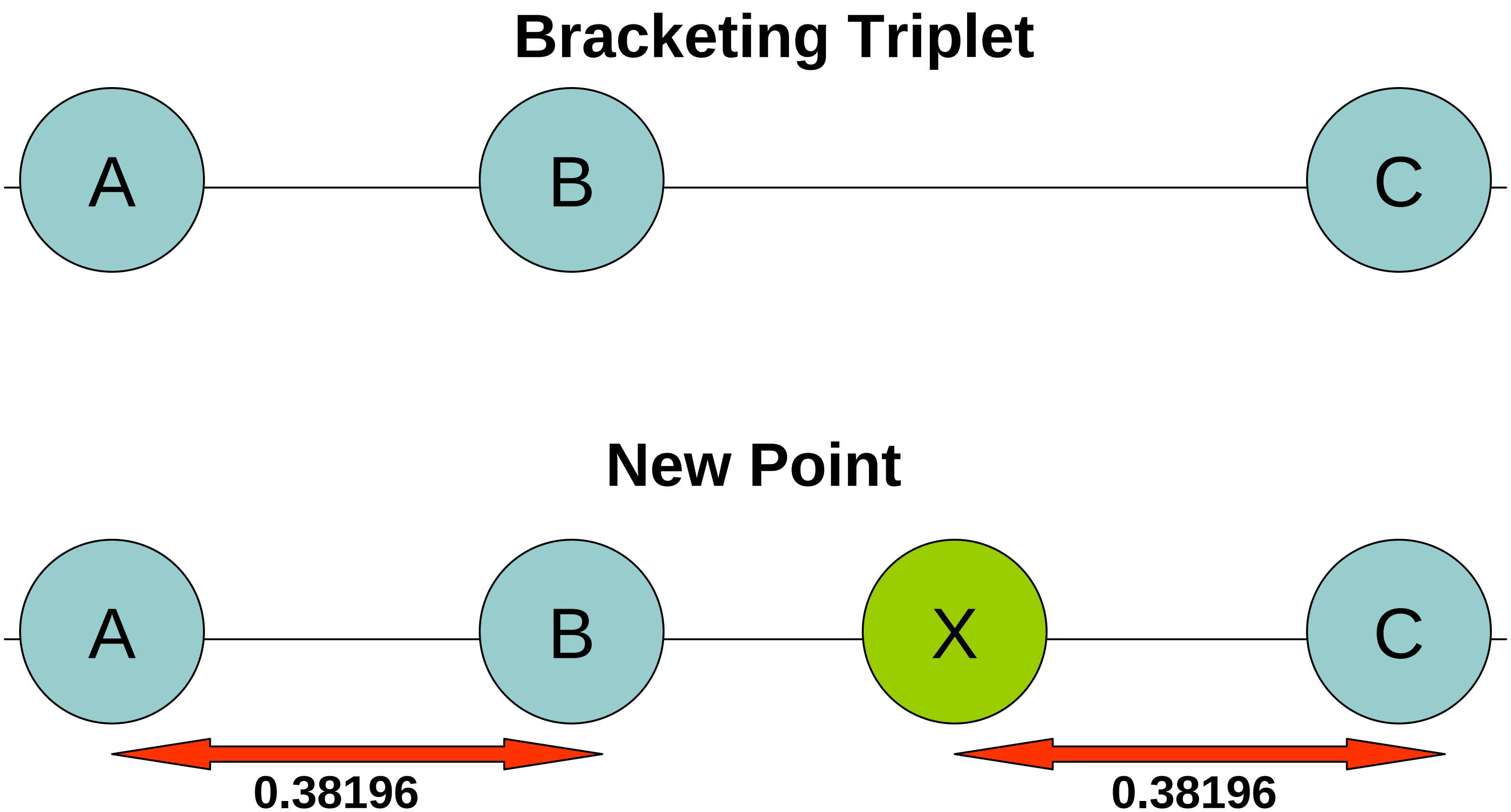
Previous Topic: One-Dimensional Optimization

- Bracketing
- Golden Search
- Quadratic Approximation

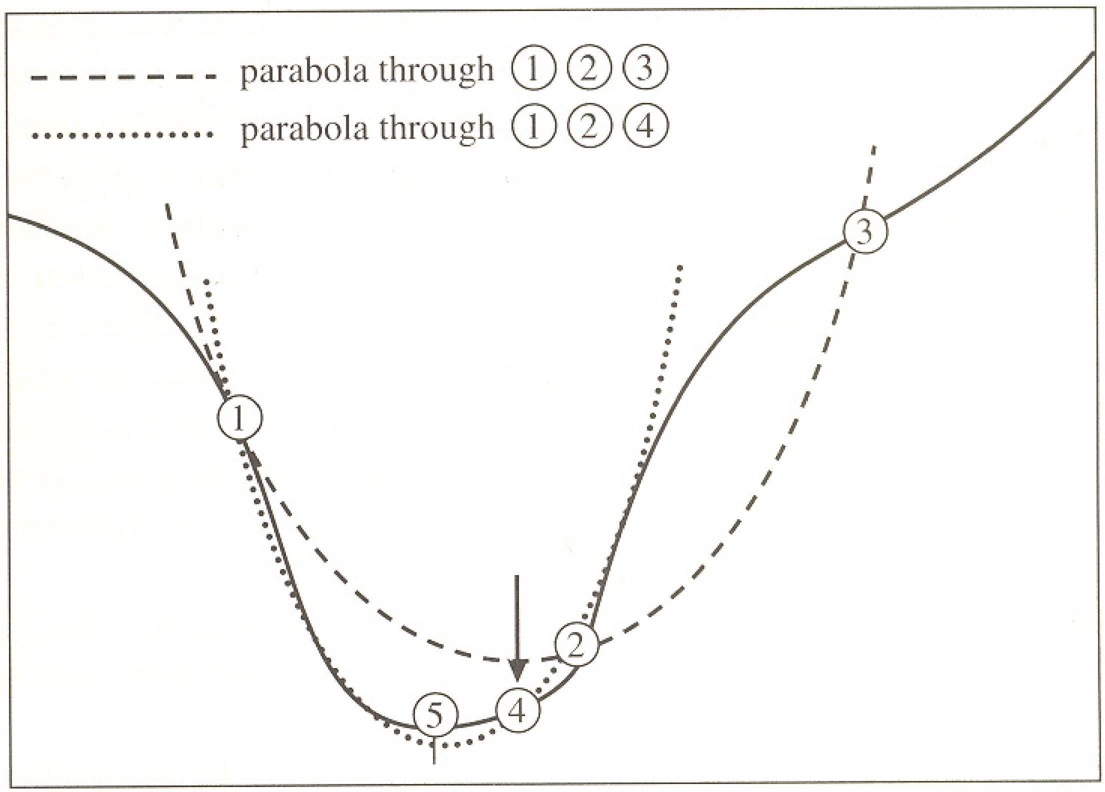
Bracketing

- Find 3 points such that
  - $a < b < c$
  - $f(b) < f(a)$ and $f(b) < f(c)$
- Locate minimum by gradually trimming bracketing interval
- Bracketing provides additional confidence in result

