The E-M Algorithm
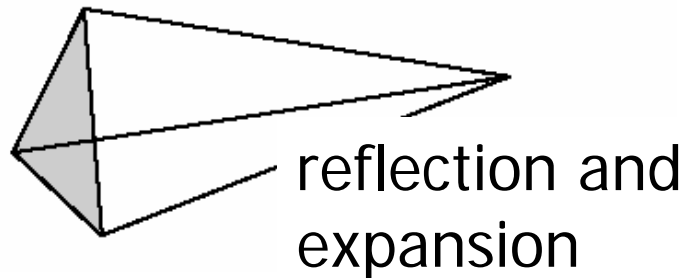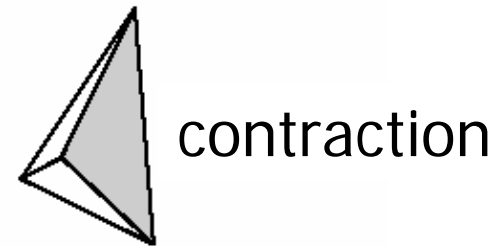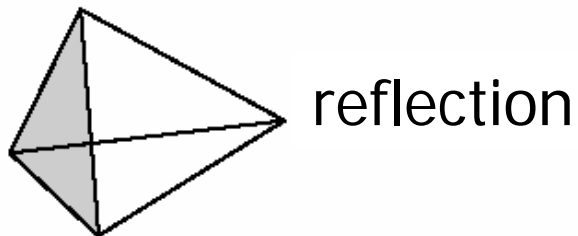
Biostatistics 615/815

Lecture 18

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   Original Simplex

low

reflection   contraction

reflection and expansion   multiple contraction
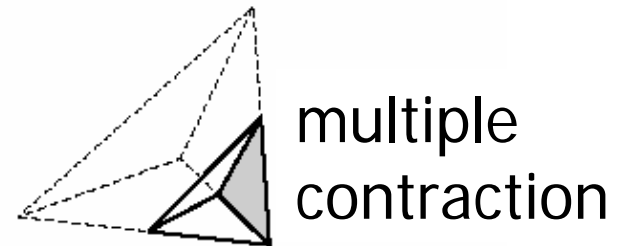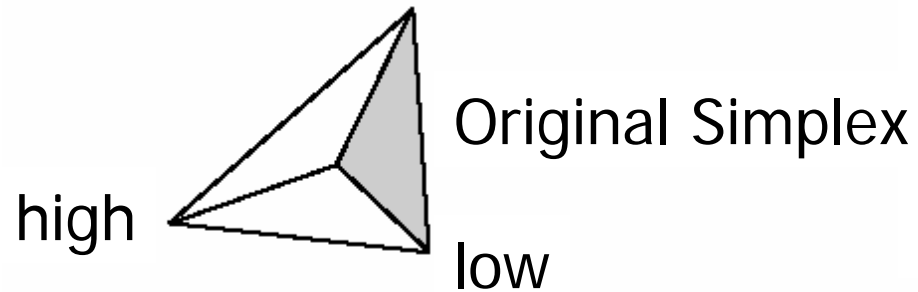
Other Strategies for Multidimensional Optimization

- 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!
