The E-M Algorithm

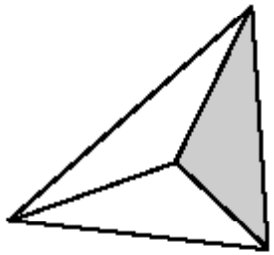
Biostatistics 615/815

Lecture 17

Last Lecture: The Simplex Method

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

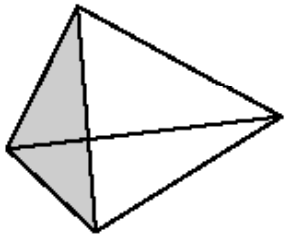
Summary:
The Simplex Method



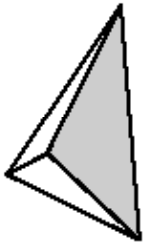
high

low

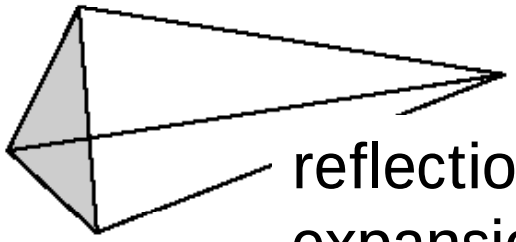
Original Simplex



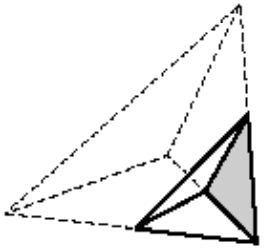
reflection



contraction



reflection and
expansion



multiple
contraction

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

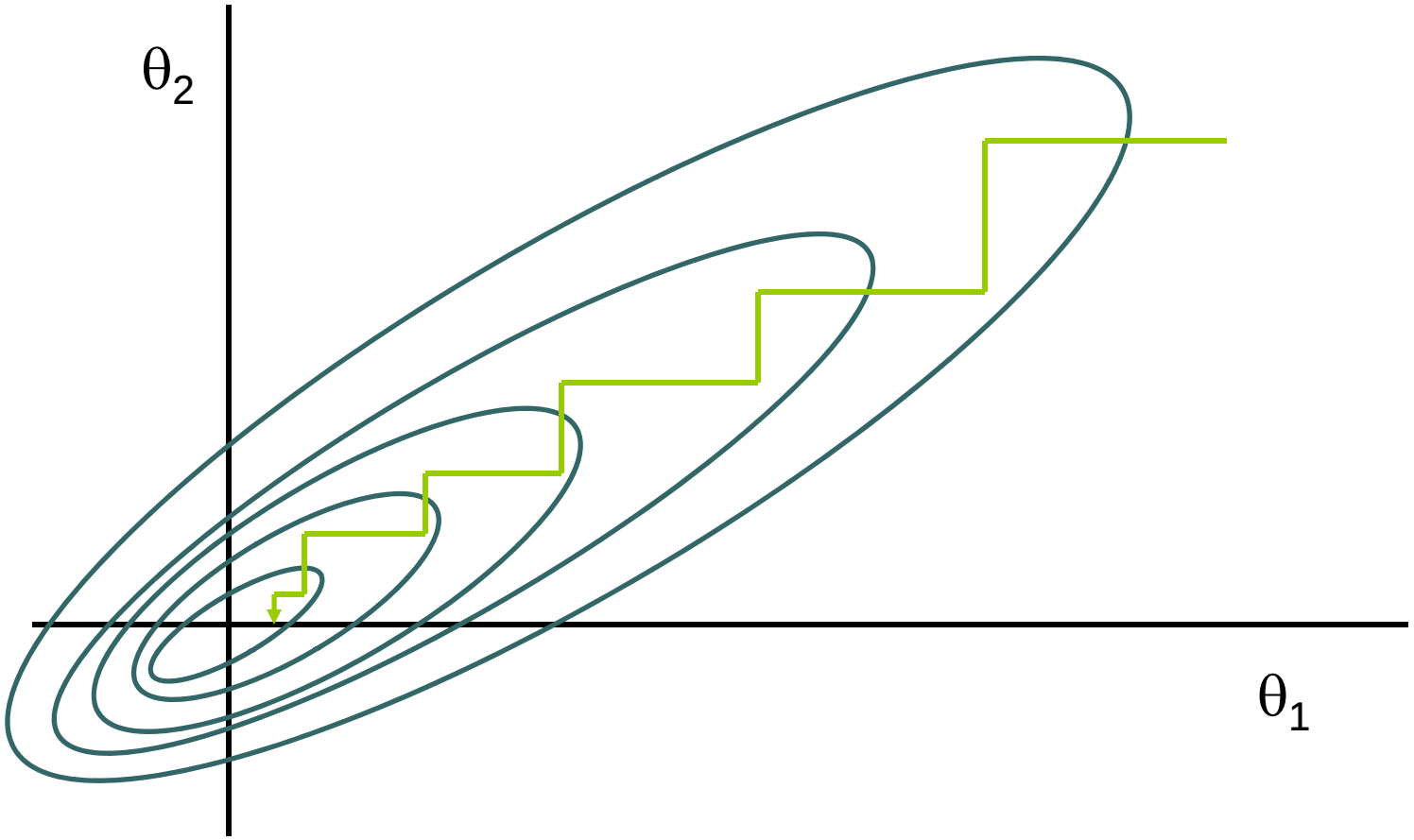
Other Methods for Minimization in Multiple Dimensions