The Golden Ratio



Parabolic Interpolation



For well behaved functions, faster than Golden Search

Today: Multidimensional Optimization

- Illustrate the method of Nelder and Mead
  - Simplex Method
  - Nicknamed "Amoeba"
- Simple and, in practice, quite robust
  - Counter examples are known
- Discuss other standard methods

C Utility Functions: Allocating Vectors

- Ease allocation of vectors.
- Peppered through today's examples

```
double * alloc_vector(int cols)
    {
    return (double *) malloc(sizeof(double) * cols);
    }

void free_vector(double * vector, int cols)
    {
    free(vector);
    }
```

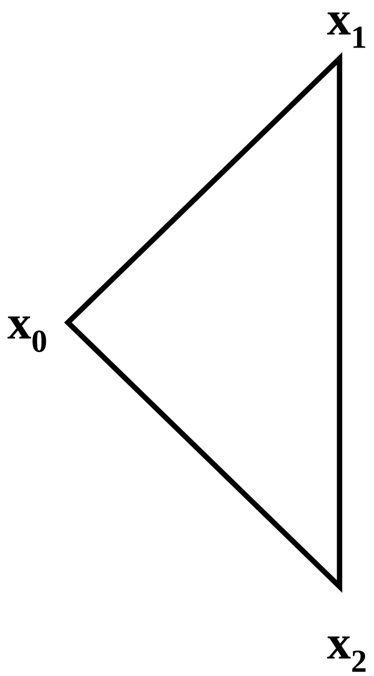
C Utility Functions: Allocating Matrices

```
double ** alloc_matrix(int rows, int cols)
   {
   int i;
   double ** matrix = (double **) malloc(sizeof(double *) * rows);

   for (i = 0; i < rows; i++)
      matrix[i] = alloc_vector(cols);
   return matrix;
   }

void free_matrix(double ** matrix, int rows, int cols)
   {
   int i;
   for (i = 0; i < rows; i++)
      free_vector(matrix[i], cols);
   free(matrix);
   }
```

The Simplex Method

- Calculate likelihoods at simplex vertices
  - Geometric shape with k+1 corners
  - E.g. a triangle in k = 2 dimensions
- Simplex *crawls*
  - Towards minimum
  - Away from maximum
- Probably the most widely used optimization method

A Simplex in Two Dimensions



- Evaluate function at vertices
- Note:
  - The highest (worst) point
  - The next highest point
  - The lowest (best) point
- Intuition:
  - Move away from high point, towards low point

C Code:
Creating A Simplex

```
double ** make_simplex(double * point, int dim)
   {
   int i, j;
   double ** simplex = alloc_matrix(dim + 1, dim);

   for (int i = 0; i < dim + 1; i++)
      for (int j = 0; j < dim; j++)
         simplex[i][j] = point[j];

   for (int i = 0; i < dim; i++)
      simplex[i][i] += 1.0;

   return simplex;
   }
```

C Code:
Evaluating Function at Vertices

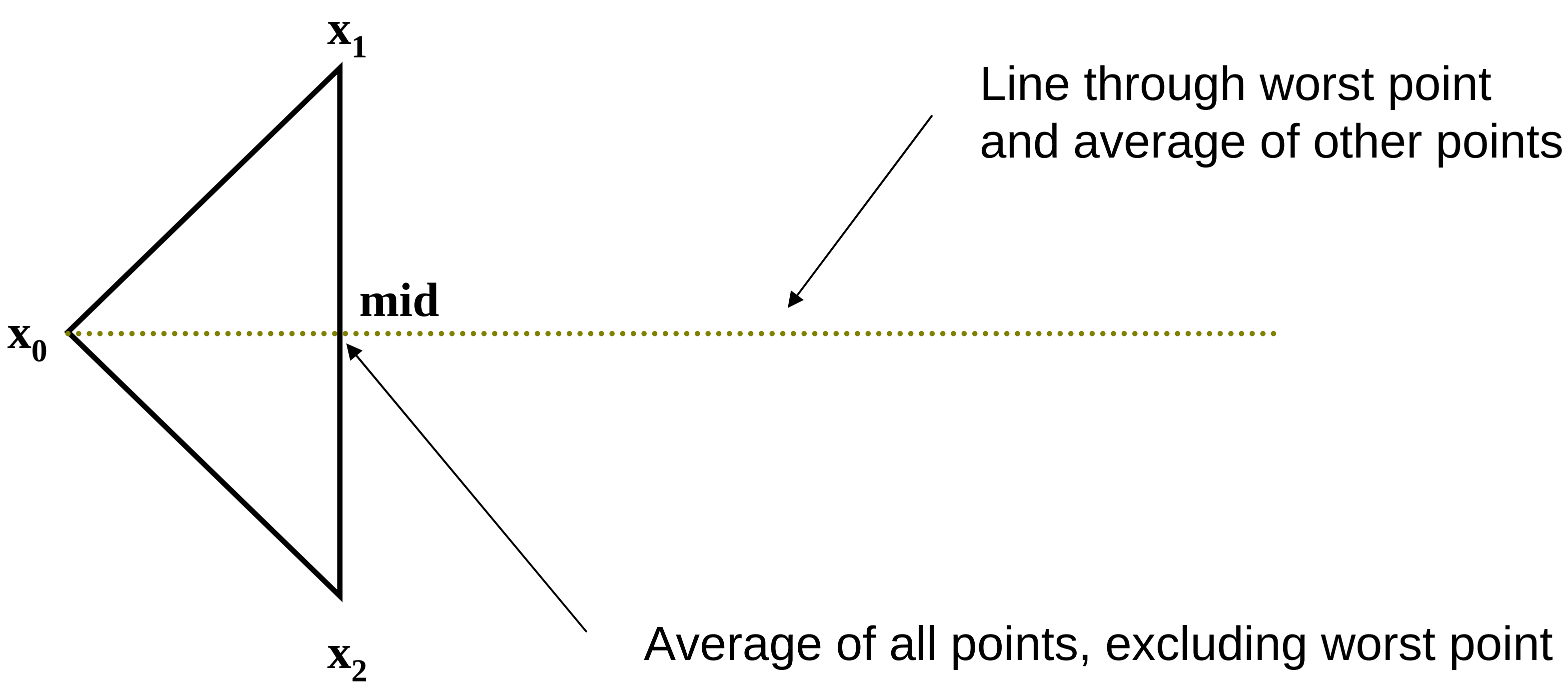
- This function is very simple
  - This is a good thing!
  - Making each function almost trivial makes debugging easy

```
void evaluate_simplex
   (double ** simplex, int dim,
    double * fx, double (* func)(double *, int))
   {
   for (int i = 0; i < dim + 1; i++)
      fx[i] = (*func)(simplex[i], dim);
   }
```

C Code: Finding Extremes

```
void simplex_extremes(double *fx, int dim, int & ihi, int & ilo,
   int & inhi)
   {
   int i;

   if (fx[0] > fx[1])
      { ihi = 0; ilo = inhi = 1; }
   else
      { ihi = 1; ilo = inhi = 0; }

   for (i = 2; i < dim + 1; i++)
      if (fx[i] <= fx[ilo])
         ilo = i;
      else if (fx[i] > fx[ihi])
         { inhi = ihi; ihi = i; }
      else if (fx[i] > fx[inhi])
         inhi = i;
   }
```

