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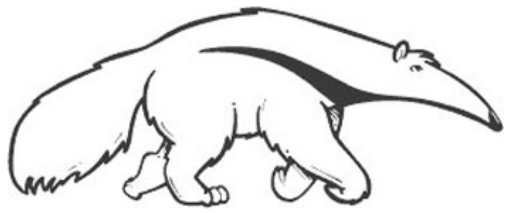
Machine Learning and Data Mining

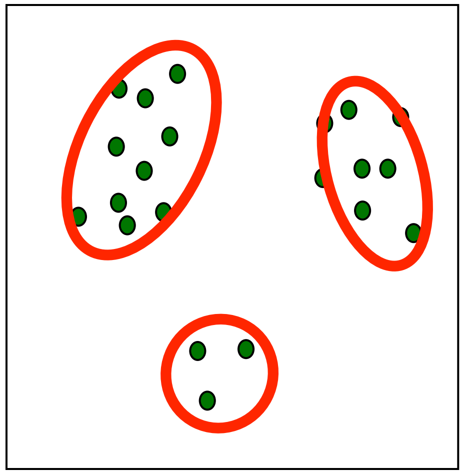
Clustering (1): Basics

Prof. Alexander Ihler



Unsupervised learning

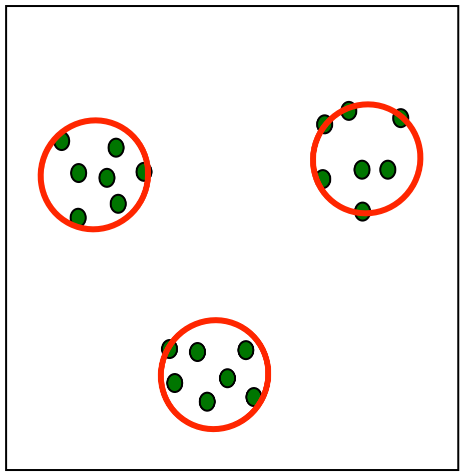
- Supervised learning
  - Predict target value (“y”) given features (“x”)
- Unsupervised learning
  - Understand patterns of data (just “x”)
  - Useful for many reasons
    - Data mining (“explain”)
    - Missing data values (“impute”)
    - Representation (feature generation or selection)
- One example: *clustering*
  - Describe data by discrete “groups” with some characteristics



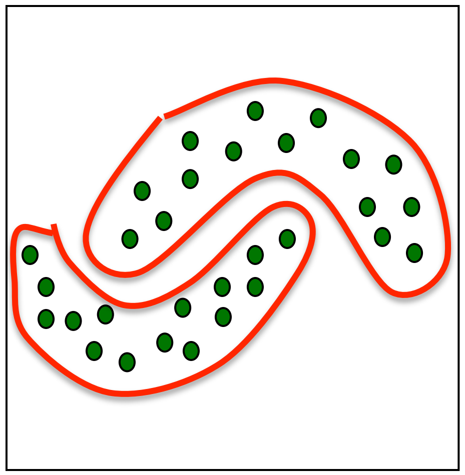
Clustering

- Clustering describes data by "groups"
- The meaning of "groups" may vary by data!

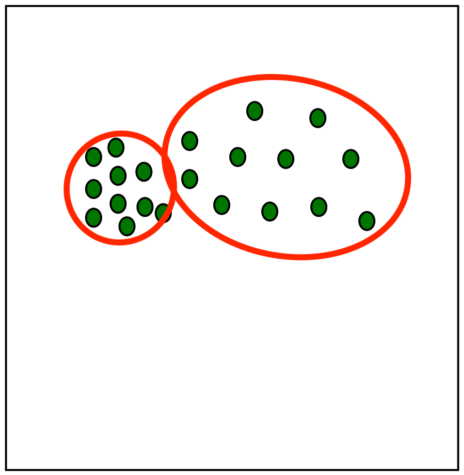
- Examples



Location



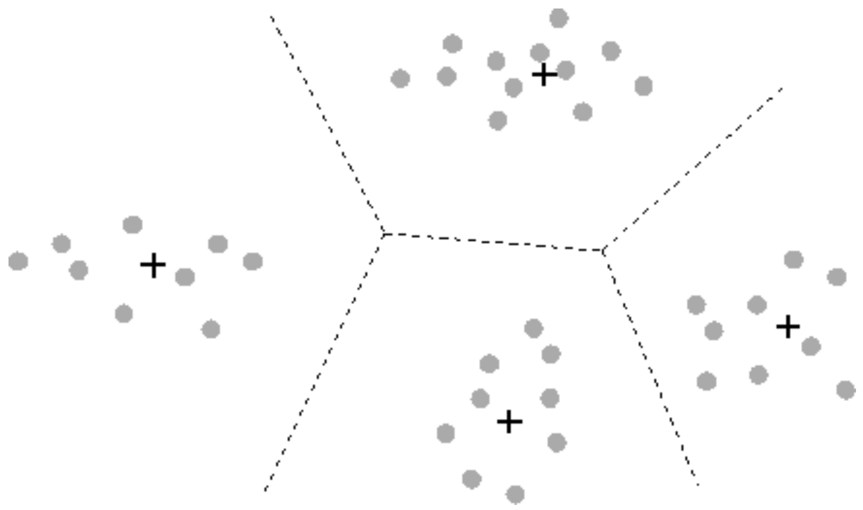
Shape

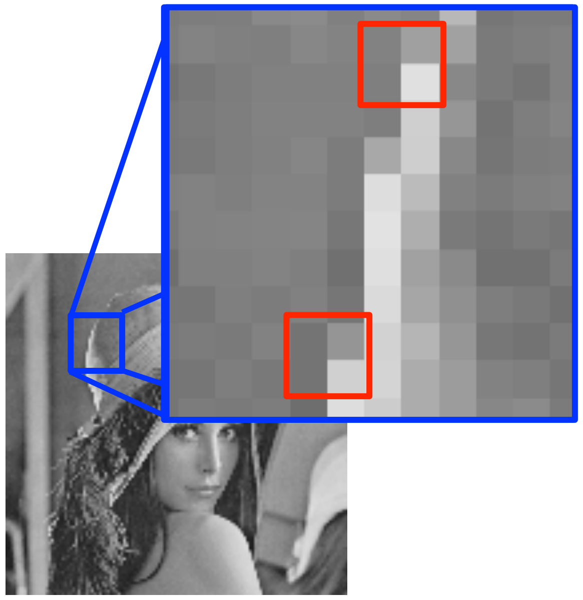


Density

Clustering and Data Compression

- Clustering is related to vector quantization
  - Dictionary of vectors (the cluster centers)
  - Each original value represented using a dictionary index
  - Each center "claims" a nearby region (Voronoi region)

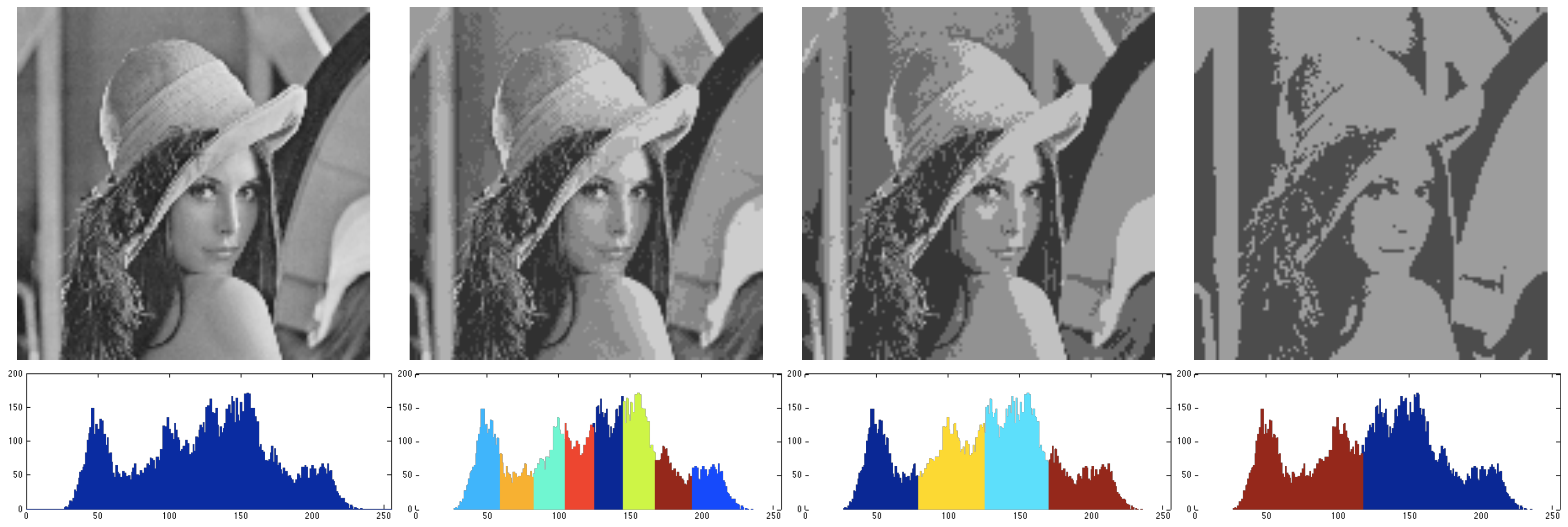




Clustering and Data Compression

- Clustering is related to vector quantization
  - Dictionary of vectors (the cluster centers)
  - Each original value represented using a dictionary index
  - Each center “claims” a nearby region (Voronoi region)

- Example in 1D: cluster pixels’ grayscale values



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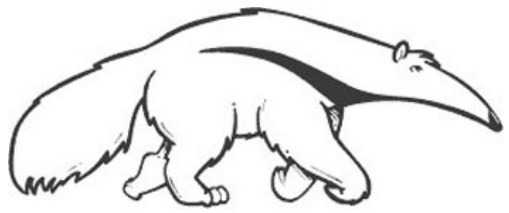
Machine Learning and Data Mining

Clustering (2):
Hierarchical Agglomerative Clustering

Prof. Alexander Ihler



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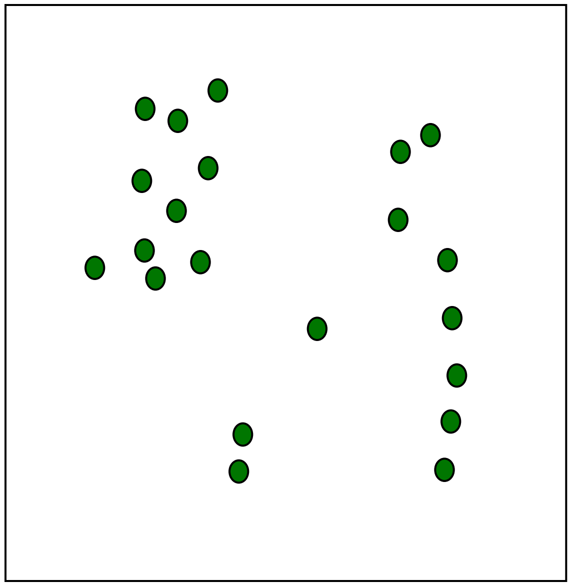
Hierarchical Agglomerative Clustering

Initially, every datum is a cluster

Data:



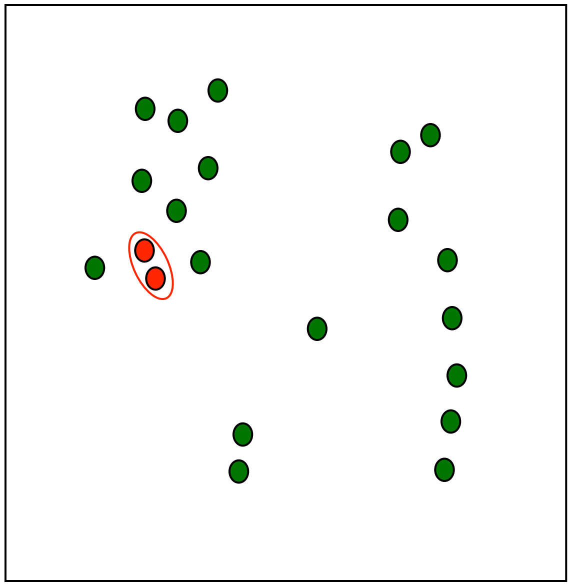
Algorithmic Complexity: O(m^2 log m) +

- A simple clustering algorithm
- Define a distance (or dissimilarity) between clusters (we'll return to this)
- Initialize: every example is a cluster
- Iterate:
  - Compute distances between all clusters
    (store for efficiency)
  - Merge two closest clusters
- Save both clustering and *sequence* of cluster operations
- "Dendrogram"

Iteration 1

Builds up a sequence of clusters ("hierarchical")

Data:



Dendrogram:

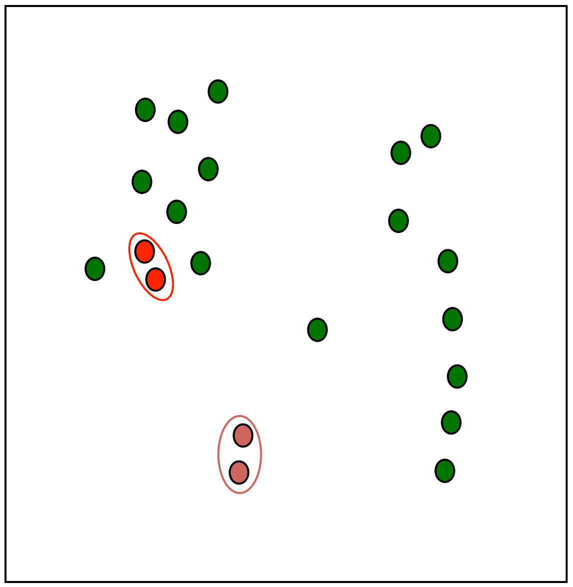
Height of the join indicates dissimilarity

Algorithmic Complexity: $O(m^2 \log m) + O(m \log m) +$

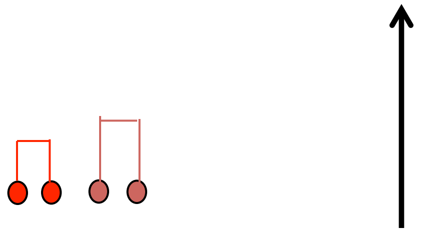
Iteration 2

Builds up a sequence of clusters ("hierarchical")

Data:



Dendrogram:

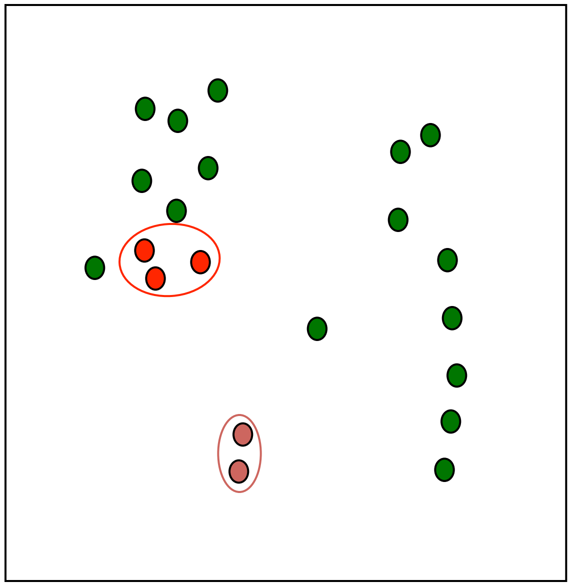


Algorithmic Complexity: O($m^2 \log m$) + 2*O(m log m) +

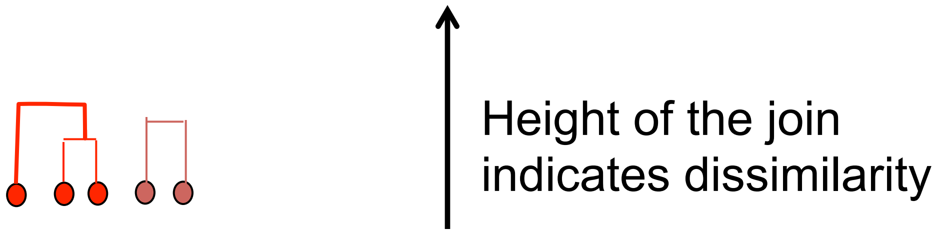
Iteration 3

Builds up a sequence of clusters ("hierarchical")

Data:



Dendrogram:

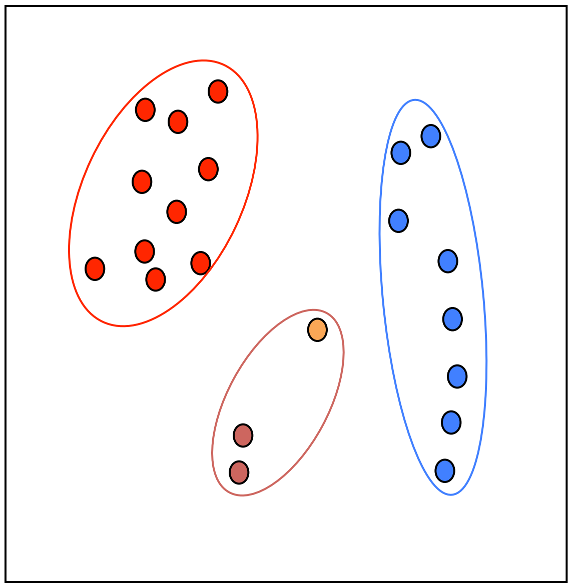


Algorithmic Complexity: $O(m^2 \log m) + 3*O(m \log m) +$

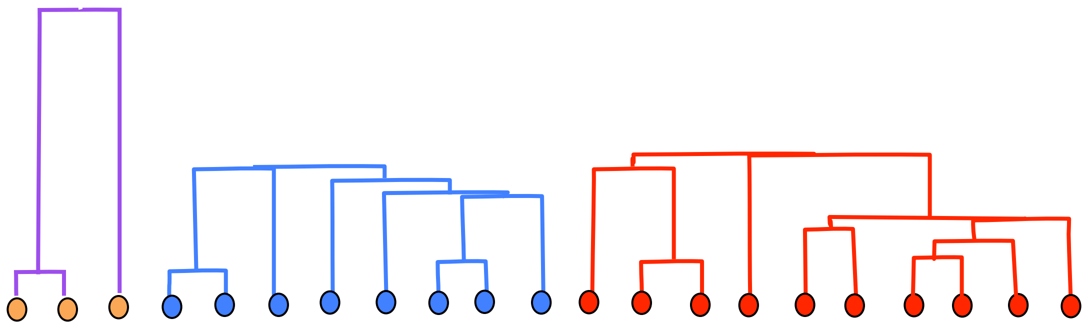
Iteration m-3

Builds up a sequence of clusters ("hierarchical")

Data:



Dendrogram:



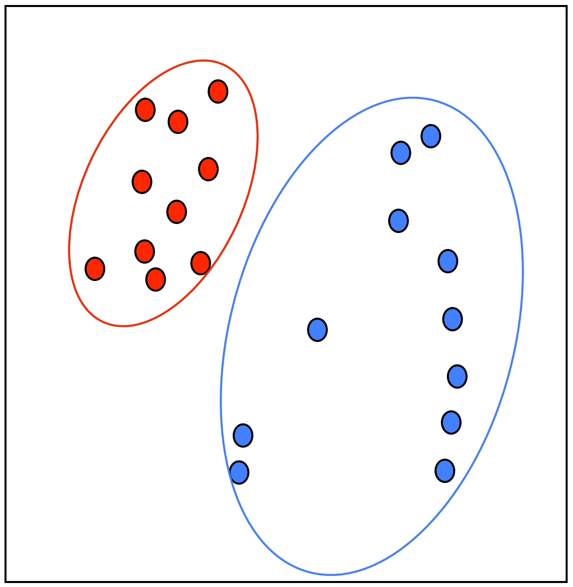
In matlab: "linkage" function (stats toolbox)
In mltools: "agglomerative"

Algorithmic Complexity: $O(m^2 \log m) + (m-3)*O(m \log m) +$

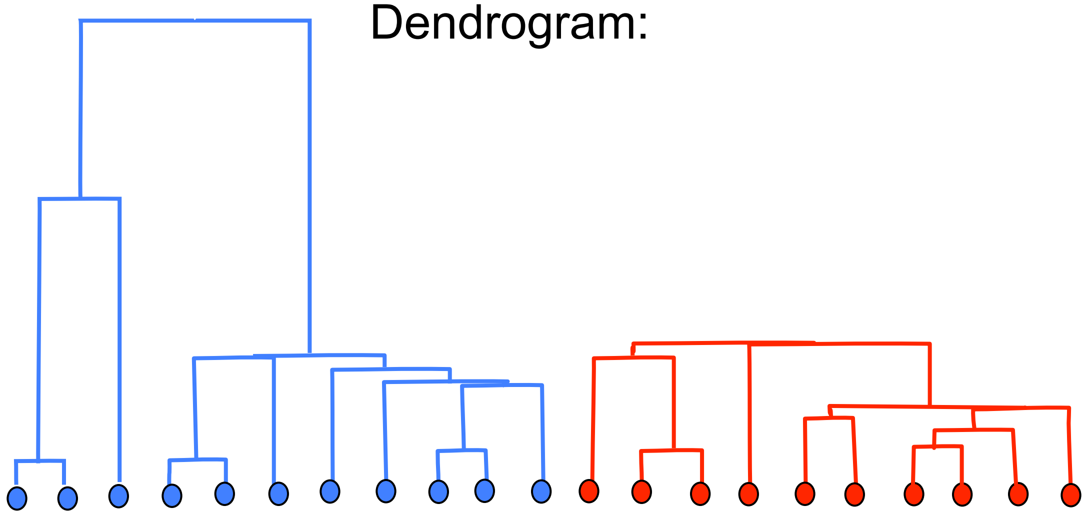
Iteration m-2

Builds up a sequence of clusters (“hierarchical”)

Data:



Dendrogram:

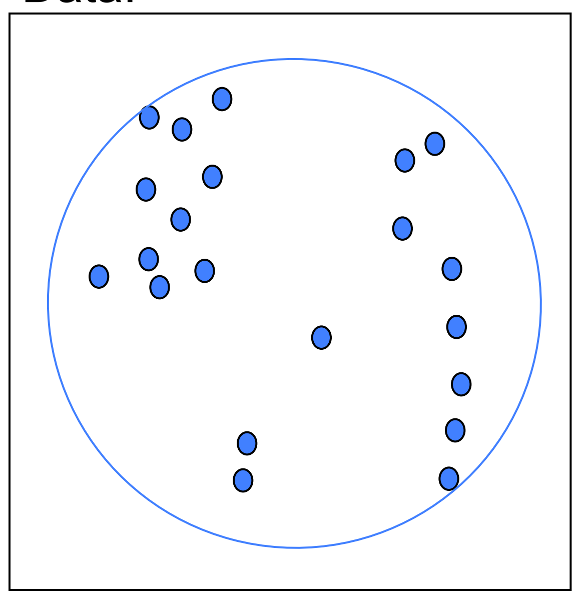


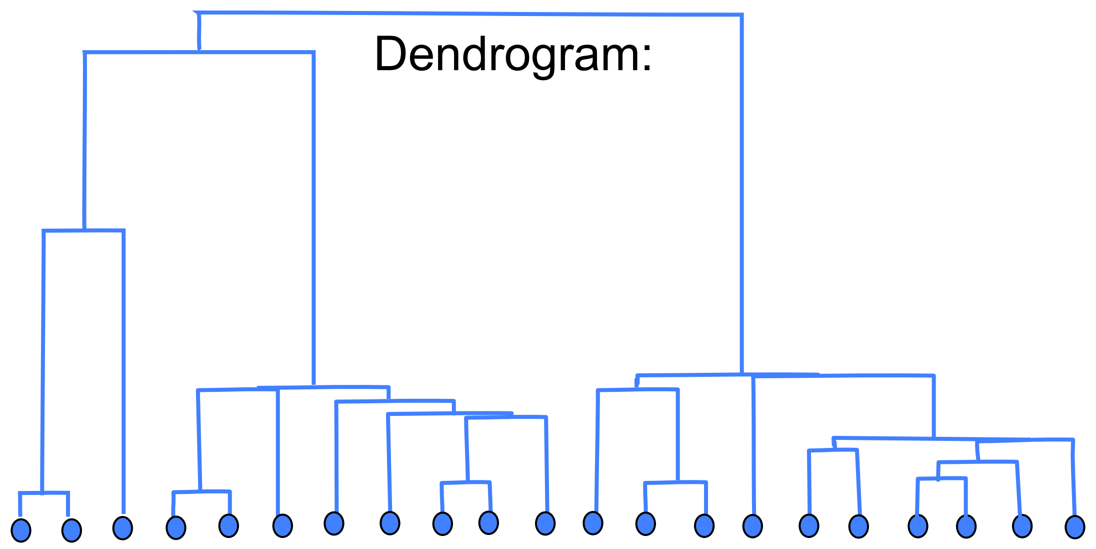
In matlab: “linkage” function (stats toolbox)
In mltools: “agglomerative”