- 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

One parameter at a time

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

The Inefficiency…



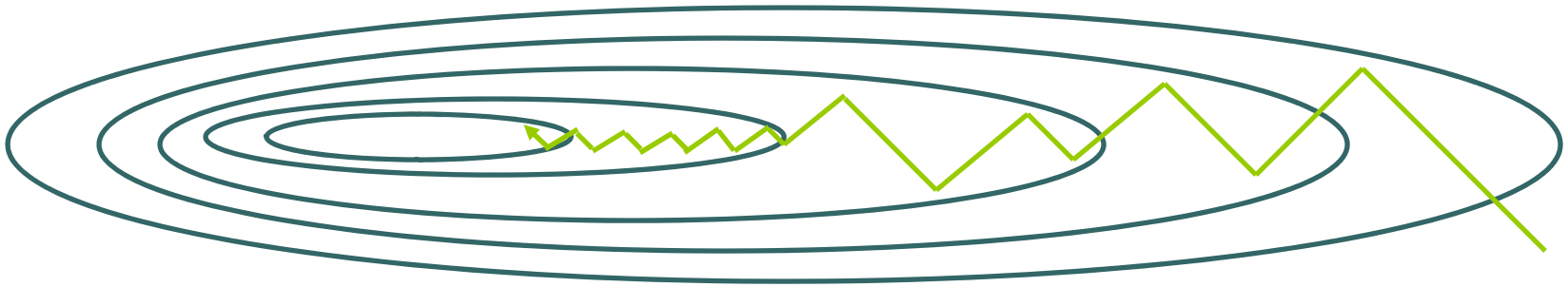
Steepest Descent

- 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...

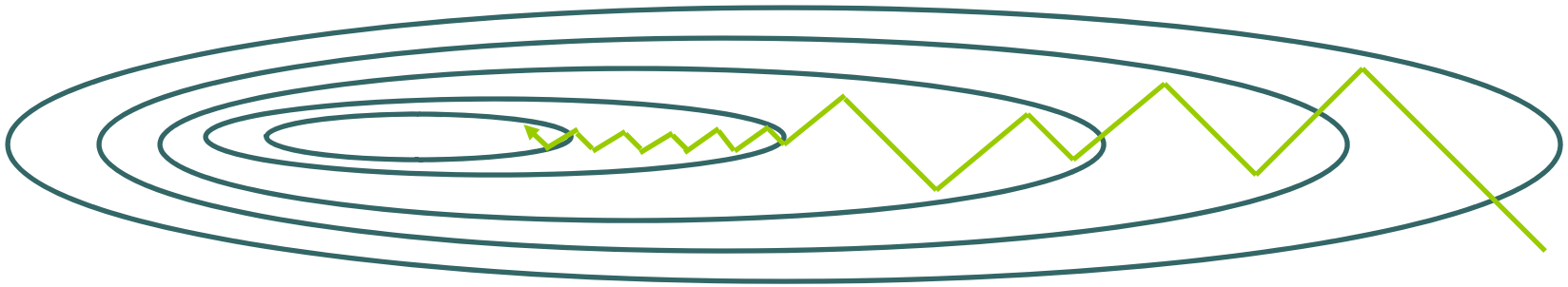


Consecutive steps are still perpendicular!

Other Strategies for Multidimensional Optimization

- Most strategies will define a series of vectors or lines through parameter space
- Estimate of minimum improved by adding an optimal multiple of each vector
- Some “intuitive” choices might be:
  - The function gradient
  - Unit vectors along one dimension

The key is to right angle turns!



Most methods that use derivatives don’t simply optimize function along current gradient or the unit vectors ...

Today ...

- The E-M algorithm
  - General algorithm for missing data problems
  - Requires "specialization" to the problem at hand
  - Frequently applied to mixture distributions

The E-M Algorithm

- Original Citation
  - Dempster, Laird and Rubin (1977)
    J Royal Statistical Society (B) **39:**1-38
  - Cited in over 9,184 research articles

- For comparison
  - Nelder and Mead (1965)
    Computer Journal **7**: 308-313
  - Cited in over 8,094 research articles

The Basic E-M Strategy

- X = (Y, Z)
  - Complete data X *(eg. what we'd like to have!)*
  - Observed data Y *(eg. individual observations)*
  - Missing data Z *(eg. class assignments)*
- The algorithm
  - Use estimated parameters to infer Z
  - Update estimated parameters using Y and Z
  - Repeat until convergence

The E-M Algorithm

- Consider a set of starting parameters
- Use these to “estimate” the missing data
- Use “complete” data to update parameters
- Repeat as necessary

Setting for the E-M Algorithm...