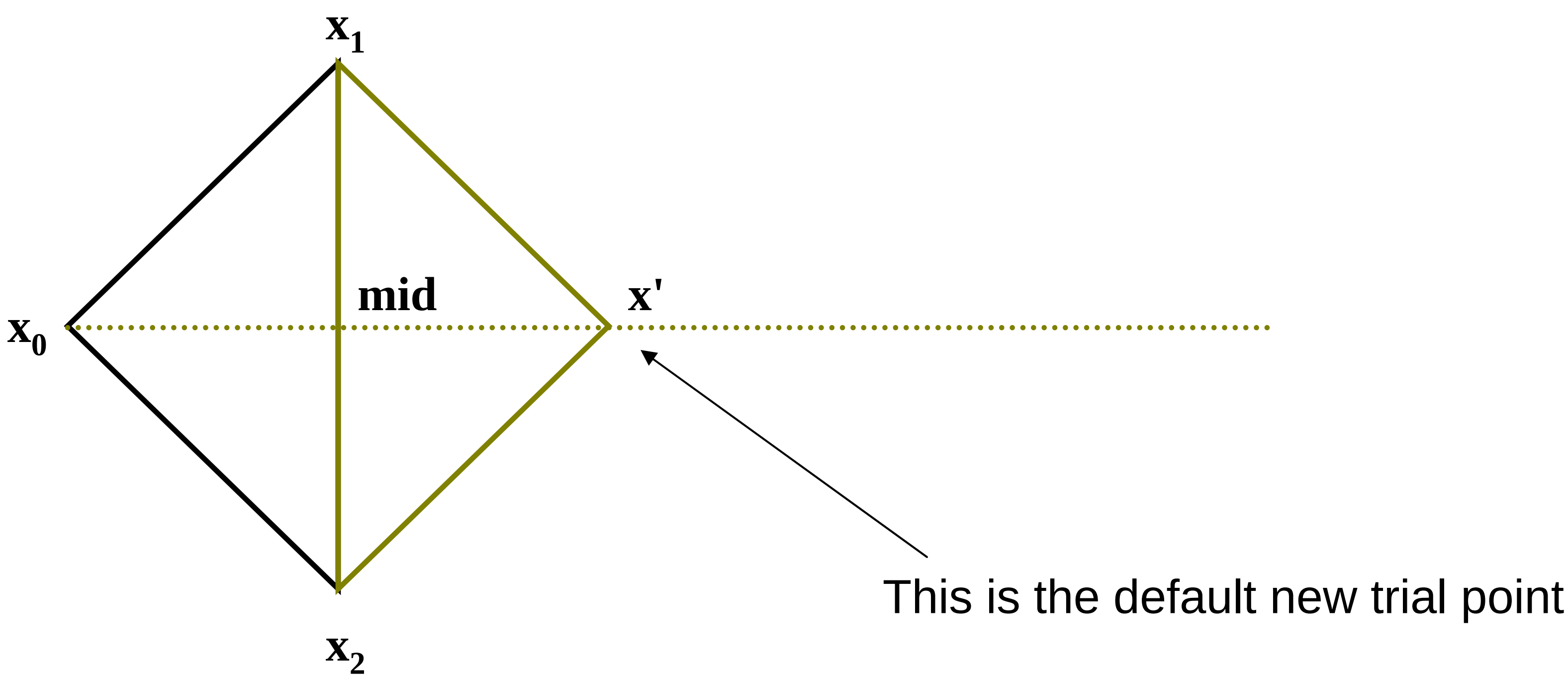
Direction for Optimization



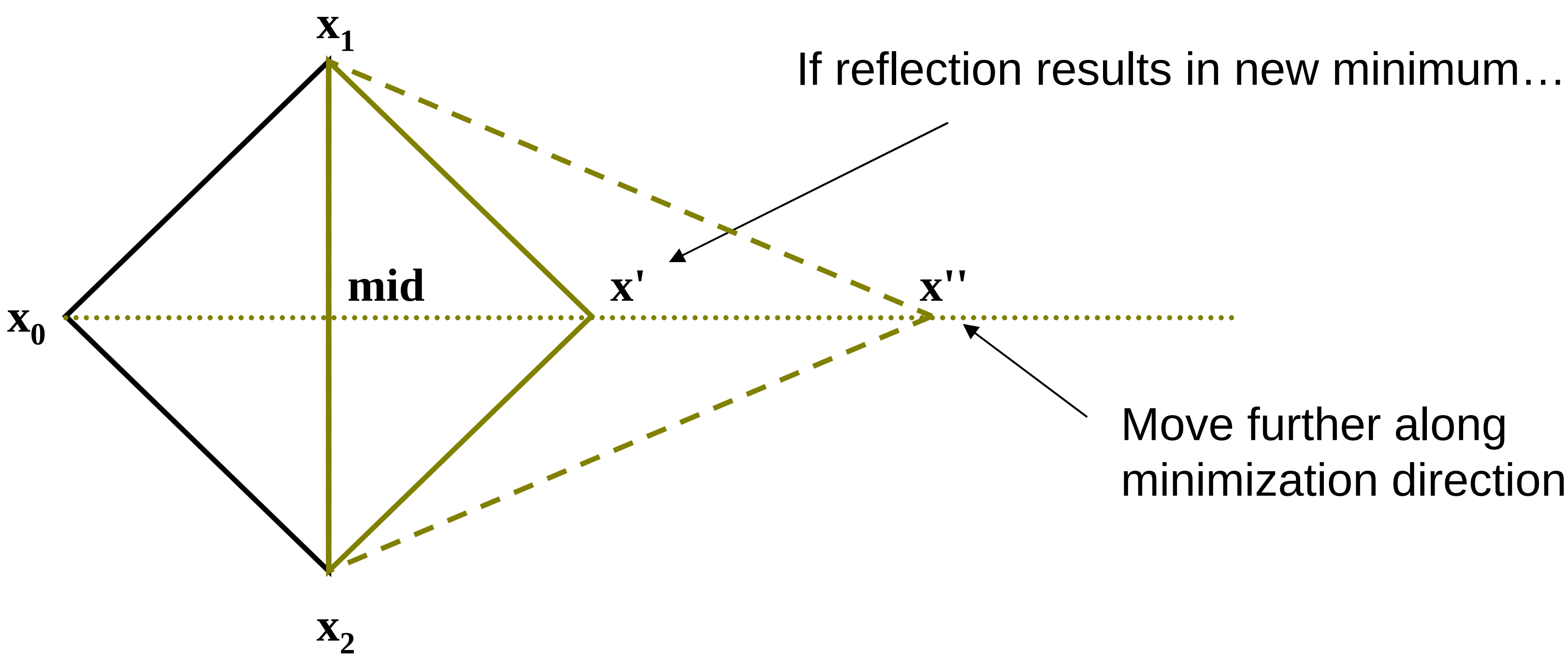
C Code:
Direction for Optimization

```
void simplex_bearings(double ** simplex, int dim,
                      double * midpoint, double * line, int ihi)
   {
   int i, j;
   for (j = 0; j < dim; j++)
      midpoint[j] = 0.0;

   for (i = 0; i < dim + 1; i++)
      if (i != ihi)
         for (j = 0; j < dim; j++)
            midpoint[j] += simplex[i][j];

   for (j = 0; j < dim; j++)
      {
      midpoint[j] /= dim;
      line[j] = simplex[ihi][j] - midpoint[j];
      }
   }
```