Algorithmic Complexity: $O(m^2 \log m) + (m-2)*O(m \log m) +$

Iteration m-1

Builds up a sequence of clusters ("hierarchical")





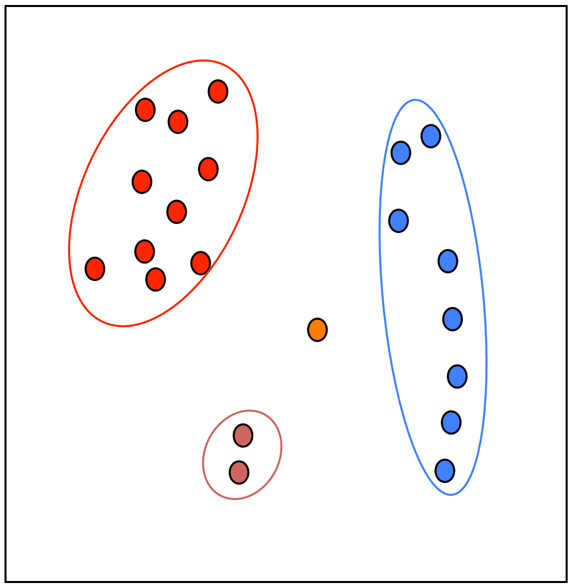
In matlab: "linkage" function (stats toolbox)
In mltools: "agglomerative"

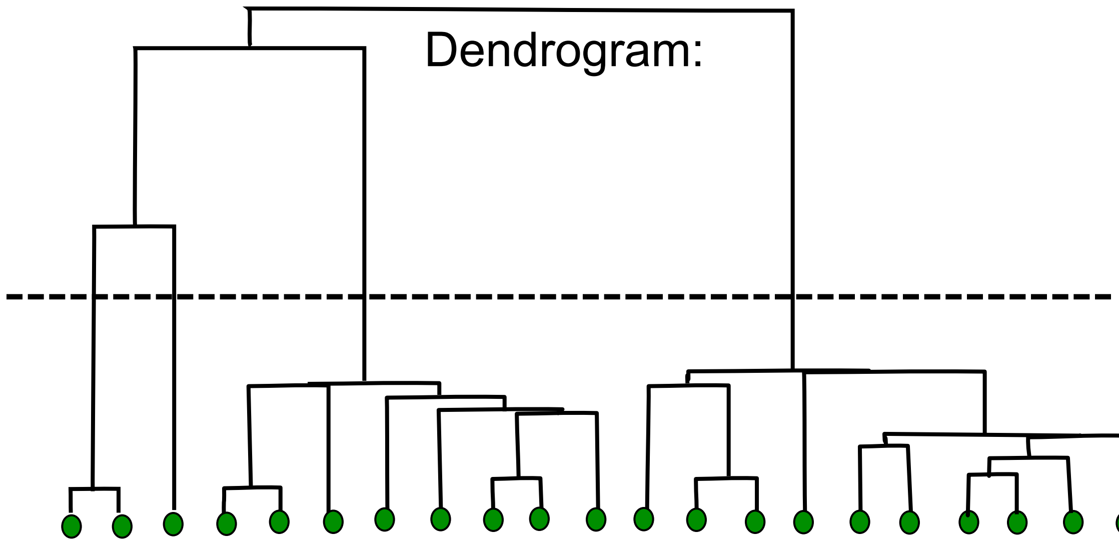
Algorithmic Complexity: $O(m^2 \log m) + (m-1)*O(m \log m) = O(m^2 \log m)$

From dendrogram to clusters

Given the sequence, can select a number of clusters or a dissimilarity threshold:

Data:



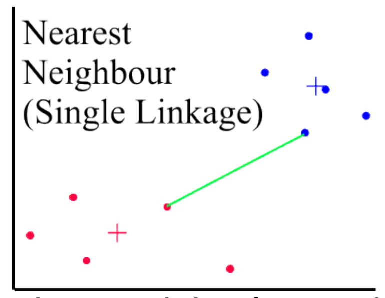


In matlab: "linkage" function (stats toolbox)
In mltools: "agglomerative"

Algorithmic Complexity: $O(m^2 \log m) + (m-1)*O(m \log m) = O(m^2 \log m)$

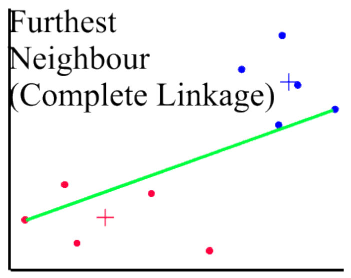
Cluster distances

$$D_{\min}(C_i, C_j) = \min_{x \in C_i,\ y \in C_j} \|x - y\|^2$$



produces minimal spanning tree.

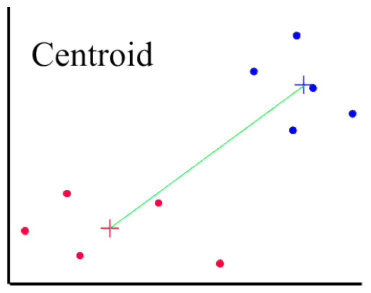
$$D_{\max}(C_i, C_j) = \max_{x \in C_i,\ y \in C_j} \|x - y\|^2$$



avoids elongated clusters.

$$D_{\text{avg}}(C_i, C_j) = \frac{1}{|C_i||C_j|} \sum_{x \in C_i,\ y \in C_j} \|x - y\|^2$$

$$D_{\text{means}}(C_i, C_j) = \|\mu_i - \mu_j\|^2$$

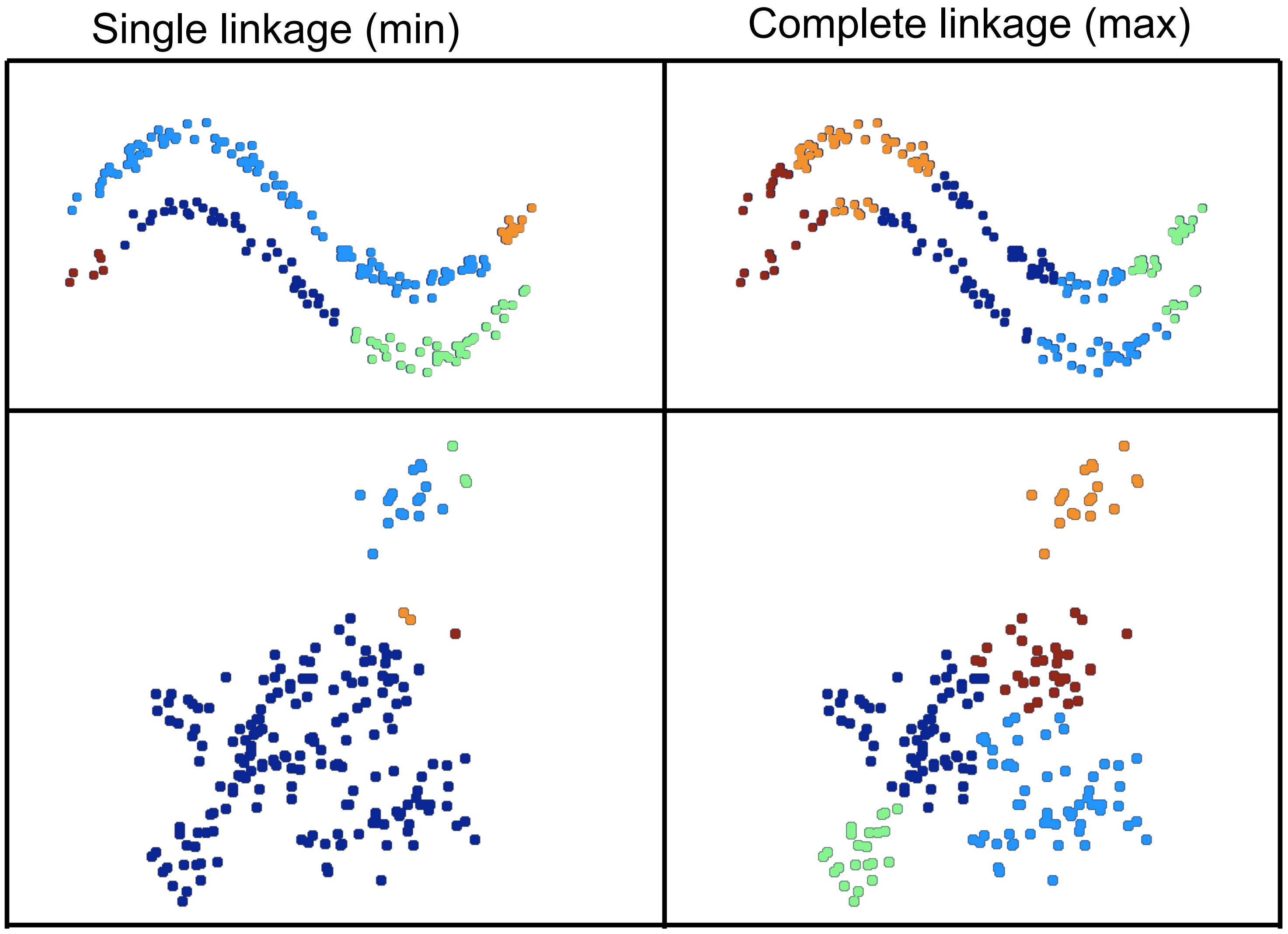


Need:

$$\begin{tikzcd} D(A,C) \arrow[dr] & \\ & D(A+B,C) \\ D(B,C) \arrow[ur] & \end{tikzcd}$$