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

Filling In Missing Data

- The missing data is the group assignment for each observation
- Complete data generated by assigning observations to groups
  - Probabilistically
  - We will use “fractional” assignments

The E-Step: Mixture of Normals

- Estimate missing data
  - Estimate assignment of observations to groups
- How?
  - Conditional on current parameter values
- Basically, “classify” each observation

Classification Probabilities

$$\Pr(Z_i = j \mid x_i, \boldsymbol{\pi}, \boldsymbol{\varphi}, \eta) = \frac{\pi_j f(x_i \mid \phi_j, \eta)}{\sum_l \pi_l f(x_i \mid \phi_l, \eta)}$$

- Results from the application of Bayes' theorem
- Implemented in `classprob()` function
  - `classprob(int j, double x, int k, double *prob, double *mean, double *sd)`

C Code: Updating Group Memberships

```
void update_class_prob(int n, double * data,
   int k, double * prob, double * mean, double * sd,
   double ** class_prob)
   {
   int i, j;

   for (i = 0; i < n; i++)
      for (j = 0; j < k; j++)
         class_prob[i][j] =
               classprob(j, data[i],
                        k, prob, mean, sd);
   }
```

The M-Step

- Update mixture parameters to maximize the likelihood of the data …
- Appears tricky, but becomes simple when we assume cluster assignments are correct
- We simply use the sample proportions, and weighted means and variances to update parameters
- This step is guaranteed never to decrease likelihood

Updating Mixture Proportions

$$\pi_i = \frac{\Pr(Z_i = j \mid x_i, \boldsymbol{\pi}, \boldsymbol{\varphi}, \eta)}{n}$$

- "Count" the observations assigned to each group

C Code: Updating Mixture Proportions

```
void update_prob(int n, double * data,
                 int k, double * prob,
                 double ** class_prob)
   {
   int i, j;

   for (int j = 0; j < k; j++)
      {
      prob[j] = 0.0;

      for (int i = 0; i < n; i++)
         prob[j] += class_prob[i][j];

      prob[j] /= n;
      }
   }
```

Updating Component Means

$$\hat{\mu}_j = \frac{\sum_i x_i \Pr(Z_i = j \mid x_i, \boldsymbol{\pi}, \boldsymbol{\varphi}, \eta)}{\sum_i \Pr(Z_i = j \mid x_i, \boldsymbol{\pi}, \boldsymbol{\varphi}, \eta)}$$

$$= \frac{\sum_i x_i \Pr(Z_i = j \mid x_i, \boldsymbol{\pi}, \boldsymbol{\varphi}, \eta)}{n\pi_j}$$

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

C Code: Update Component Means

```
void update_mean(int n, double * data,
                 int k, double * prob, double * mean,
                 double ** class_prob)
   {
   int i, j;

   for (int j = 0; j < k; j++)
      {
      mean[j] = 0.0;

      for (int i = 0; i < n; i++)
         mean[j] += data[i] * class_prob[i][j];

      mean[j] /= n * prob[j] + TINY;
      }
   }
```

Updating Component Variances

$$\hat{\sigma}_i^2 = \frac{\sum_i (x_i - \mu_i)^2 \Pr(Z_i = j \mid x_i, \boldsymbol{\pi}, \boldsymbol{\varphi}, \eta)}{n\pi_j}$$

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

C Code:
Update Component Std Deviations

```
void update_sd(int n, double * data,
               int k, double * prob, double * mean, double * sd,
               double ** class_prob)
   {
   int i, j;

   for (int j = 0; j < k; j++)
      {
      sd[j] = 0.0;

      for (int i = 0; i < n; i++)
         sd[j] += square(data[i] - mean[j]) * class_prob[i][j];

      sd[j] /= (n * prob[j] + TINY);
      sd[j] = sqrt(sd[j]);
      }
   }
```

C Code: Update Mixture

```
void update_parameters
       (int n, double * data,
        int k, double * prob, double * mean, double * sd,
        double ** class_prob)
   {
   // First, we update the mixture proportions
   update_prob(n, data, k, prob, class_prob);

   // Next, update the mean for each component
   update_mean(n, data, k, prob, mean, class_prob);

   // Finally, update the standard deviation
   update_sd(n, data, k, prob, mean, sd, class_prob);
   }
```

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

C Code:
The E-M Algorithm

```
double em(int n, double * data,
          int k, double * prob, double * mean, double * sd,
          double eps)
   {
   double llk = 0, prev_llk = 0;
   double ** class_prob = alloc_matrix(n, k);

   start_em(n, data, k, prob, mean, sd);
   do {
      prev_llk = llk;
      update_class_prob(n, data, k, prob, mean, sd, class_prob);
      update_parameters(n, data, k, prob, mean, sd, class_prob);
      llk = mixLLK(n, data, k, prob, mean, sd);
   } while ( !check_tol(llk, prev_llk, eps) );

   return llk;
   }
```

Picking Starting Parameters

- Mixing proportions
  - Assumed equal
- Means for each group
  - Pick one observation as the group mean
- Variances for each group
  - Use overall variance