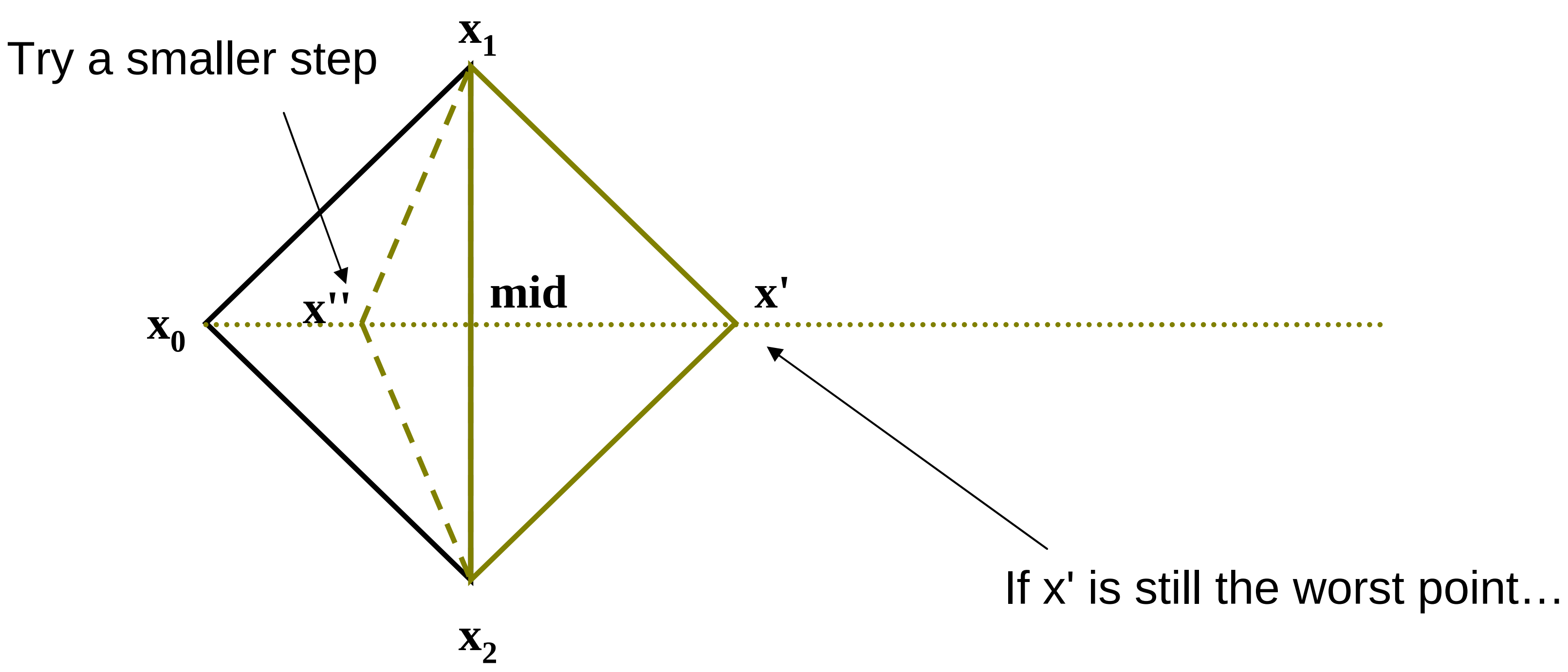
Reflection



Reflection and Expansion



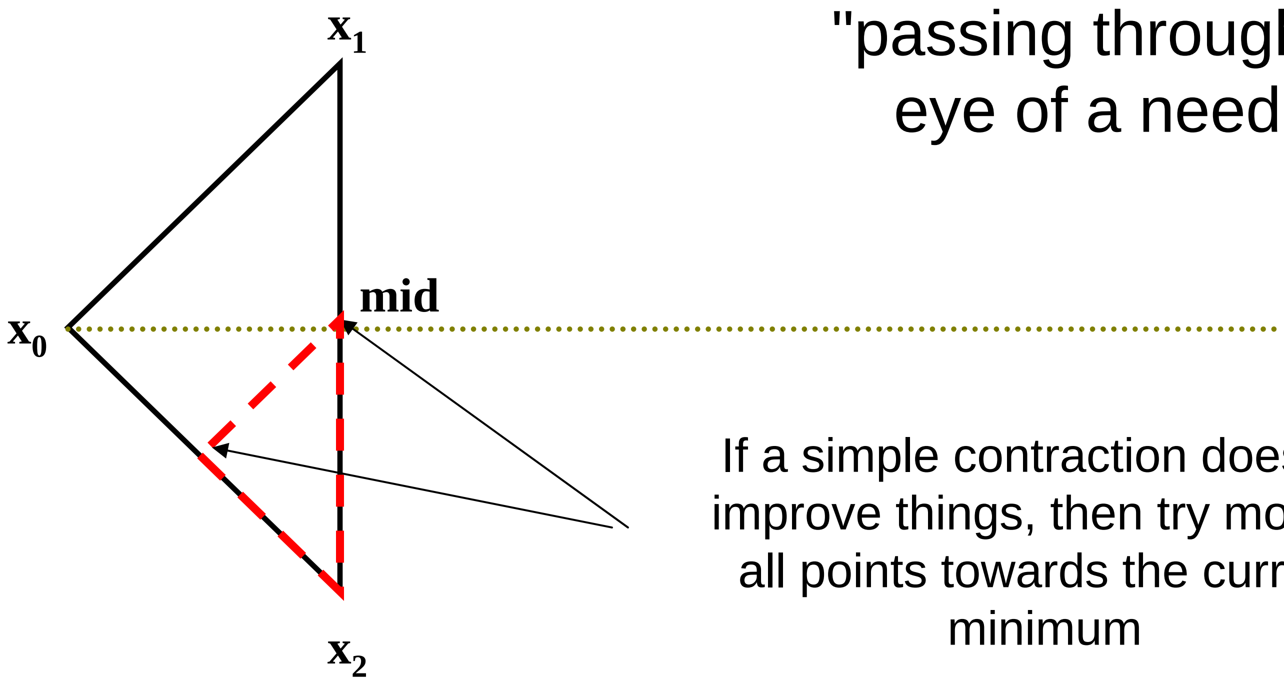
Contraction (One Dimension)



C Code: Updating The Simplex

```
int update_simplex(double * point, int dim, double & fmax,
                   double * midpoint, double * line, double scale,
                   double (* func)(double *, int))
   {
   int i, update = 0; double * next = alloc_vector(dim), fx;

   for (i = 0; i < dim; i++)
      next[i] = midpoint[i] + scale * line[i];
   fx = (*func)(next, dim);

   if (fx < fmax)
      {
      for (i = 0; i < dim; i++)
         point[i] = next[i];
      fmax = fx;
      update = 1;
      }

   free_vector(next, dim);
   return update;
   }
```

Contraction ...