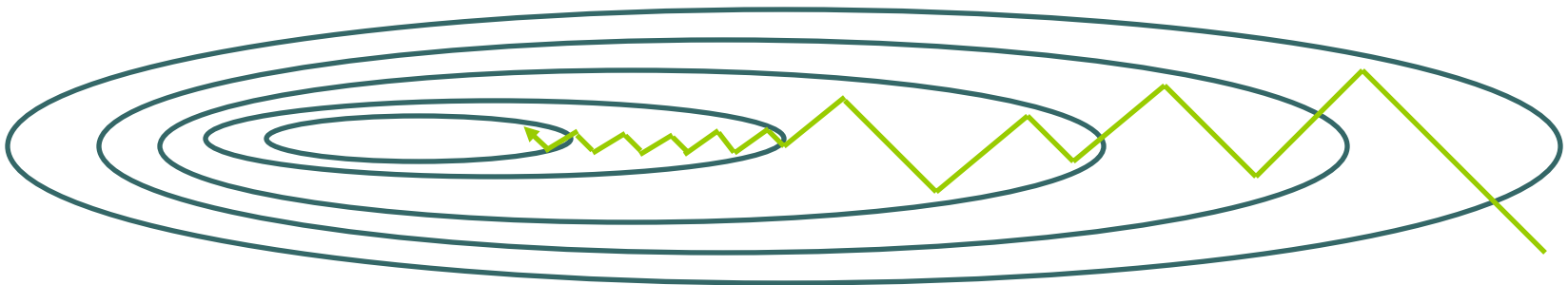
Most methods that use derivatives don't simply optimize function along current gradient or the unit vectors …

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 6,082 research articles

- For comparison
  - Nelder and Mead (1965)
    Computer Journal **7**: 308-313
  - Cited in over 6,762 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