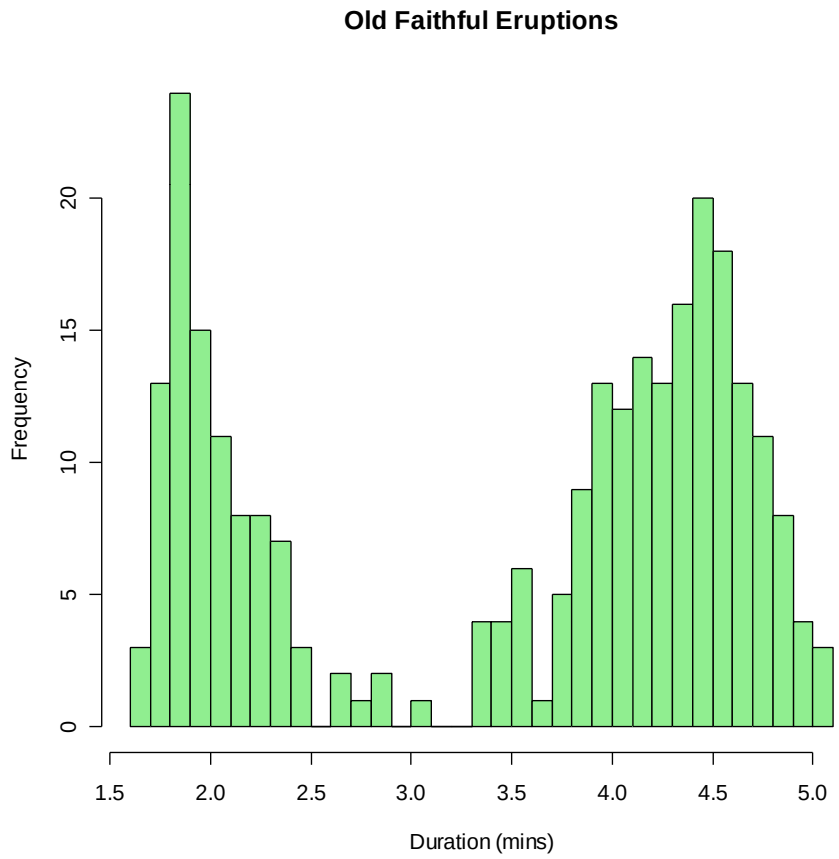
C Code:
Picking Starting Parameters

```
void start_em(int n, double * data,
              int k, double * prob, double * mean, double * sd)
   {
   int i, j; double mean1 = 0.0, sd1 = 0.0;

   for (i = 0; i < n; i++)
      mean1 += data[i];
   mean1 /= n;
   for (i = 0; i < n; i++)
      sd1 += square(data[i] - mean1);
   sd1 = sqrt(sd1 / n);

   for (j = 0; j < k; j++)
      {
      prob[j] = 1.0 / k;
      mean[j] = data[rand() % n];
      sd[j] = sd1;
      }
   }
```

Example Application
Old Faithful Eruptions (n = 272)



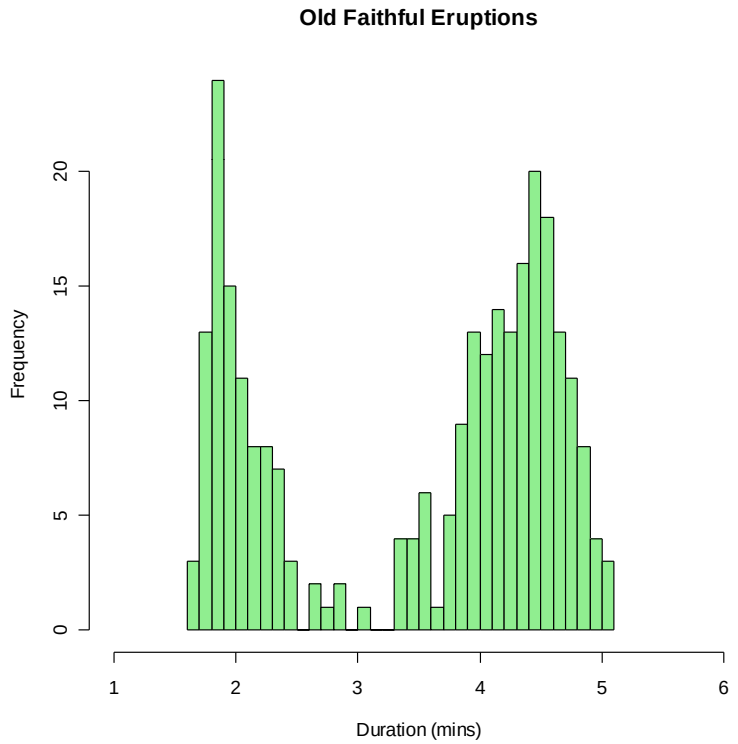
Using Simplex Method
A Mixture of Two Normals