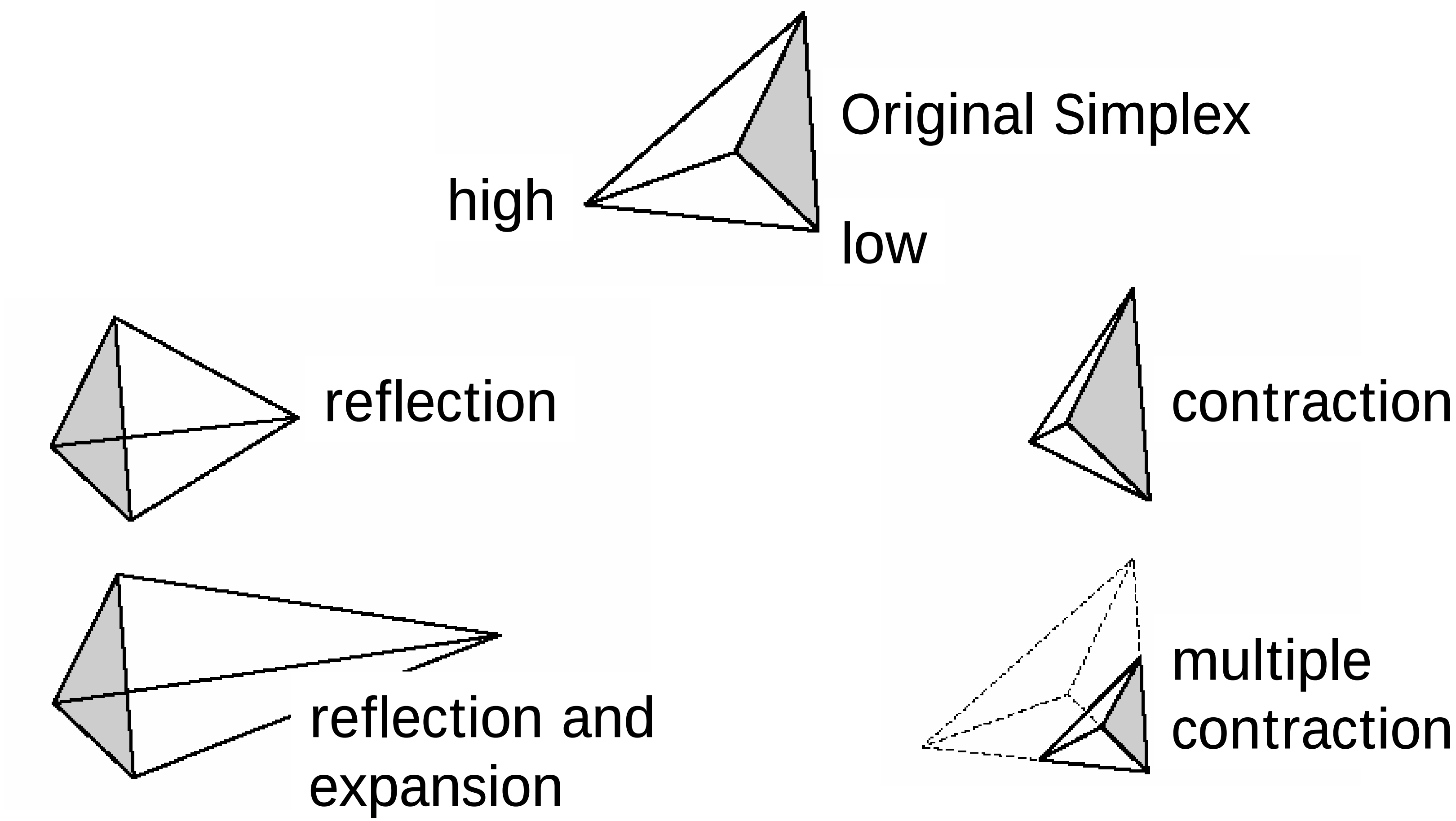
"passing through the eye of a needle"

If a simple contraction doesn't improve things, then try moving all points towards the current minimum

C Code: Contracting The Simplex

```
void contract_simplex(double ** simplex, int dim,
                      double * fx, int ilo,
                      double (*func)(double *, int))
   {
   int i, j;

   for (int i = 0; i < dim + 1; i++)
      if (i != ilo)
         {
         for (int j = 0; j < dim; j++)
            simplex[i][j] = (simplex[ilo][j]+simplex[i][j])*0.5;
         fx[i] = (*func)(simplex[i], dim);
         }
   }
```

Summary: The Simplex Method



C Code: Minimization Routine (Part I)

- Declares local variables and allocates memory

```
double amoeba(double *point, int dim,
              double (*func)(double *, int),
              double tol)
   {
   int    ihi, ilo, inhi, j;
   double fmin;
   double *  fx = alloc_vector(dim + 1);
   double *  midpoint = alloc_vector(dim);
   double *  line = alloc_vector(dim);
   double ** simplex = make_simplex(point, dim);

   evaluate_simplex(simplex, dim, fx, func);
```

C Code:
Minimization Route (Part II)

```
while (true)
     {
     simplex_extremes(fx, dim, ihi, ilo, inhi);
     simplex_bearings(simplex, dim, midpoint, line, ihi);

     if (check_tol(fx[ihi], fx[ilo], tol)) break;

     update_simplex(simplex[ihi], dim, fx[ihi],
                    midpoint, line, -1.0, func);

     if (fx[ihi] < fx[ilo])
        update_simplex(simplex[ihi], dim, fx[ihi],
                       midpoint, line, -2.0, func);
     else if (fx[ihi] >= fx[inhi])
        if (!update_simplex(simplex[ihi], dim, fx[ihi],
                            midpoint, line, 0.5, func))
           contract_simplex(simplex, dim, fx, ilo, func);
     }
```

C Code: Minimization Routine (Part III)

- Store the result and free memory

```
for (j = 0; j < dim; j++)
   point[j] = simplex[ilo][j];
fmin = fx[ilo];

free_vector(fx, dim);
free_vector(midpoint, dim);
free_vector(line, dim);
free_matrix(simplex, dim + 1, dim);

return fmin;
}
```