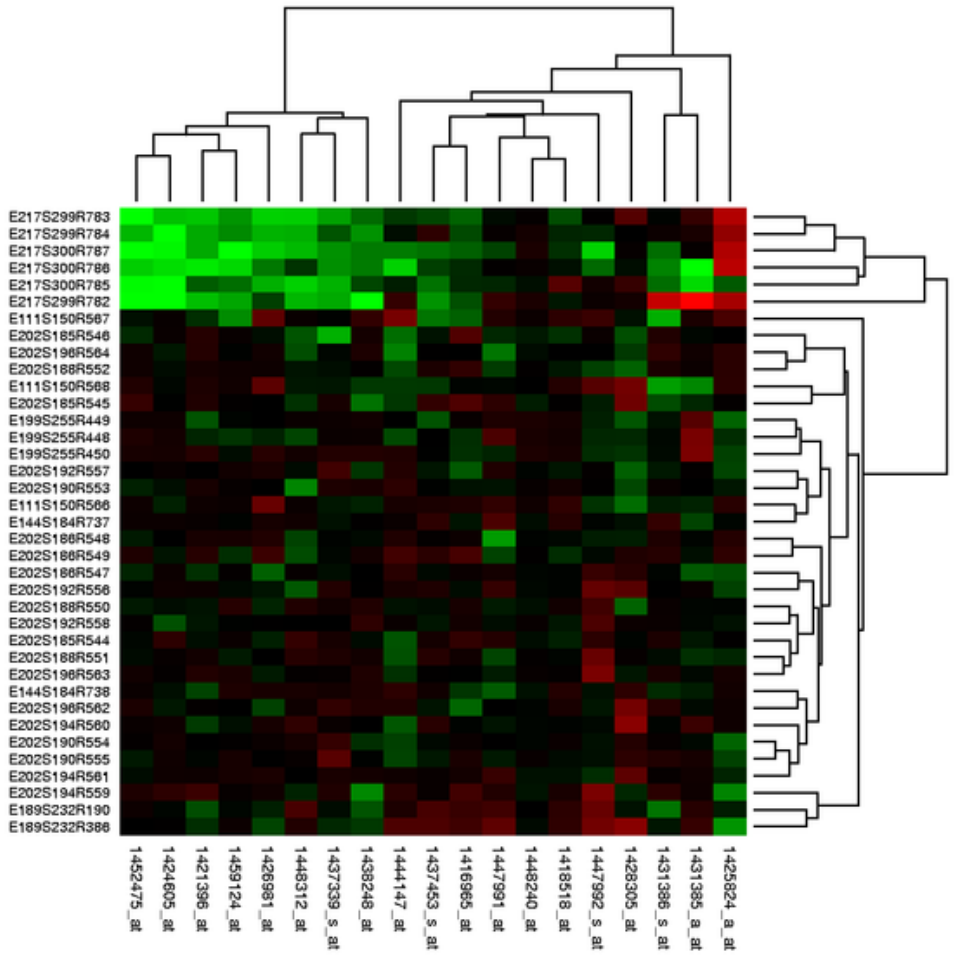
Cluster distances

- Dissimilarity choice will affect clusters created



Example: microarray expression

- Measure gene expression
- Various experimental conditions
  - Disease v. normal
  - Time
  - Subjects
- Explore similarities
  - What genes change together?
  - What conditions are similar?
- Cluster on both genes and conditions



Matlab: "clustergram" (bioinfo toolbox)

Summary

- Agglomerative clustering
  - Choose a cluster distance / dissimilarity scoring method
  - Successively merge closest pair of clusters
  - "Dendrogram" shows sequence of merges & distances
  - Complexity: $O(m^2 \log m)$

- "Clustergram" for understanding data matrix
  - Build clusters on rows (data) and columns (features)
  - Reorder data & features to expose behavior across groups

- Agglomerative clusters depend critically on dissimilarity
  - Choice determines characteristics of "found" clusters

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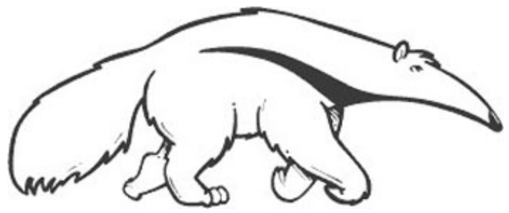
Machine Learning and Data Mining

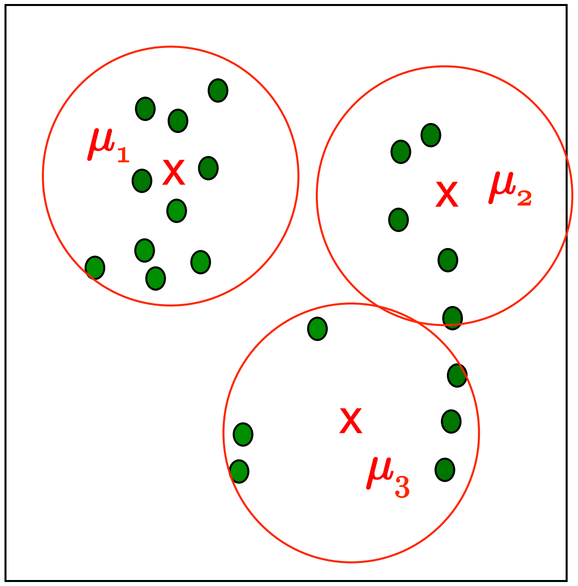
Clustering (3):
k-Means Clustering

Prof. Alexander Ihler



K-Means Clustering

- A simple clustering algorithm
- Iterate between
  - Updating the assignment of data to clusters
  - Updating the cluster's summarization



Notation:

Data example i has features x_i

Assume K clusters

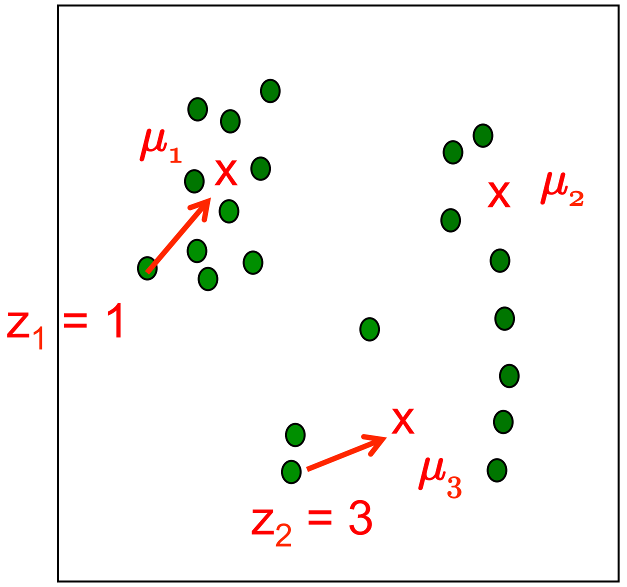
Each cluster c "described" by a center μ_c

Each cluster will "claim" a set of nearby points

Matlab: "kmeans" (stats toolbox)

K-Means Clustering

- A simple clustering algorithm
- Iterate between
  - Updating the assignment of data to clusters
  - Updating the cluster's summarization



Notation:

Data example i has features x_i

Assume K clusters

Each cluster c "described" by a center μ_c

Each cluster will "claim" a set of nearby points

"Assignment" of ith example: $z_i \in 1..K$

Matlab: "kmeans" (stats toolbox)

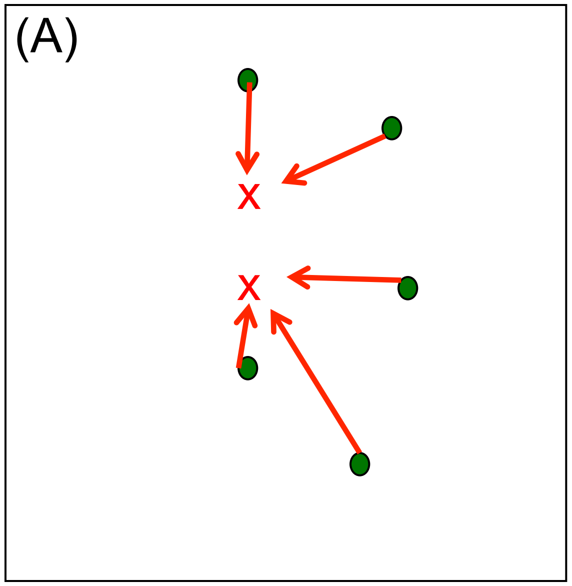
K-Means Clustering

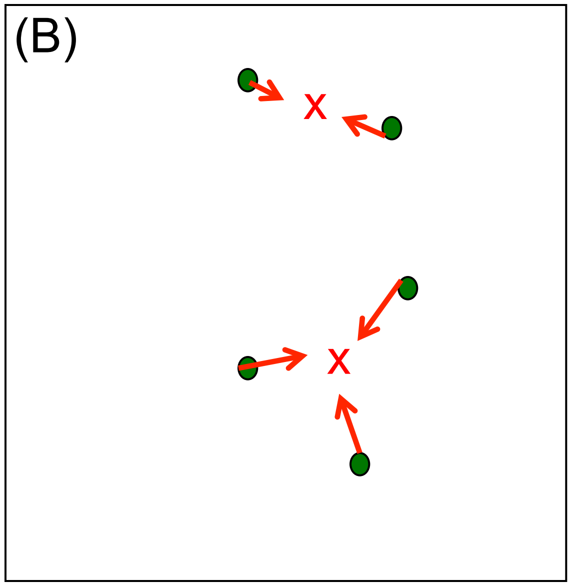
- Iterate until convergence:
  - (A) For each datum, find the closest cluster

$$z_i = \arg\min_c \|x_i - \mu_c\|^2 \qquad \forall i$$

  - (B) Set each cluster to the mean of all assigned data:

$$\forall c, \qquad \mu_c = \frac{1}{m_c} \sum_{i \in S_c} x_i \qquad\qquad S_c = \{i : z_i = c\},\ m_c = |S_c|$$





K-Means Clustering

- Optimizing the cost function:

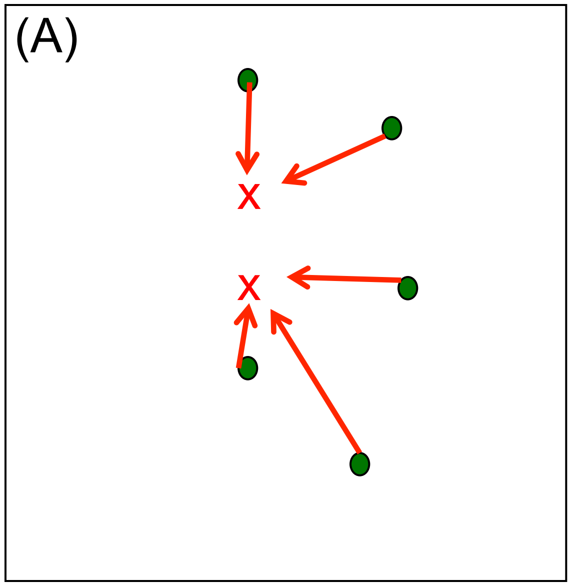
$$C(\underline{z}, \underline{\mu}) = \sum_i \|x_i - \mu_{z_i}\|^2$$

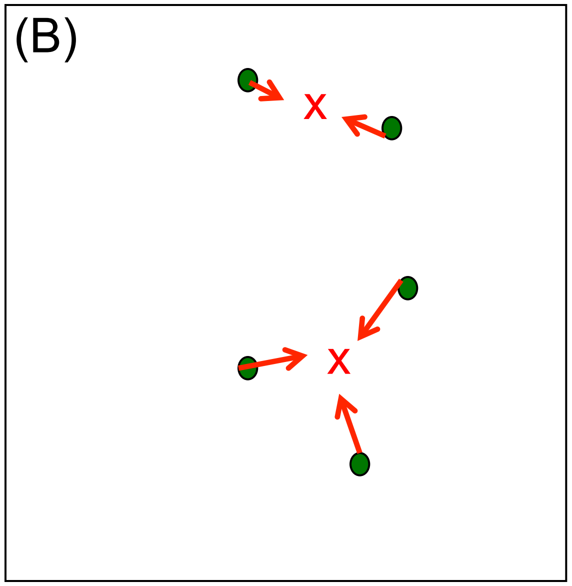
- Coordinate descent:

Descent => guaranteed to converge
New means = same assignments
Same assignments = same means
Same means = same assignments
…

Over the cluster assignments:
Only one term in sum depends on z_i
Minimized by selecting closest μ_c

Over the cluster centers:
Cluster c only depends on x_i with z_i=c
Minimized by selecting the mean