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

```c
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);
}
```

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

```c
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

```c
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

```c
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

```c
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

```c
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

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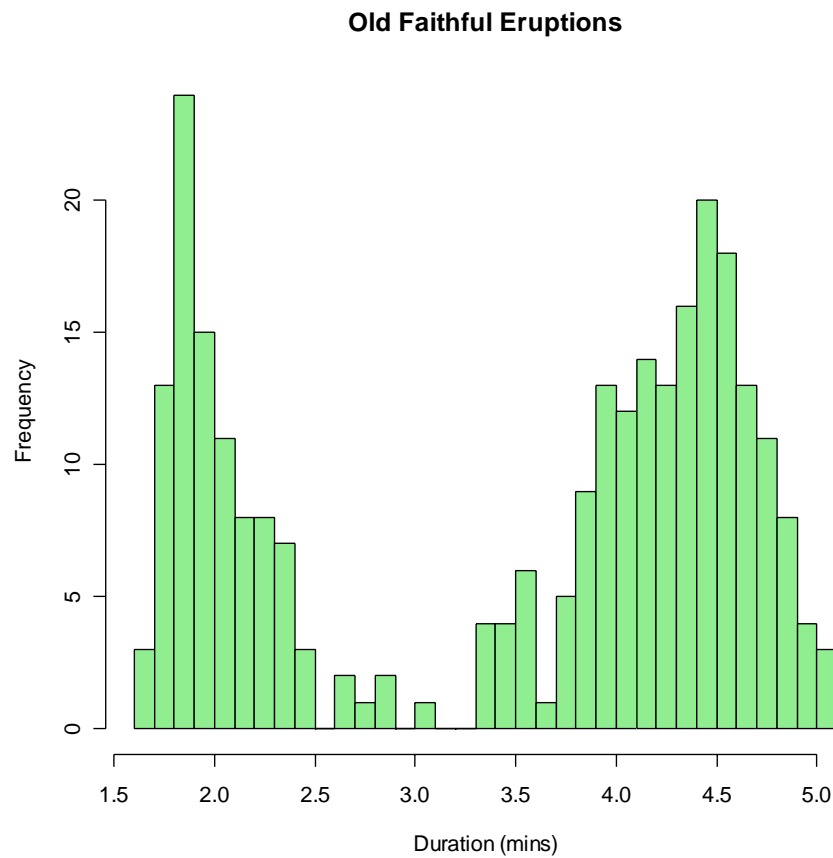void start_em(int n, double * data,
              int k, double * prob, double * mean, double * sd)
   {
   int i, j; double mean1 = 0.0, sd1 = 0.0;

   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)