C Code:
Checking Convergence

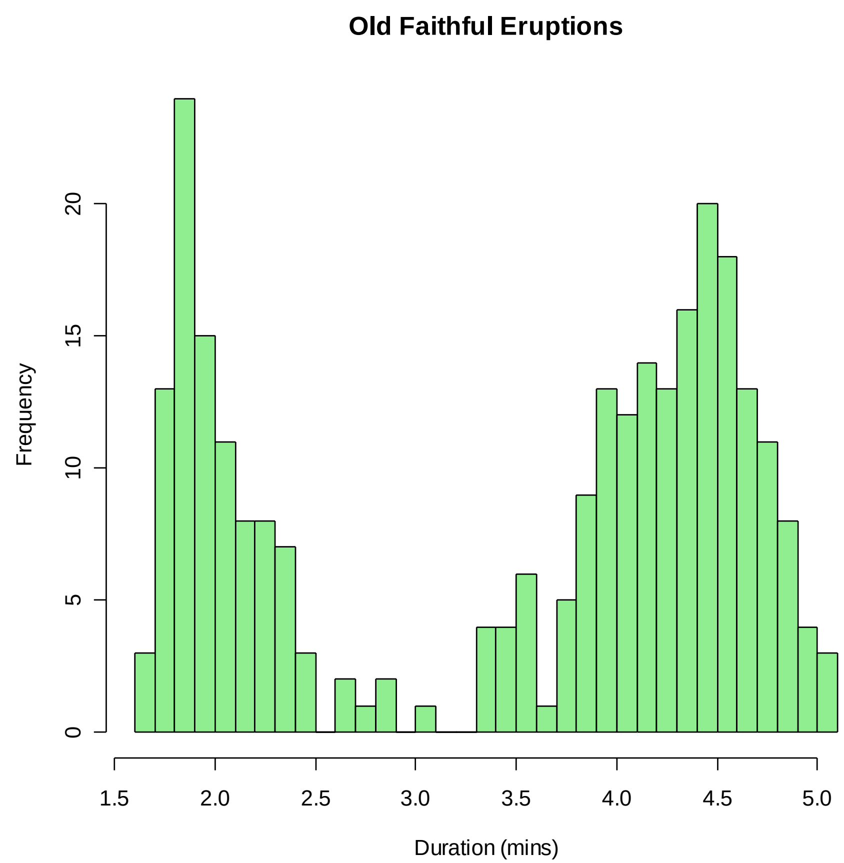
```
#include <math.h>

#define ZEPS 1e-10

int check_tol(double fmax, double fmin, double ftol)
   {
   double delta = fabs(fmax - fmin);
   double accuracy = (fabs(fmax) + fabs(fmin)) * ftol;

   return (delta < (accuracy + ZEPS));
   }
```

amoeba()

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

- Typical usage:
  - `my_func(double * x, int n) { … }`
  - `amoeba(point, dim, my_func, 1e-7);`

Example Application
Old Faithful Eruptions (n = 272)



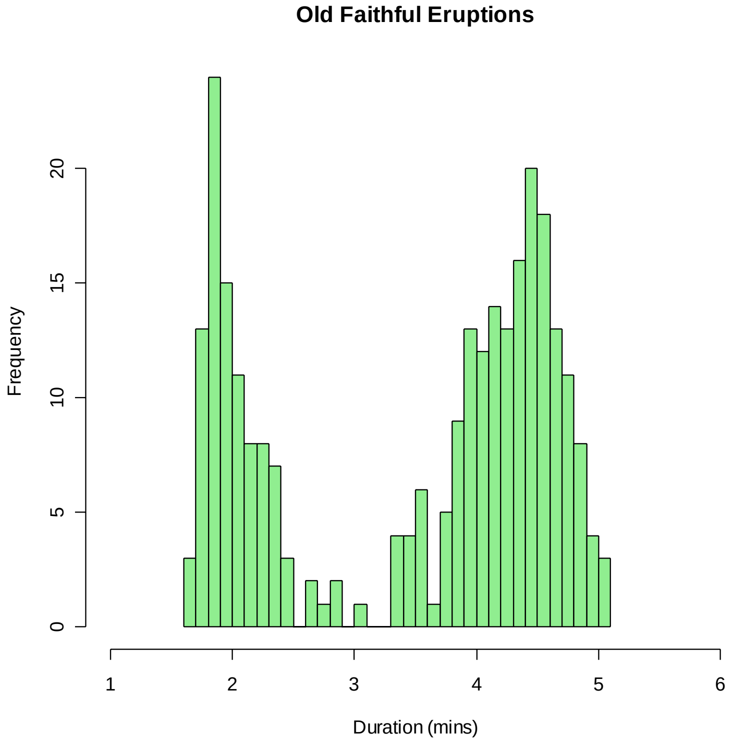
Fitting a Normal Distribution

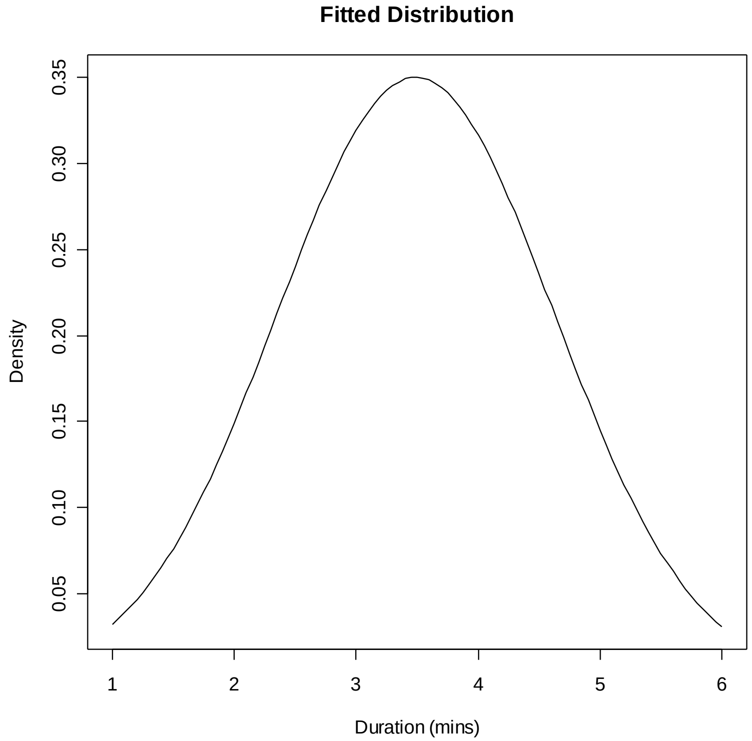
- Fit two parameters
  - Mean
  - Variance

- Requires ~165 likelihood evaluations
  - Mean = 3.4878
  - Variance = 1.2979

  - Maximum log-likelihood = -421.42

Nice fit, eh?


Old Faithful Eruptions
Frequency
0
5
10
15
20
1
2
3
4
5
6
Duration (mins)


Fitted Distribution
Density
0.05
0.10
0.15
0.20
0.25
0.30
0.35
1
2
3
4
5
6
Duration (mins)