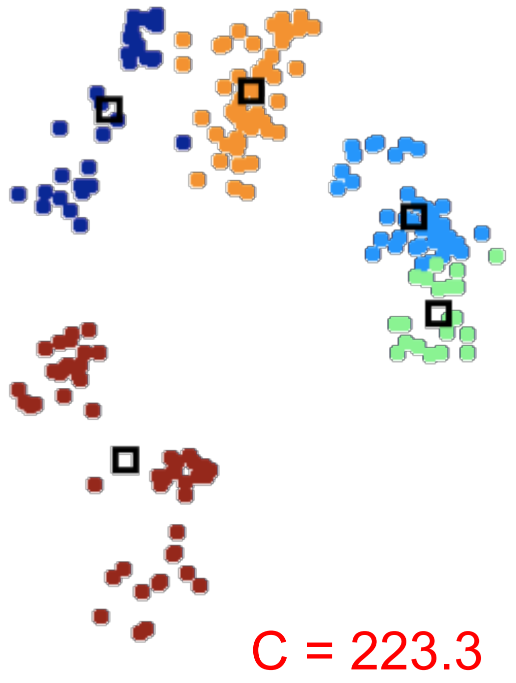


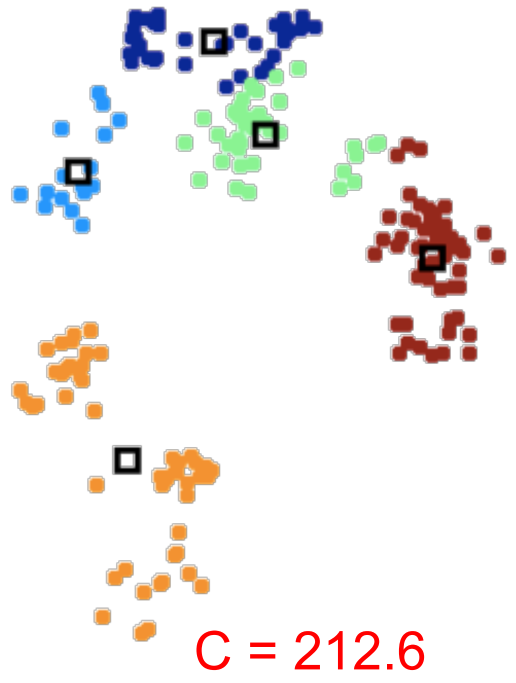


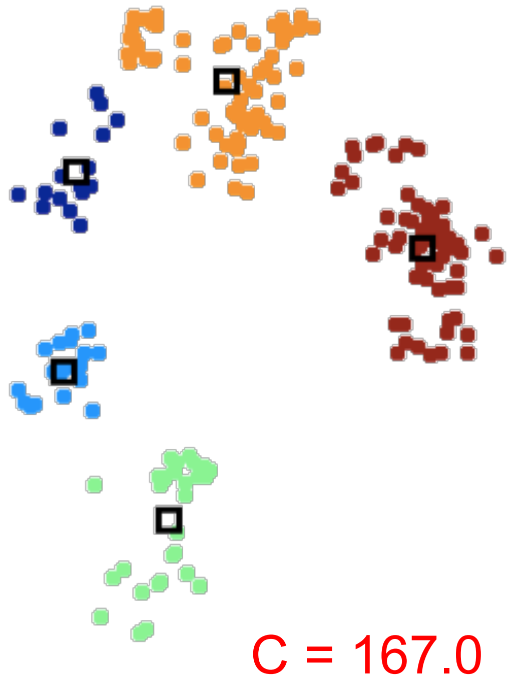
Initialization

- Multiple local optima, depending on initialization

- Try different (randomized) initializations
- Can use cost C to decide which we prefer

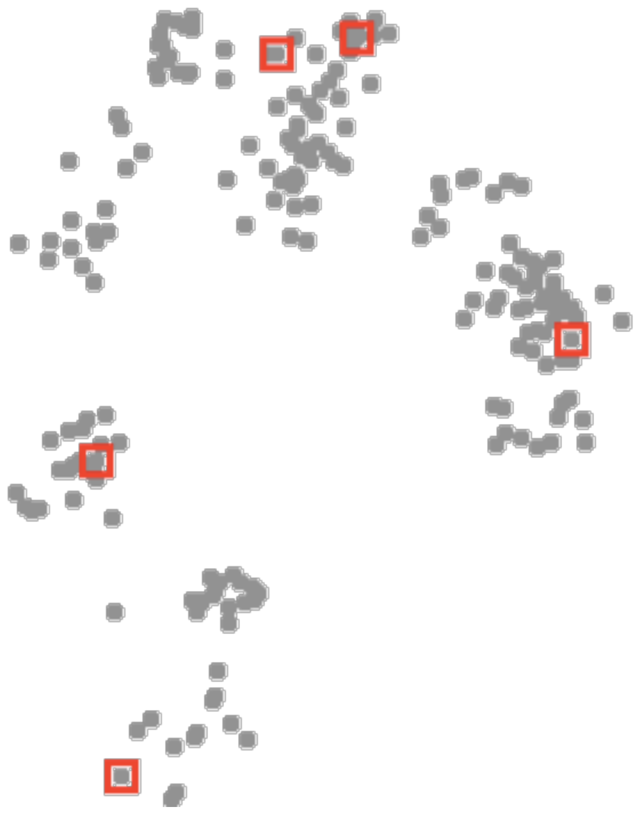






Initialization methods

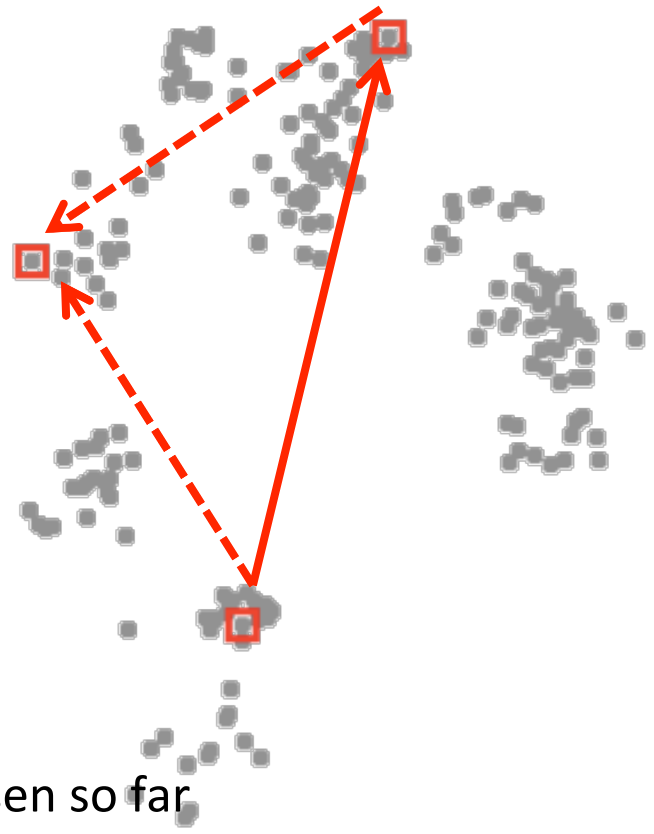
- Random
  - Usually, choose random data index
  - Ensures centers are near some data
  - Issue: may choose nearby points



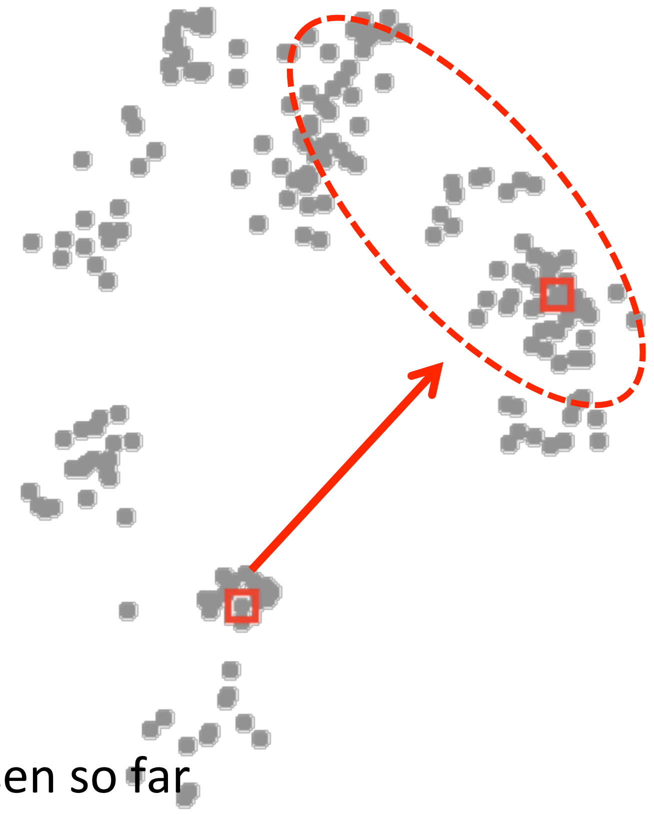
Initialization methods

- Random
  - Usually, choose random data index
  - Ensures centers are near some data
  - Issue: may choose nearby points

- Distance-based
  - Start with one random data point
  - Find the point farthest from the clusters chosen so far
  - Issue: may choose outliers



Initialization methods



- Random
  - Usually, choose random data index
  - Ensures centers are near some data
  - Issue: may choose nearby points
- Distance-based
  - Start with one random data point
  - Find the point farthest from the clusters chosen so far
  - Issue: may choose outliers
- Random + distance (“k-means++”) (Arthur & Vassilvitskii, 2007)
  - Choose next points “far but randomly”

    $p(x) \propto$ squared distance from x to current centers
  - Likely to put a cluster far away, in a region with lots of data

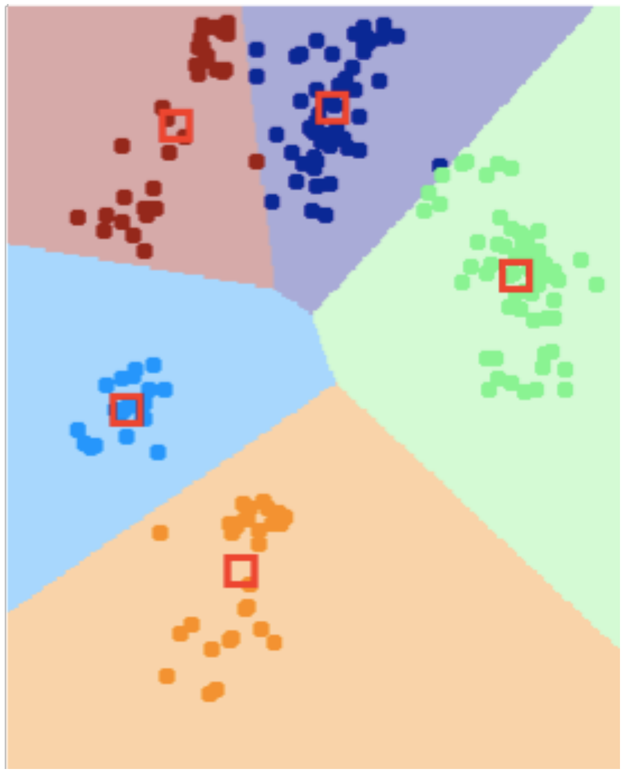
Out-of-sample points

- Often want to use clustering on new data
- Easy for k-means: choose nearest cluster center

```
# perform clustering
Z , mu , score = kmeans(X, K);

# cluster id = nearest center
L = knnClassify(mu, range(K), 1);

# assign in- or out-of-sample points
Z = L.predict(X);
```