Old Faithful Eruptions

Using Simplex Method
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

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

Old Faithful Eruptions
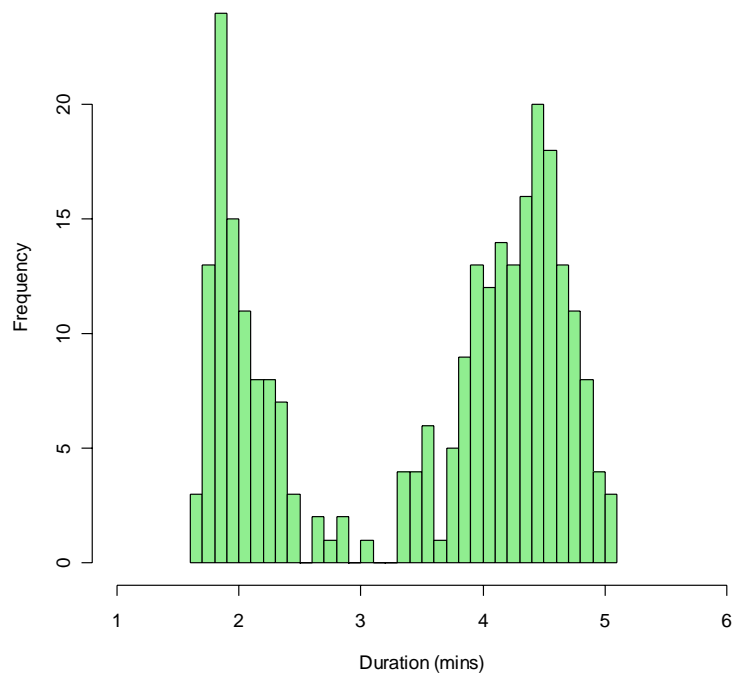
Fitted Distribution
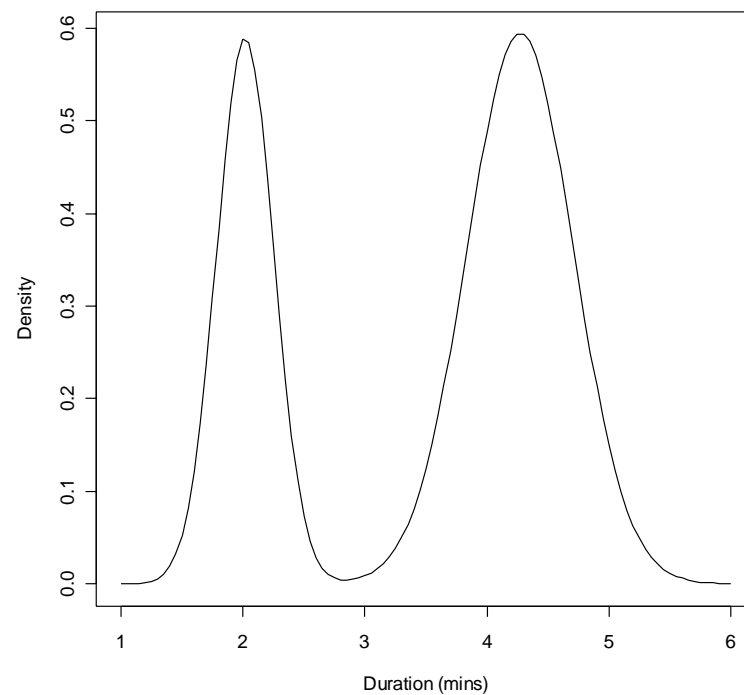
Simplex Method:
A Mixture of Three Normals

- 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