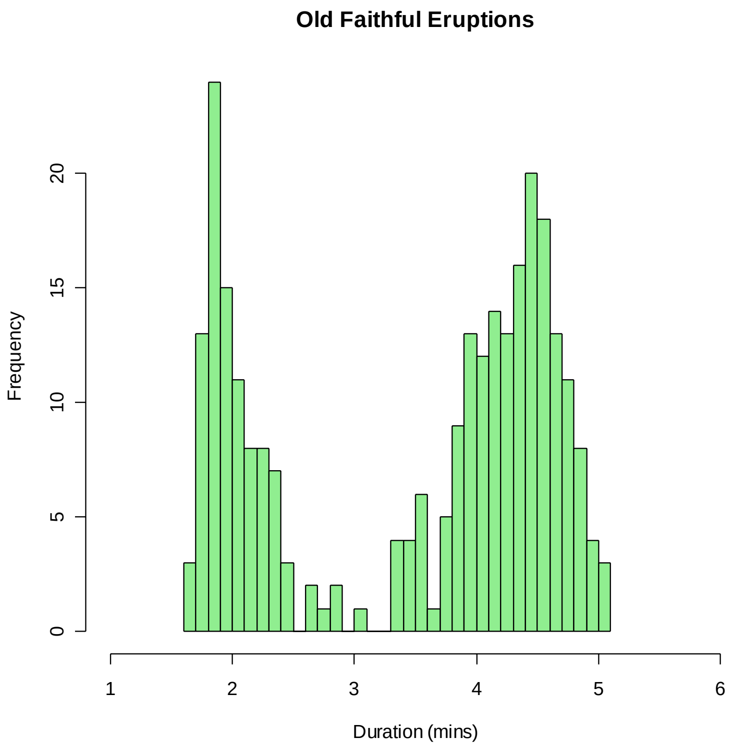
A Mixture of Two Normals

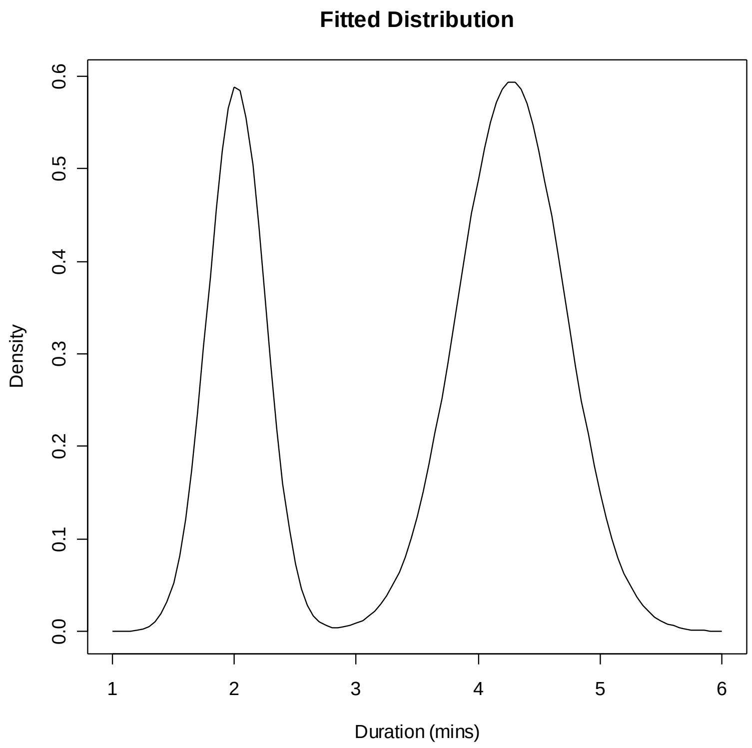
- Fit 5 parameters
  - Proportion in the first component
  - Two means
  - Two variances

- Required about ~700 evaluations
  - First component contributes 0.34841 of mixture
  - Means are 2.0186 and 4.2734
  - Variances are 0.055517 and 0.19102

  - Maximum log-likelihood = -276.36

Two Components



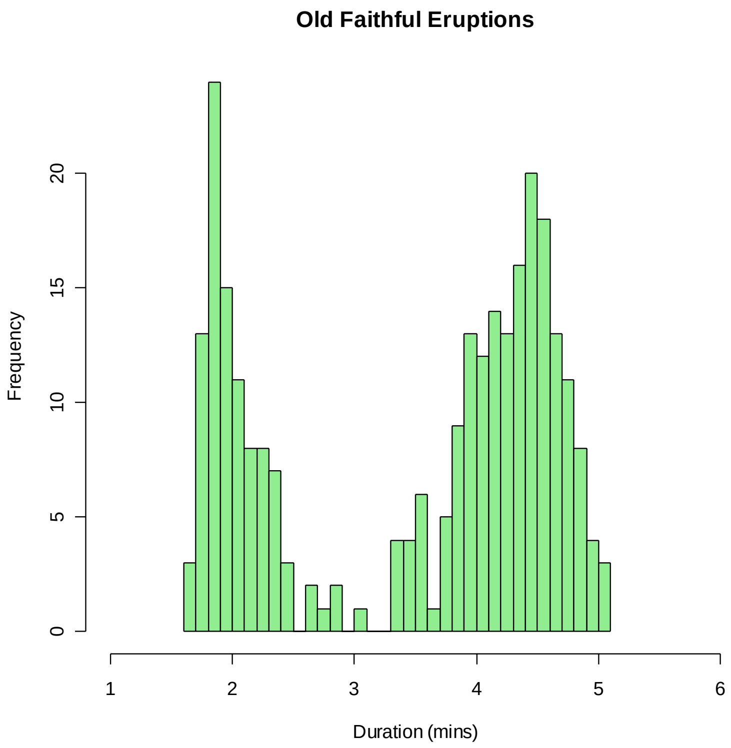


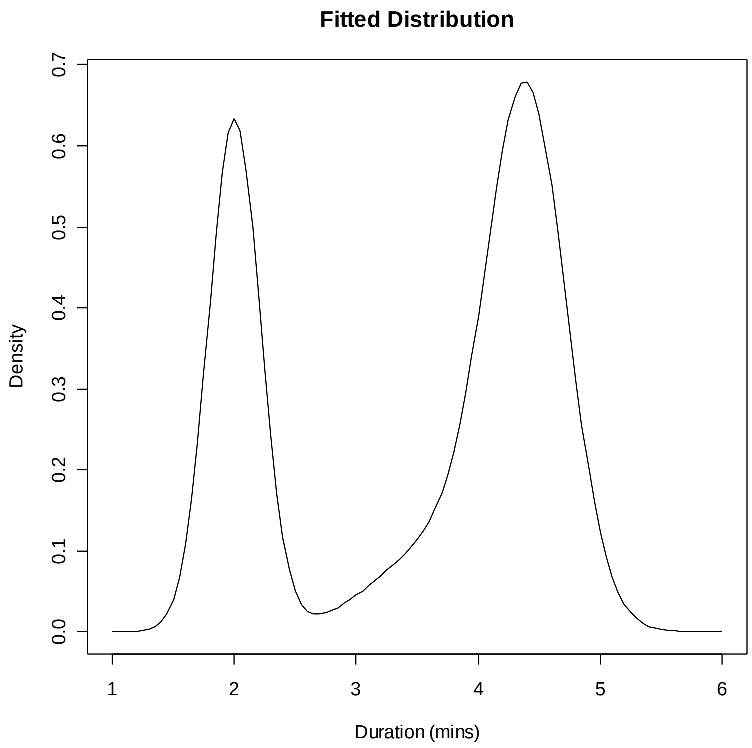
A Mixture of Three Normals

- Fit 8 parameters
  - Proportion in the first two components
  - Three means
  - Three variances
- Required about ~1400 evaluations
  - Did not always converge!
- One of the best solutions …
  - Components contributing .339, 0.512 and 0.149
  - Component means are 2.002, 4.401 and 3.727
  - Variances are 0.0455, 0.106, 0.2959

  - Maximum log-likelihood = -267.89

Three Components





Tricky Minimization Questions

- Fitting variables that are constrained
  - Proportions vary between 0 and 1
  - Variances must be positive
- Selecting the number of components
- Checking convergence