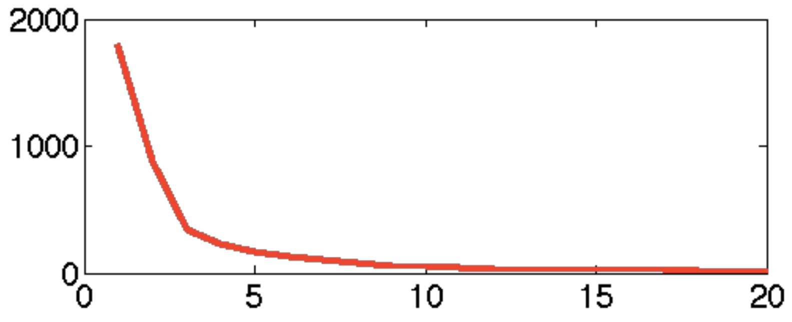
Choosing the number of clusters

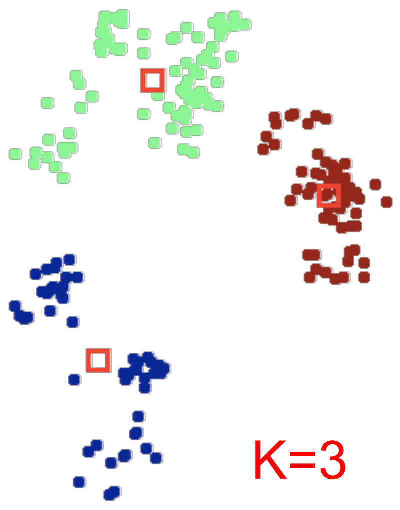
- With cost function

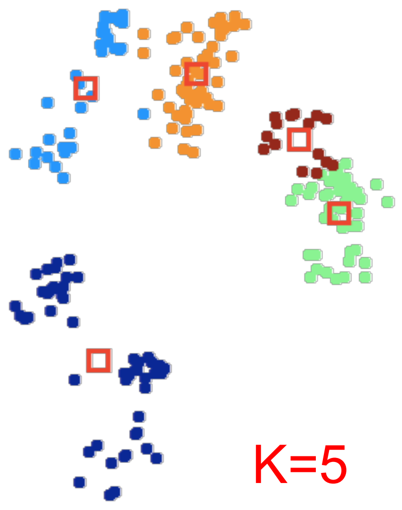
$$C(\underline{z}, \underline{\mu}) = \sum_i \|x_i - \mu_{z_i}\|^2$$

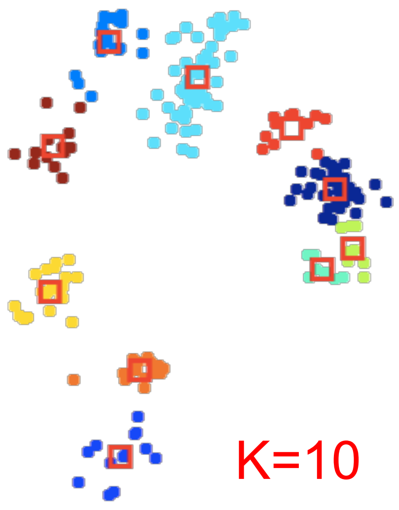
  what is the optimal value of k?

- Cost always decreases with k!
- A model complexity issue…









Choosing the number of clusters

- With cost function

$$C(\underline{z},\underline{\mu}) = \sum_i \|x_i - \mu_{z_i}\|^2$$

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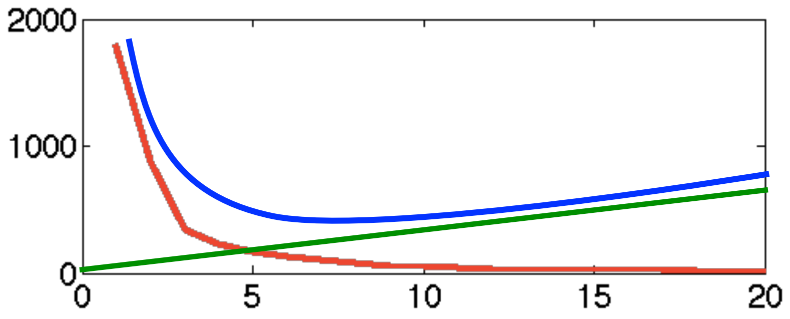

- One solution is to penalize for complexity
  - Add penalty: Total = Error + Complexity
  - Now more clusters can increase cost, if they don't help "enough"

  - Ex: simplified BIC penalty

$$J(\underline{z},\underline{\mu}) = \log\left[\frac{1}{m\,d}\sum_i \|x_i - \mu_{z_i}\|^2\right] + k\frac{\log m}{m}$$

  - More precise version: see e.g. "X-means" (Pelleg & Moore 2000)

Summary

- K-Means clustering
  - Clusters described as locations (“centers”) in feature space
- Procedure
  - Initialize cluster centers
  - Iterate: assign each data point to its closest cluster center
  - : move cluster centers to minimize mean squared error
- Properties
  - Coordinate descent on MSE criterion
  - Prone to local optima; initialization important
- Out-of-sample data
- Choosing the # of clusters, K
  - Model selection problem; penalize for complexity (BIC, etc.)

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Machine Learning and Data Mining

Clustering (4):
Gaussian Mixtures & EM

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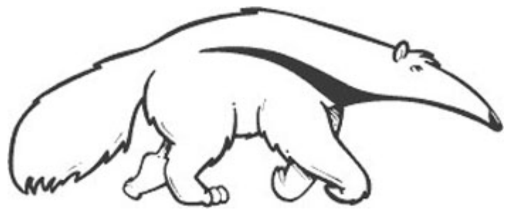

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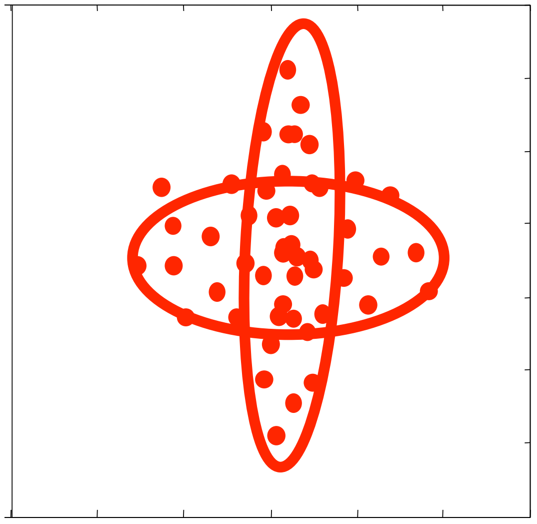
Mixtures of Gaussians

- K-means algorithm
  - Assigned each example to exactly one cluster
  - What if clusters are overlapping?
    - Hard to tell which cluster is right
    - Maybe we should try to remain uncertain
  - Used Euclidean distance
  - What if cluster has a non-circular shape?

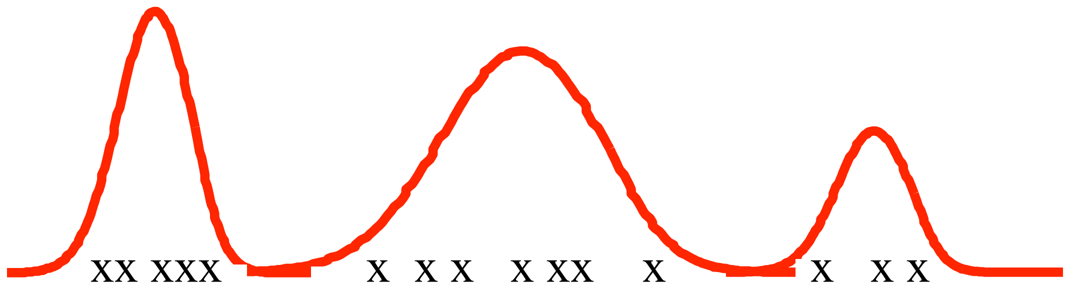
- Gaussian mixture models
  - Clusters modeled as Gaussians
    - Not just by their mean
  - EM algorithm: assign data to cluster with some *probability*
  - Gives probability model of x! ("generative")



Mixtures of Gaussians

- Start with parameters describing each cluster
- Mean μ_c , variance σ_c , "size" π_c
- Probability distribution:

$$p(x) = \sum_c \pi_c \, \mathcal{N}(x \; ; \; \mu_c, \sigma_c)$$



Mixtures of Gaussians

- Start with parameters describing each cluster
- Mean μ_c , variance σ_c , "size" π_c
- Probability distribution: $p(x) = \sum_c \pi_c \, \mathcal{N}(x \; ; \; \mu_c, \sigma_c)$
- Equivalent "latent variable" form:

$$p(z = c) = \pi_c$$

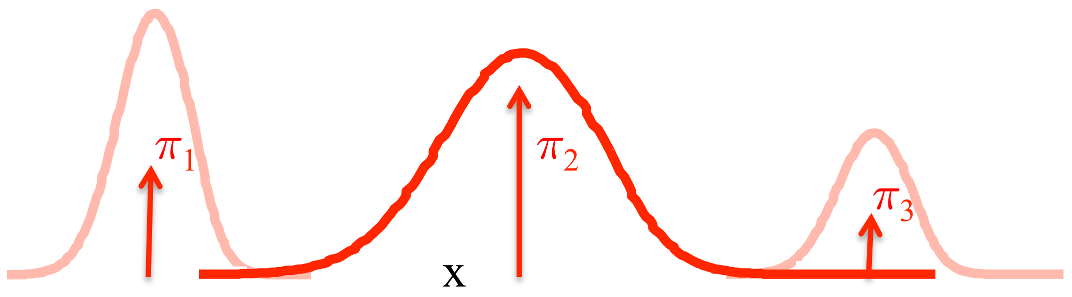
Select a mixture component with probability π

$$p(x|z = c) = \mathcal{N}(x \; ; \; \mu_c, \sigma_c)$$

Sample from that component's Gaussian

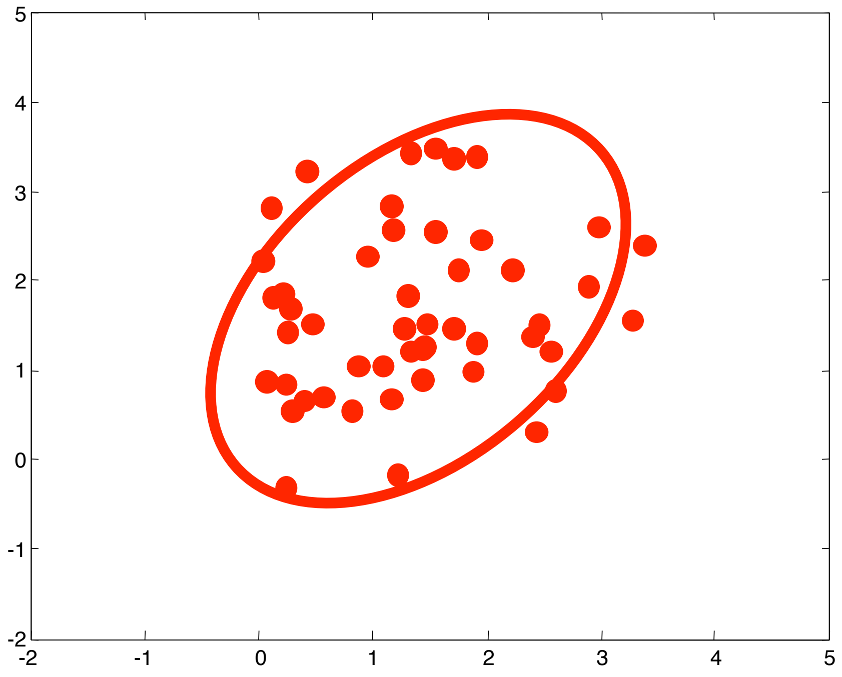
"Latent assignment" z:
we observe x, but z is hidden

p(x) = marginal over x



Multivariate Gaussian models

$$\mathcal{N}(\underline{x}\ ;\ \underline{\mu}, \Sigma) = \frac{1}{(2\pi)^{d/2}} |\Sigma|^{-1/2} \exp\left\{ -\frac{1}{2} (\underline{x} - \underline{\mu})^T \Sigma^{-1} (\underline{x} - \underline{\mu}) \right\}$$



Maximum Likelihood estimates

$$\hat{\mu} = \frac{1}{m} \sum_i x^{(i)}$$

$$\hat{\Sigma} = \frac{1}{m} \sum_i (x^{(i)} - \hat{\mu})^T (x^{(i)} - \hat{\mu})$$