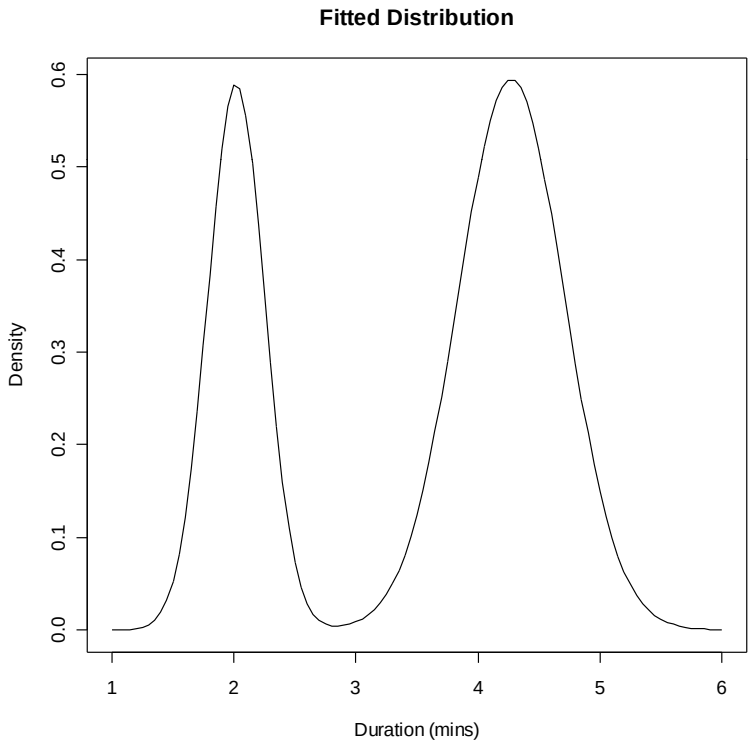
- Fit 5 parameters
  - Proportion in 1st component, 2 means, 2 variances
- 44/50 runs found minimum
- Required about ~700 evaluations
  - First component contributes 0.348 of mixture
  - Means are 2.018 and 4.273
  - Variances are 0.055 and 0.191
  - Maximum log-likelihood = -276.36

Using E-M Algorithm
A Mixture of Two Normals

- Fit 5 parameters
- 50/50 runs found maximum
- Required about ~25 evaluations
  - First component contributes 0.348 of mixture
  - Means are 2.018 and 4.273
  - Variances are 0.055 and 0.191
  - Maximum log-likelihood = -276.36

Two Components

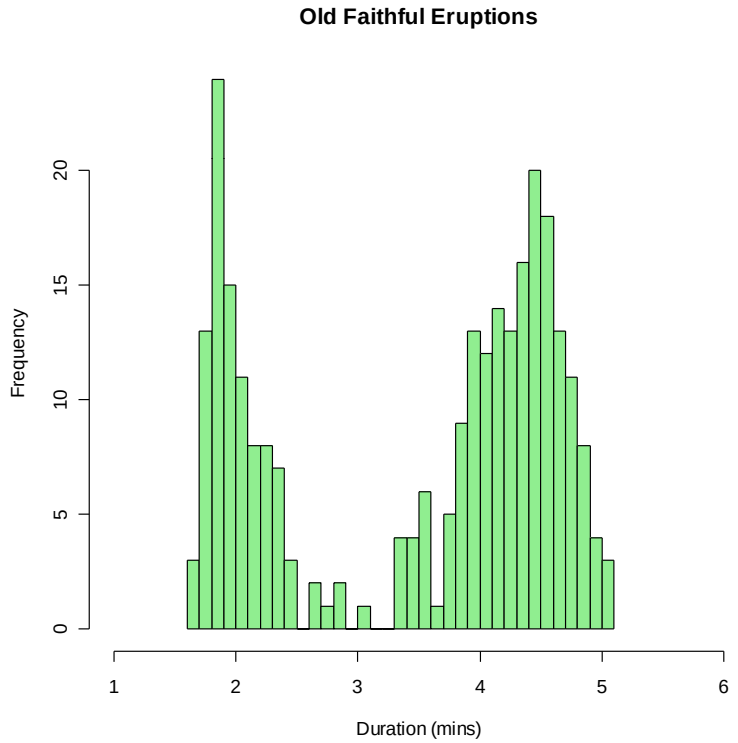


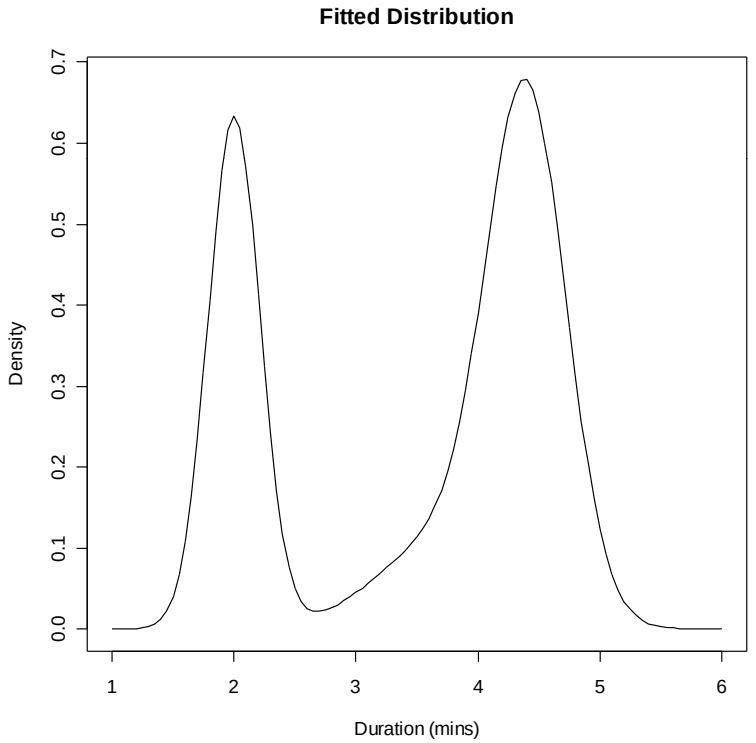


Simplex Method: A Mixture of Three Normals

- Fit 8 parameters
  - 2 proportions, 3 means, 3 variances
- Required about ~1400 evaluations
  - Found best solution in 7/50 runs
  - Other solutions effectively included only 2 components
- 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