Old Faithful Eruptions
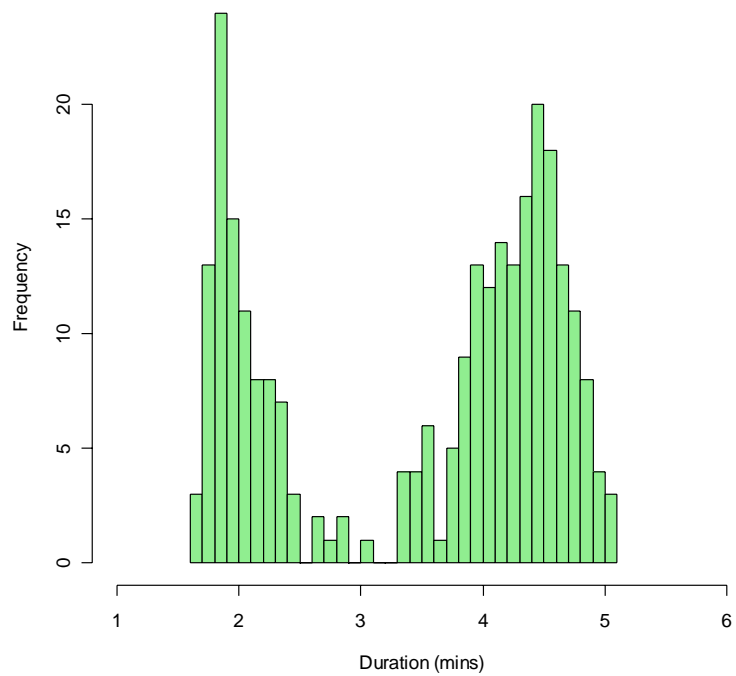
Fitted Distribution
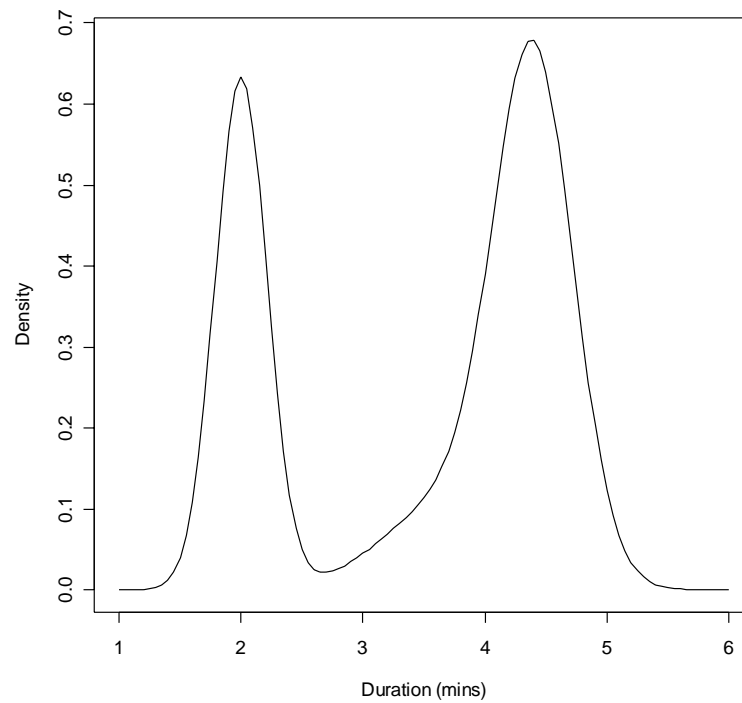
E-M Algorithm:
A Mixture of Three Normals

- 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

Old Faithful Eruptions
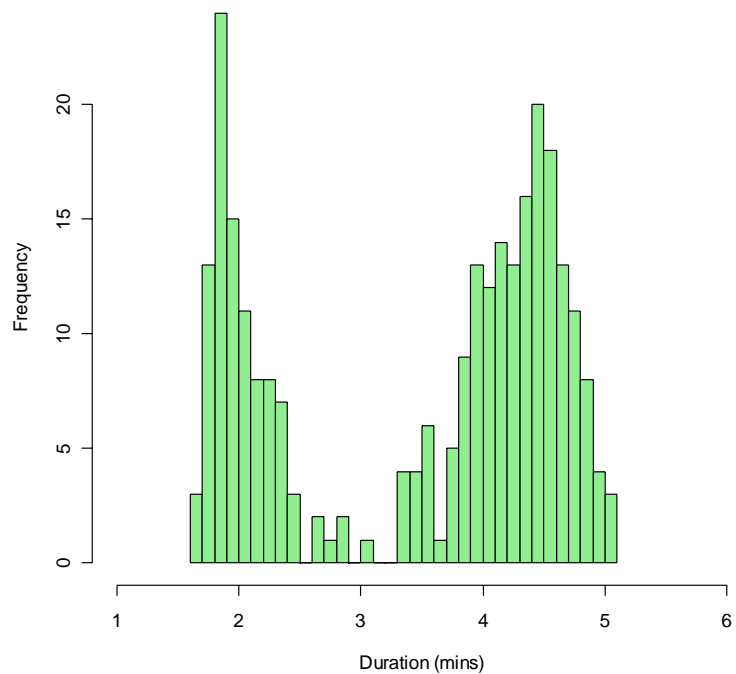
Fitted Density
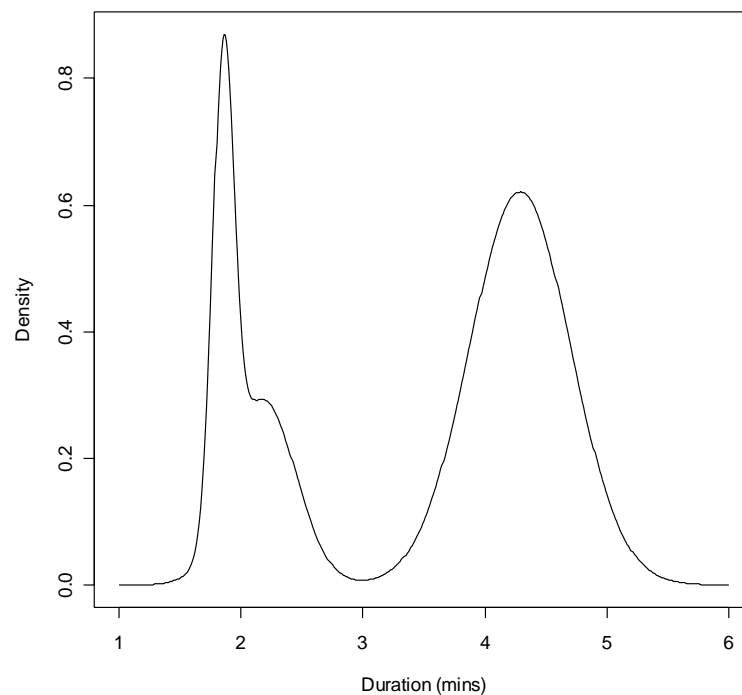
Convergence for E-M Algorithm