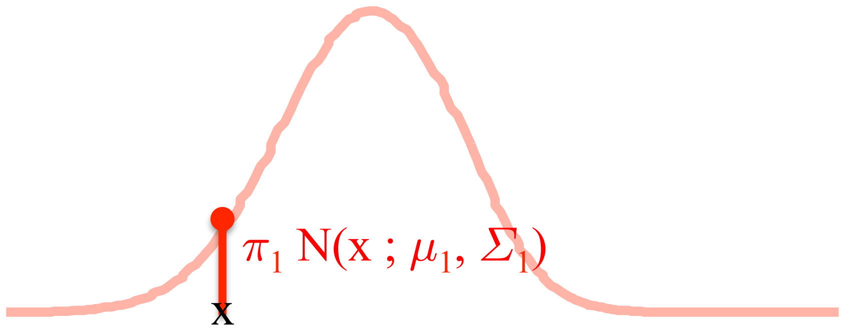
We' ll model each cluster using one of these Gaussian "bells"…

EM Algorithm: E-step

- Start with clusters: Mean μ_c, Covariance Σ_c, "size" π_c

- E-step ("Expectation")
  - For each datum (example) x_i,
  - Compute "r_{ic}", the probability that it belongs to cluster c
    - Compute its probability under model c
    - Normalize to sum to one (over clusters c)

$$r_{ic} = \frac{\pi_c \mathcal{N}(x_i \; ; \; \mu_c, \Sigma_c)}{\sum_{c'} \pi_{c'} \mathcal{N}(x_i \; ; \; \mu_{c'}, \Sigma_{c'})}$$



EM Algorithm: E-step

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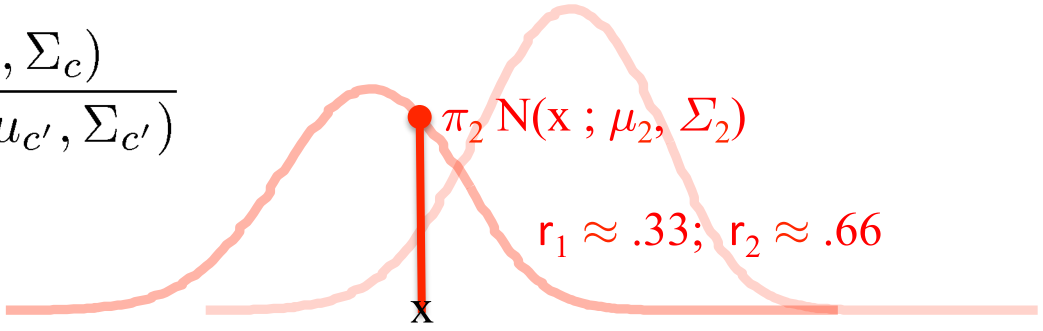

π_2 N(x ; μ_2, Σ_2)
$r_1 \approx .33$; $r_2 \approx .66$
x

  - If x_i is very likely under the cth Gaussian, it gets high weight
  - Denominator just makes r's sum to one

EM Algorithm: M-step

- Start with assignment probabilities r_{ic}
- Update parameters: mean μ_c, Covariance Σ_c, "size" π_c

- M-step ("Maximization")
  - For each cluster (Gaussian) z = c,
  - Update its parameters using the (weighted) data points

$$m_c = \sum_i r_{ic}$$

Total responsibility allocated to cluster c

$$\pi_c = \frac{m_c}{m}$$

Fraction of total assigned to cluster c

$$\mu_c = \frac{1}{m_c} \sum_i r_{ic} x^{(i)}$$

$$\Sigma_c = \frac{1}{m_c} \sum_i r_{ic} (x^{(i)} - \mu_c)^T (x^{(i)} - \mu_c)$$

Weighted mean of assigned data

Weighted covariance of assigned data
(use new weighted means here)

Expectation-Maximization

- Each step increases the log-likelihood of our model

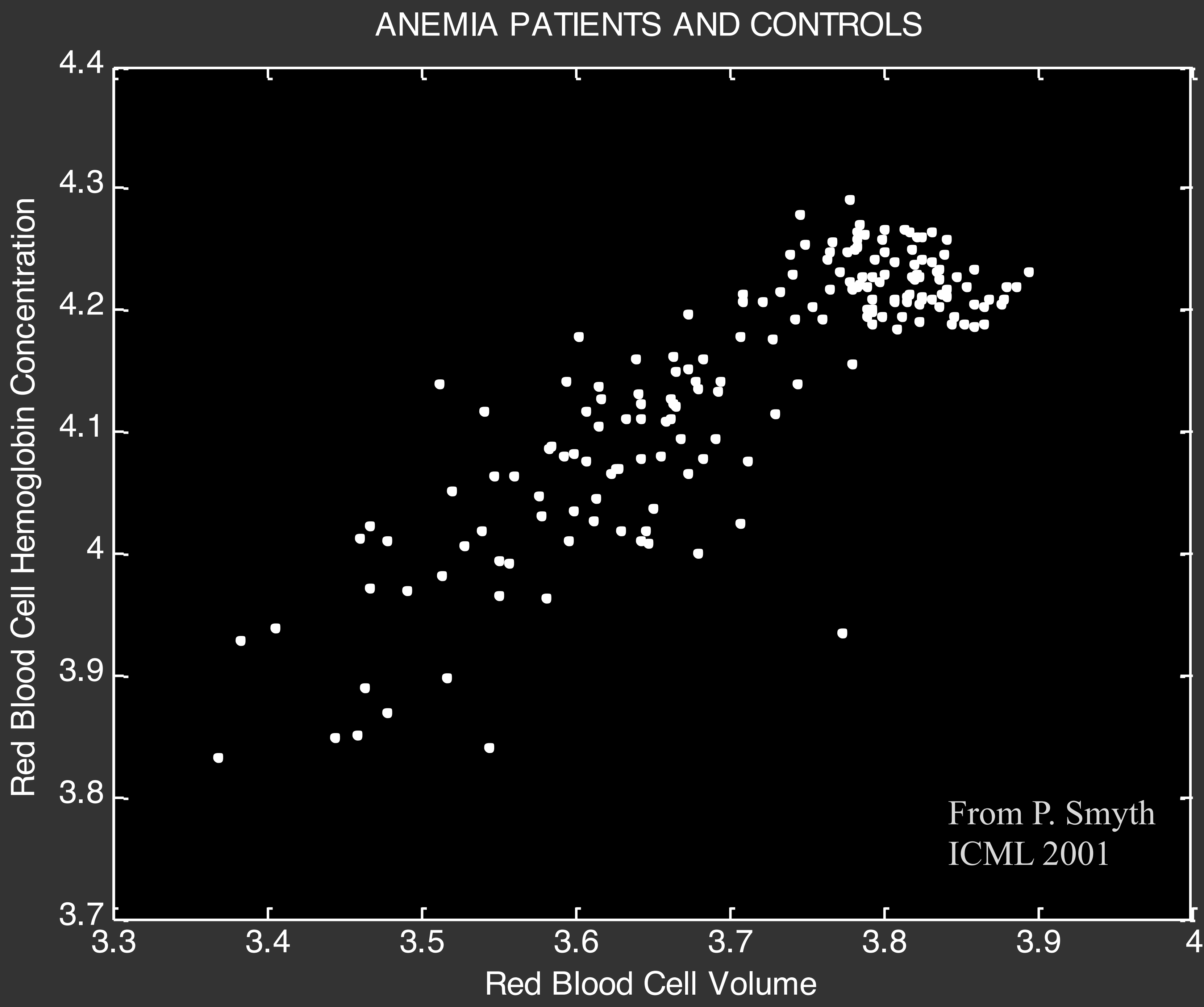
$$\log p(\underline{X}) = \sum_i \log \left[\sum_c \pi_c \, \mathcal{N}(x_i \; ; \; \mu_c, \Sigma_c) \right]$$

(we won't derive this here, though)

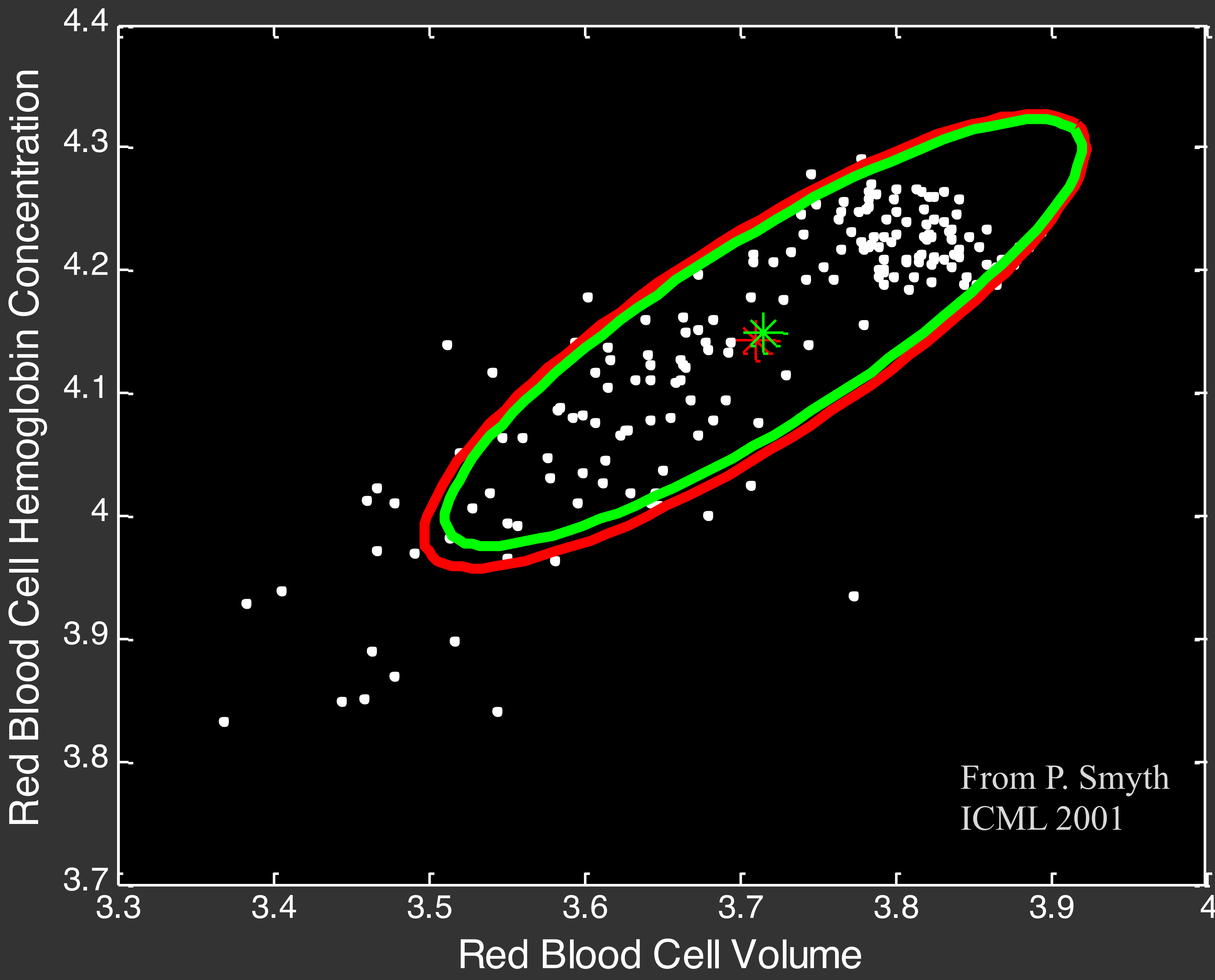
- Iterate until convergence
  - Convergence guaranteed – another ascent method
  - Local optima: initialization often important

- What should we do
  - If we want to choose a single cluster for an "answer"?
  - With new data we didn't see during training?