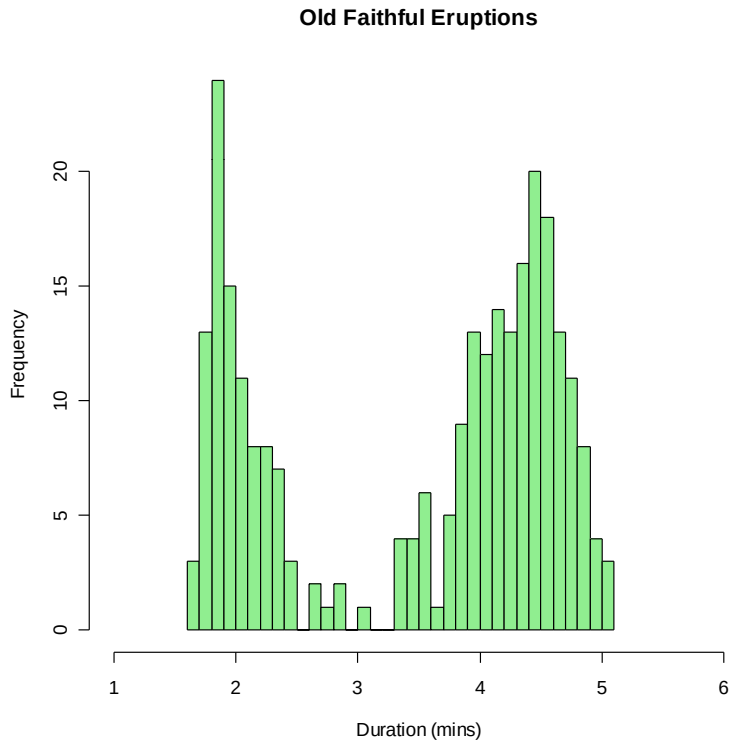


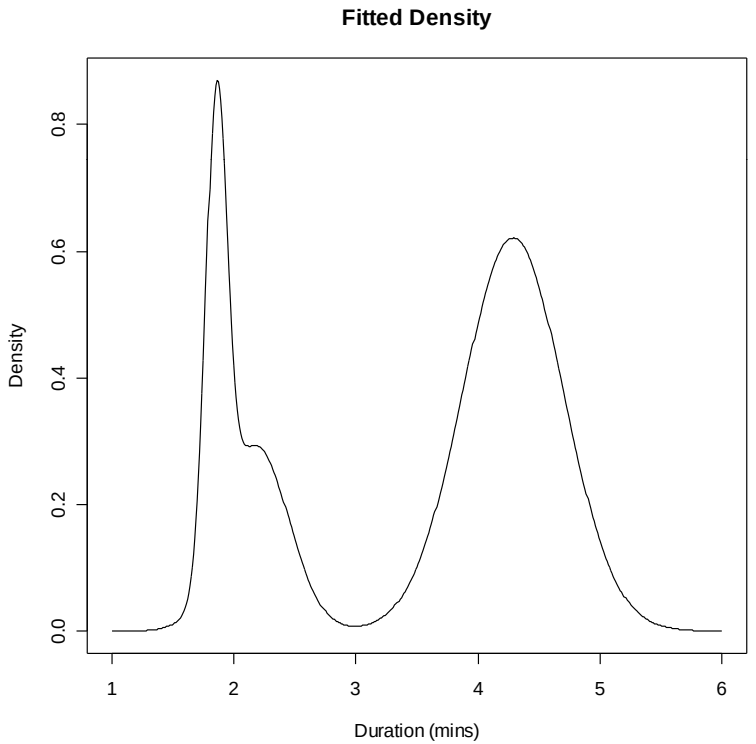


E-M Algorithm: A Mixture of Three Normals

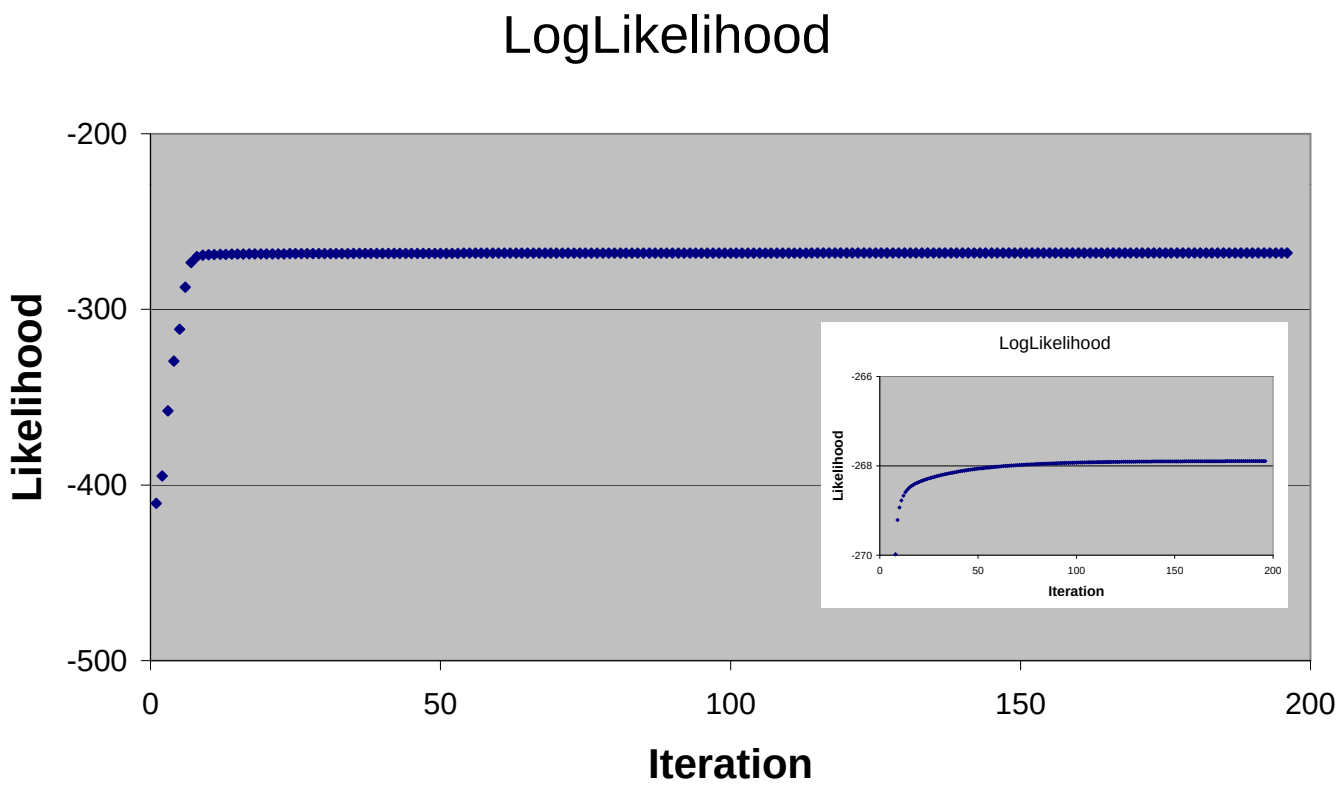
- Fit 8 parameters
  - 2 proportions, 3 means, 3 variances
- Required about ~150 evaluations
  - Found log-likelihood of ~267.89 in 42/50 runs
  - Found log-likelihood of ~263.91 in 7/50 runs
- The best solutions …
  - Components contributing .160, 0.195 and 0.644
  - Component means are 1.856, 2.182 and 4.289
  - Variances are 0.00766, 0.0709 and 0.172
  - Maximum log-likelihood = -263.91