Improvements to amoeba()

- Different scaling along each dimension
  - If parameters have different impact on the likelihood
- Track total function evaluations
  - Avoid getting stuck if function does not cooperate
- Rotate simplex
  - If the current simplex is leading to slow improvement

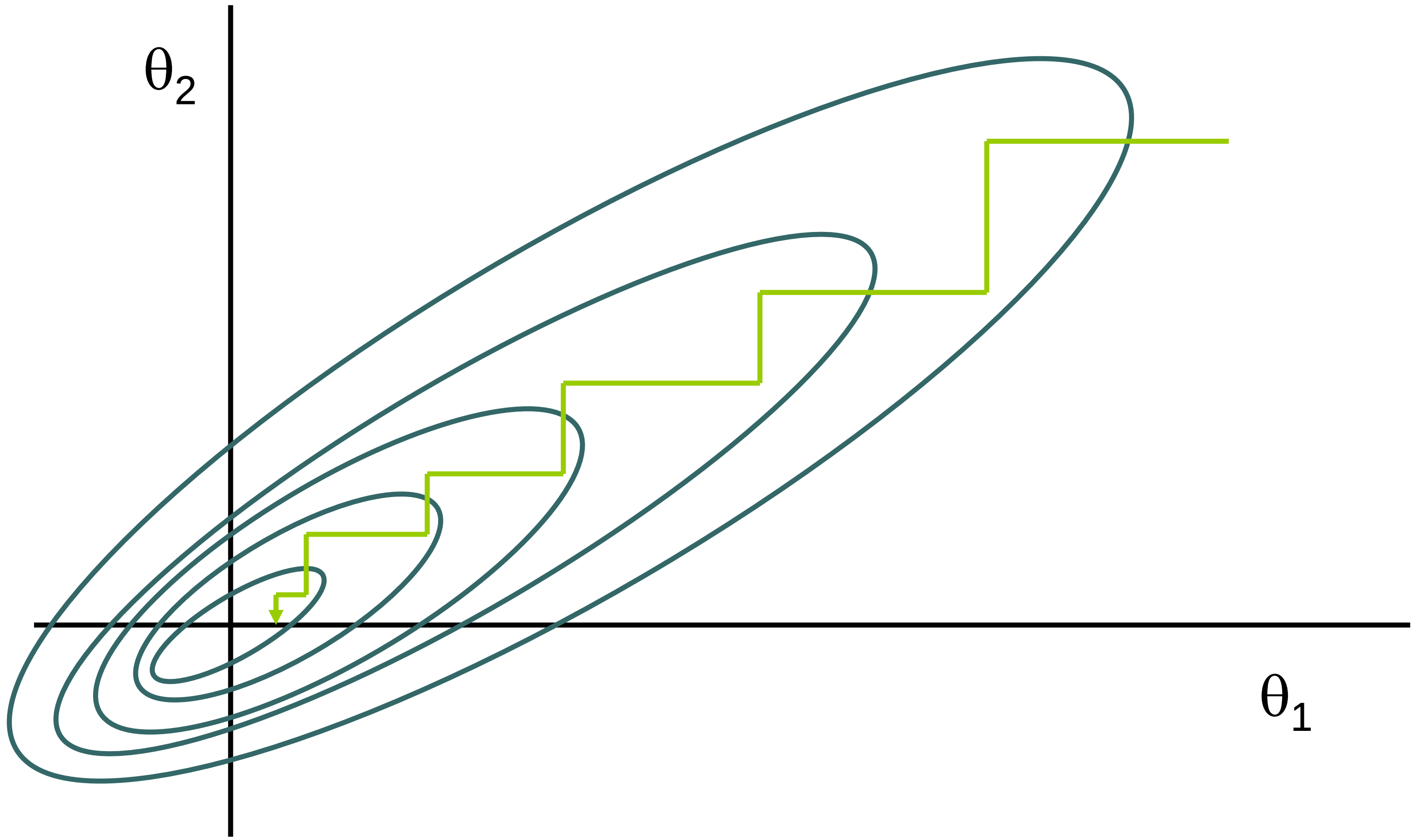
optim() Function in R

- optim(point, function, method)
  - Point – starting point for minimization
  - Function that accepts point as argument
  - Method can be
    - "Nelder-Mead" for simplex method (default)
    - "BFGS", "CG" and other options use gradient

One parameter at a time

- Simple but inefficient approach
- Consider
  - Parameters $\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_k)$
  - Function f $(\boldsymbol{\theta})$
- Maximize $\boldsymbol{\theta}$ with respect to each θ_i in turn
  - Cycle through parameters

The Inefficiency…



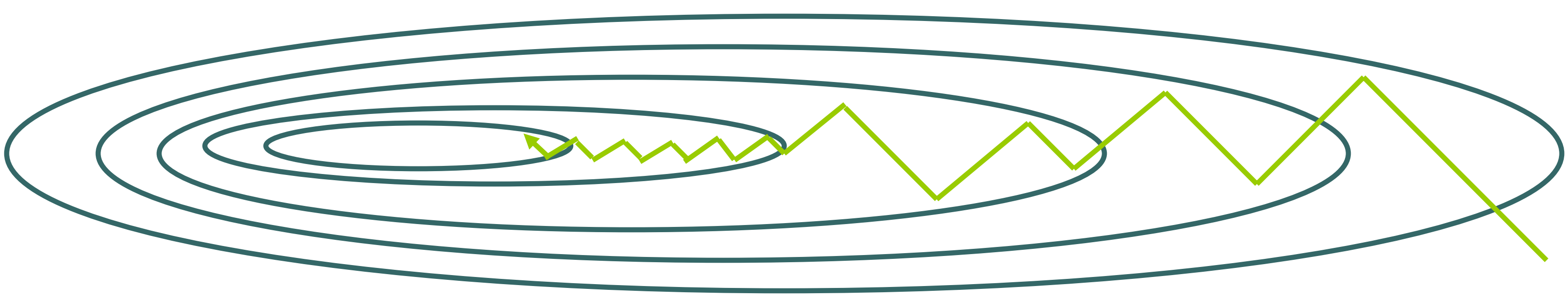
Steepest Descent

- Consider
  - Parameters $\theta = (\theta_1, \theta_2, \ldots, \theta_k)$
  - Function $f(\theta; x)$
- Score vector

$$S = \frac{d \ln f}{d\theta} = \left(\frac{d \ln f}{d\theta_1}, \quad \ldots, \quad \frac{d \ln f}{d\theta_k} \right)$$

  - Find maximum along $\theta + \delta S$

Still inefficient…



Consecutive steps are still perpendicular!

Multidimensional Minimization

- Typically, sophisticated methods will…
- Use derivatives
  - May be calculated numerically. How?
- Select a direction for minimization, using:
  - Weighted average of previous directions
  - Current gradient
  - Avoid right angle turns

Recommended Reading

- Numerical Recipes in C (or C++, or Fortran)
  - Press, Teukolsky, Vetterling, Flannery
  - Chapter 10.4
- Clear description of Simplex Method
  - Other sub-chapters illustrate more sophisticated methods
- Online at
  - http://www.numerical-recipes.com/