LogLikelihood
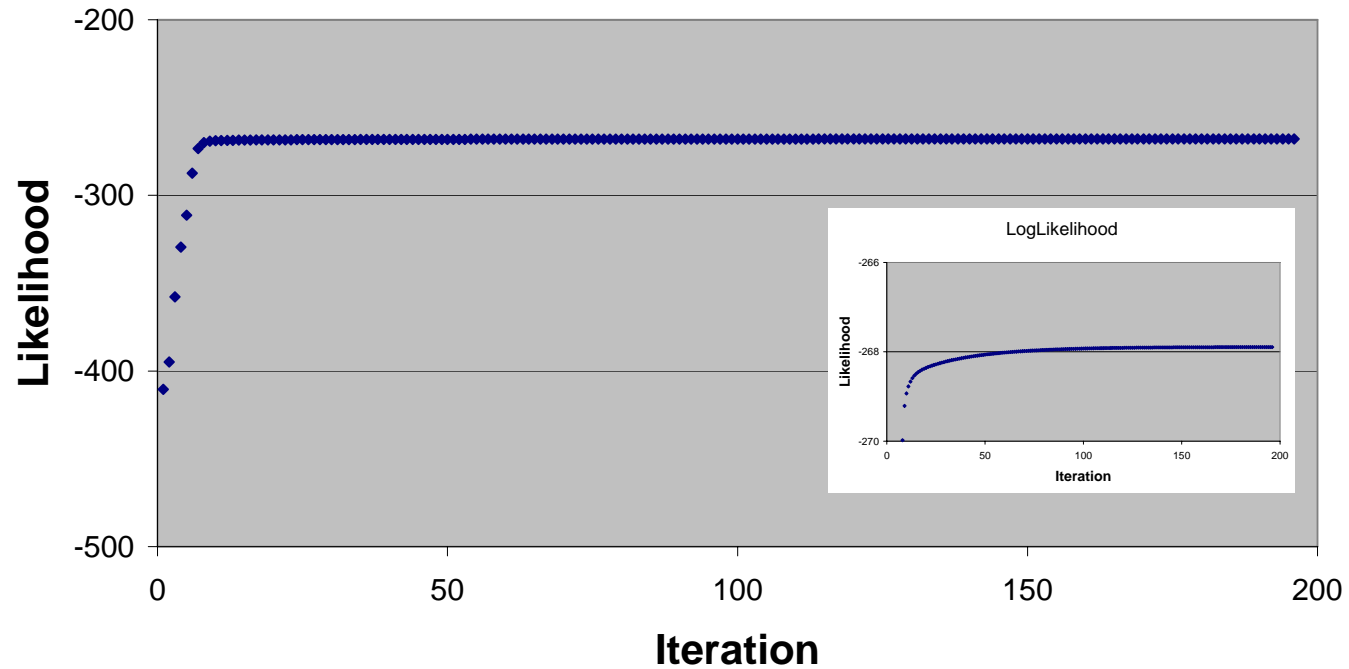
Convergence for E-M Algorithm

Mixture Means
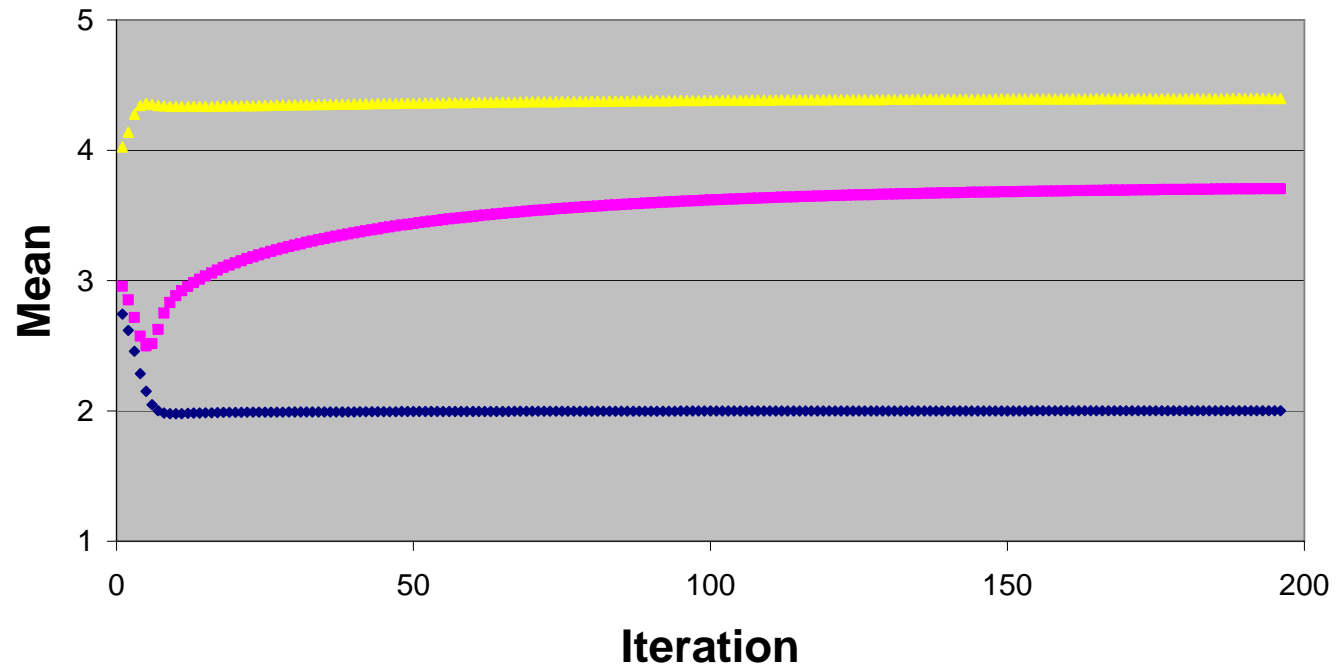
E-M Algorithm:
A Mixture of Four Normals

- 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
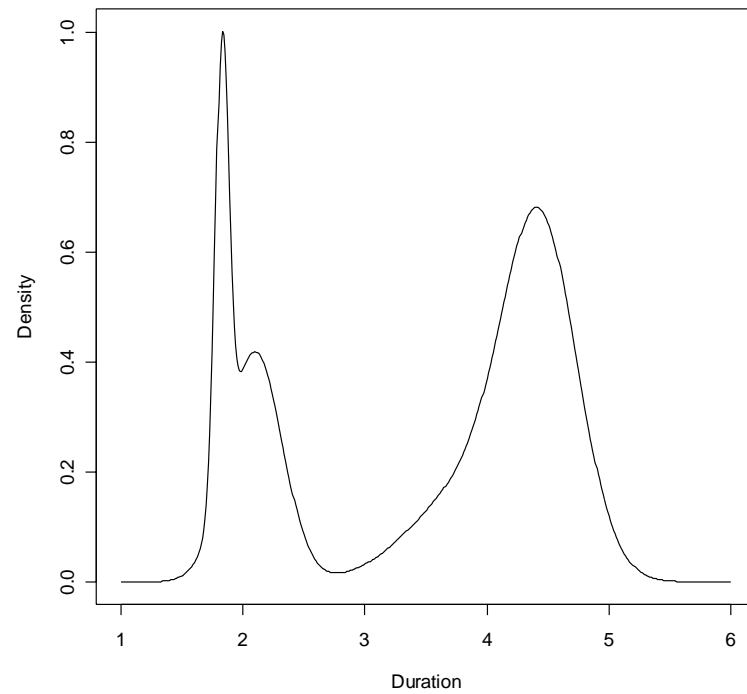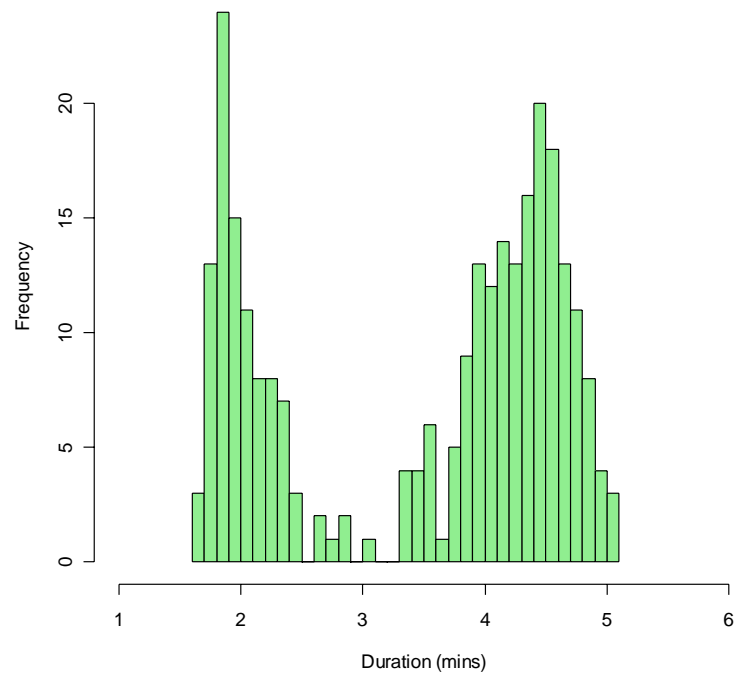
Today ...

- 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