Three Components

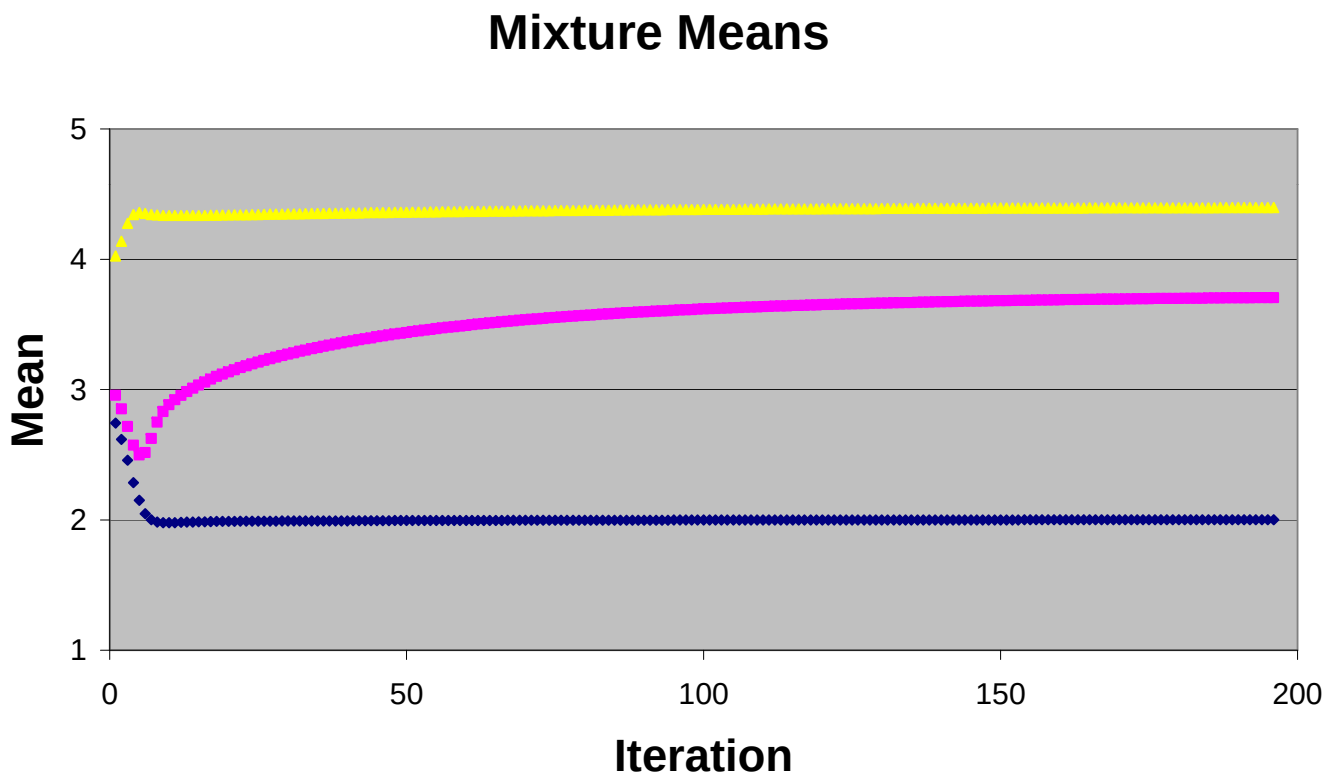




Convergence for E-M Algorithm



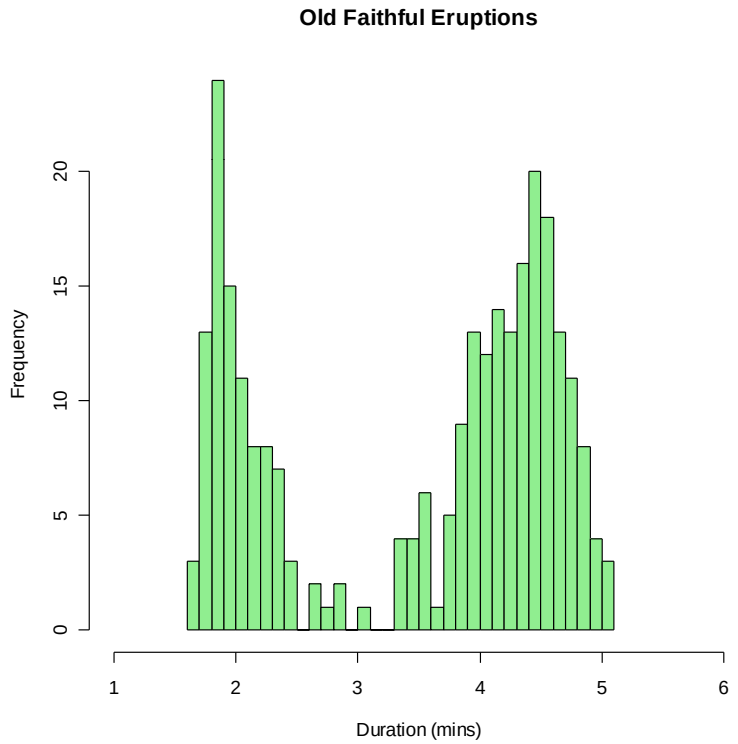
Convergence for E-M Algorithm

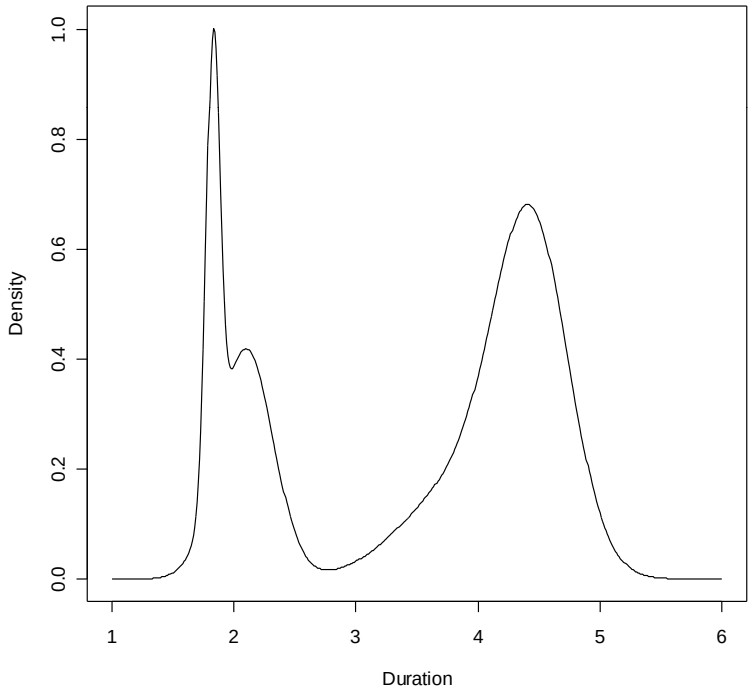


E-M Algorithm: A Mixture of Four Normals

- Fit 11 parameters
  - 3 proportions, 4 means, 4 variances
- Required about ~300 evaluations
  - Found log-likelihood of ~267.89 in 1/50 runs
  - Found log-likelihood of ~263.91 in 2/50 runs
  - Found log-likelihood of ~257.46 in 47/50 runs
- "Appears" more reliable than with 3 components

Four Components





Today ...

- The E-M algorithm
- Missing data formulation
- Application to mixture distributions
  - Consider multiple starting points

Further Reading

- There is a nice discussion of the E-M algorithm, with application to mixtures at:

  http://en.wikipedia.org/wiki/EM_algorithm