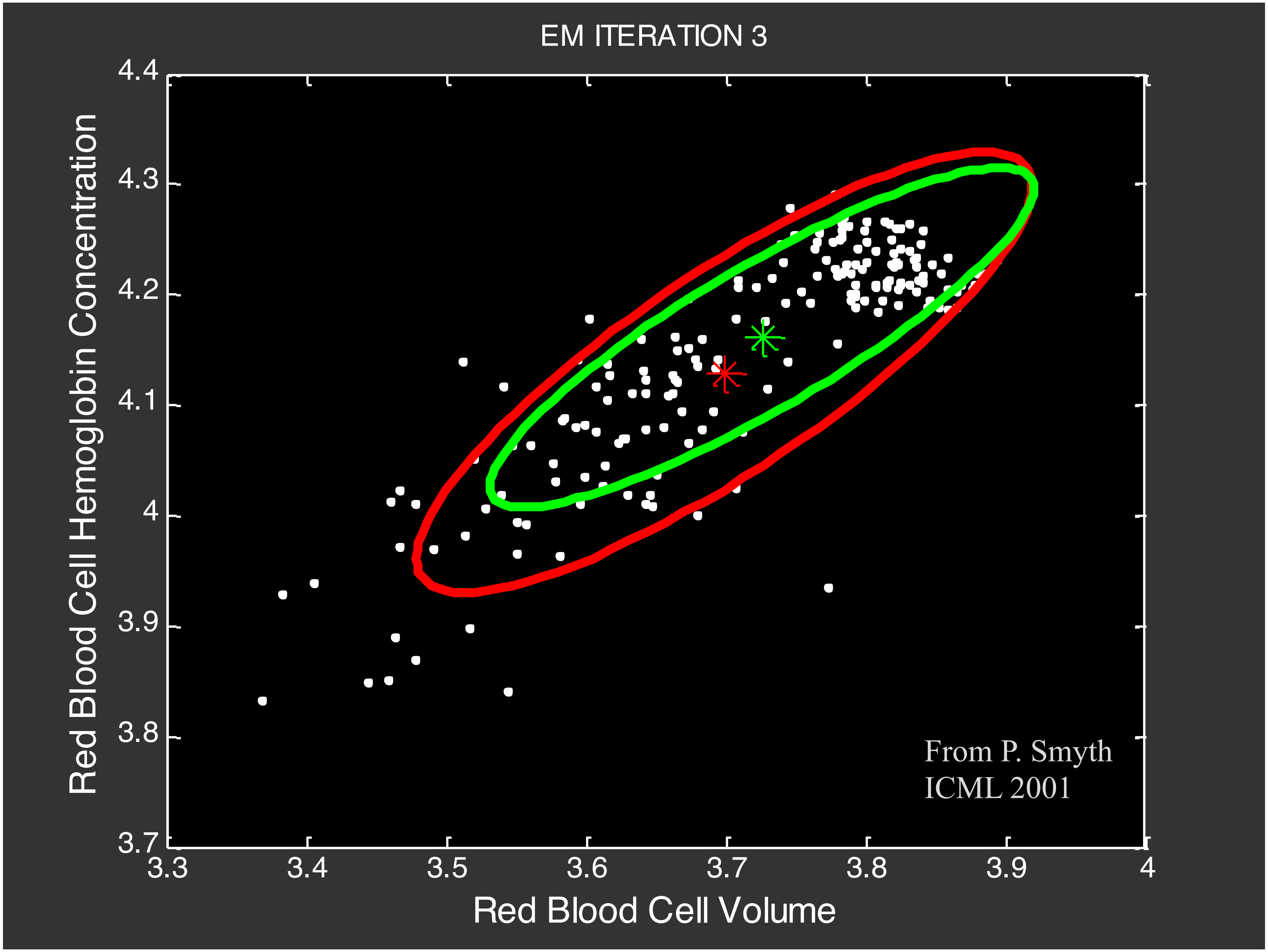
- Choosing the number of clusters
  - Can use penalized likelihood of training data (like k-means
  - True probability model: can use log-likelihood of test data, log p(x')

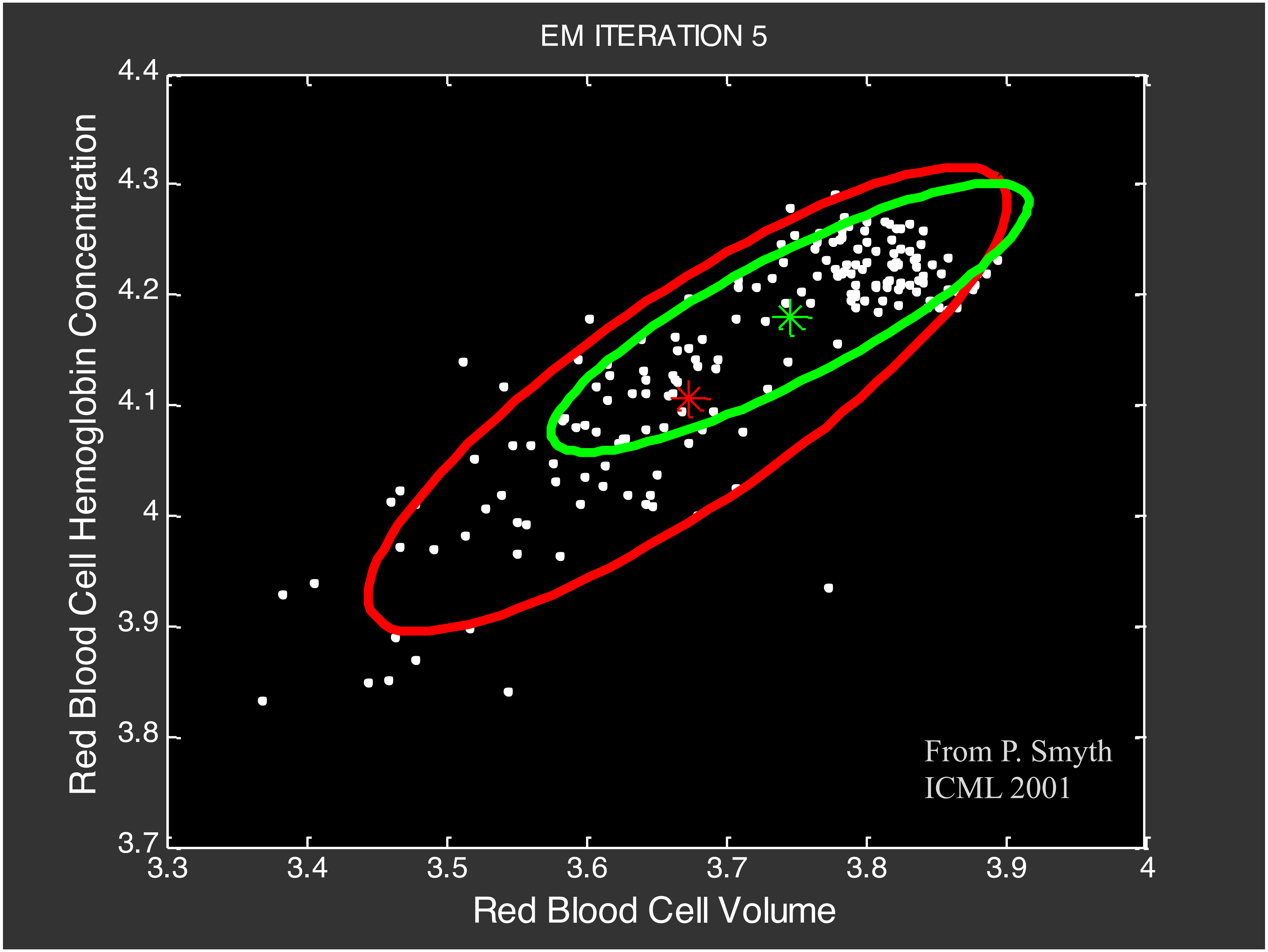

ANEMIA PATIENTS AND CONTROLS
Red Blood Cell Hemoglobin Concentration
4.4
4.3
4.2
4.1
4
3.9
3.8
3.7
3.3
3.4
3.5
3.6
3.7
3.8
3.9
4
Red Blood Cell Volume
From P. Smyth
ICML 2001

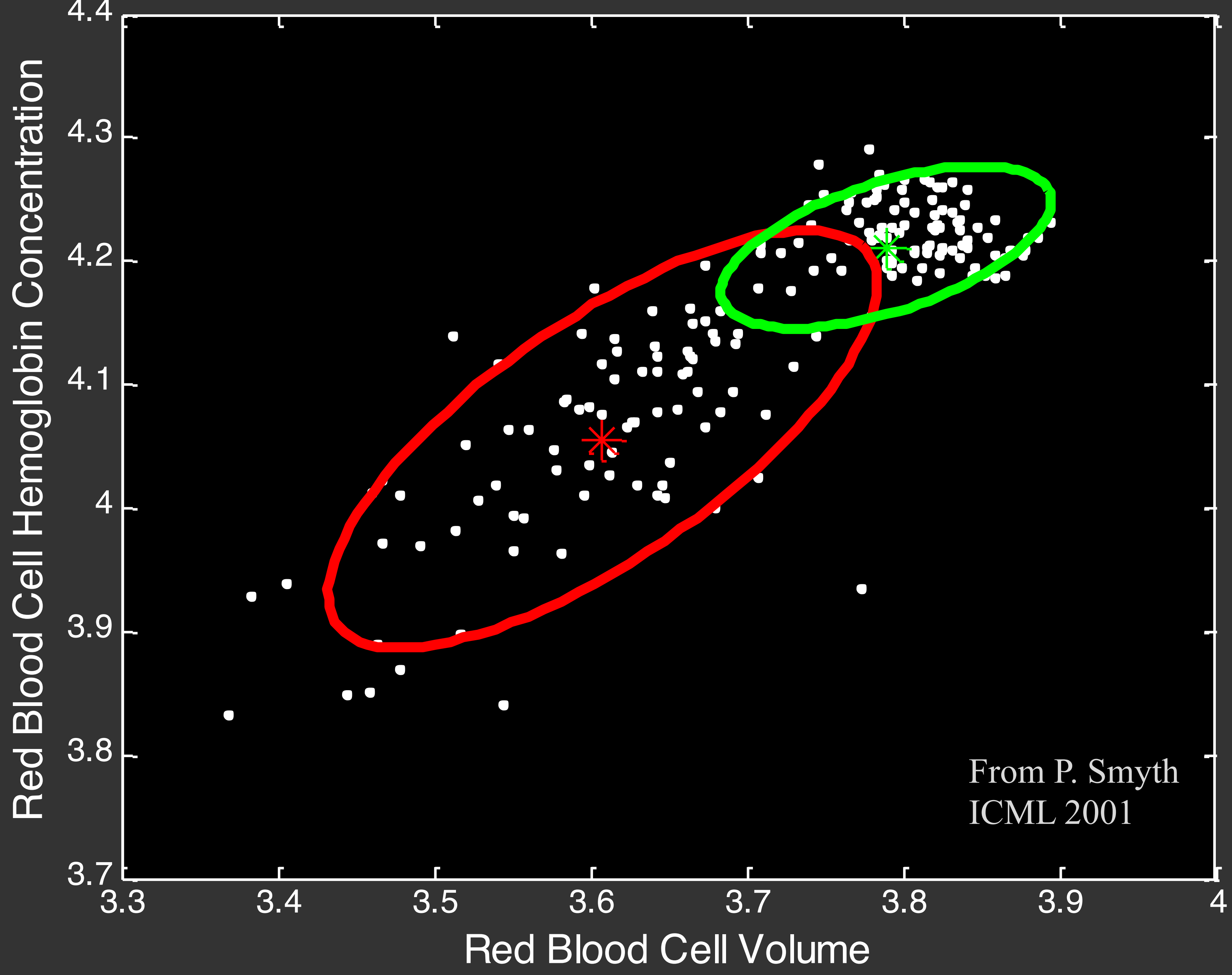
EM ITERATION 1

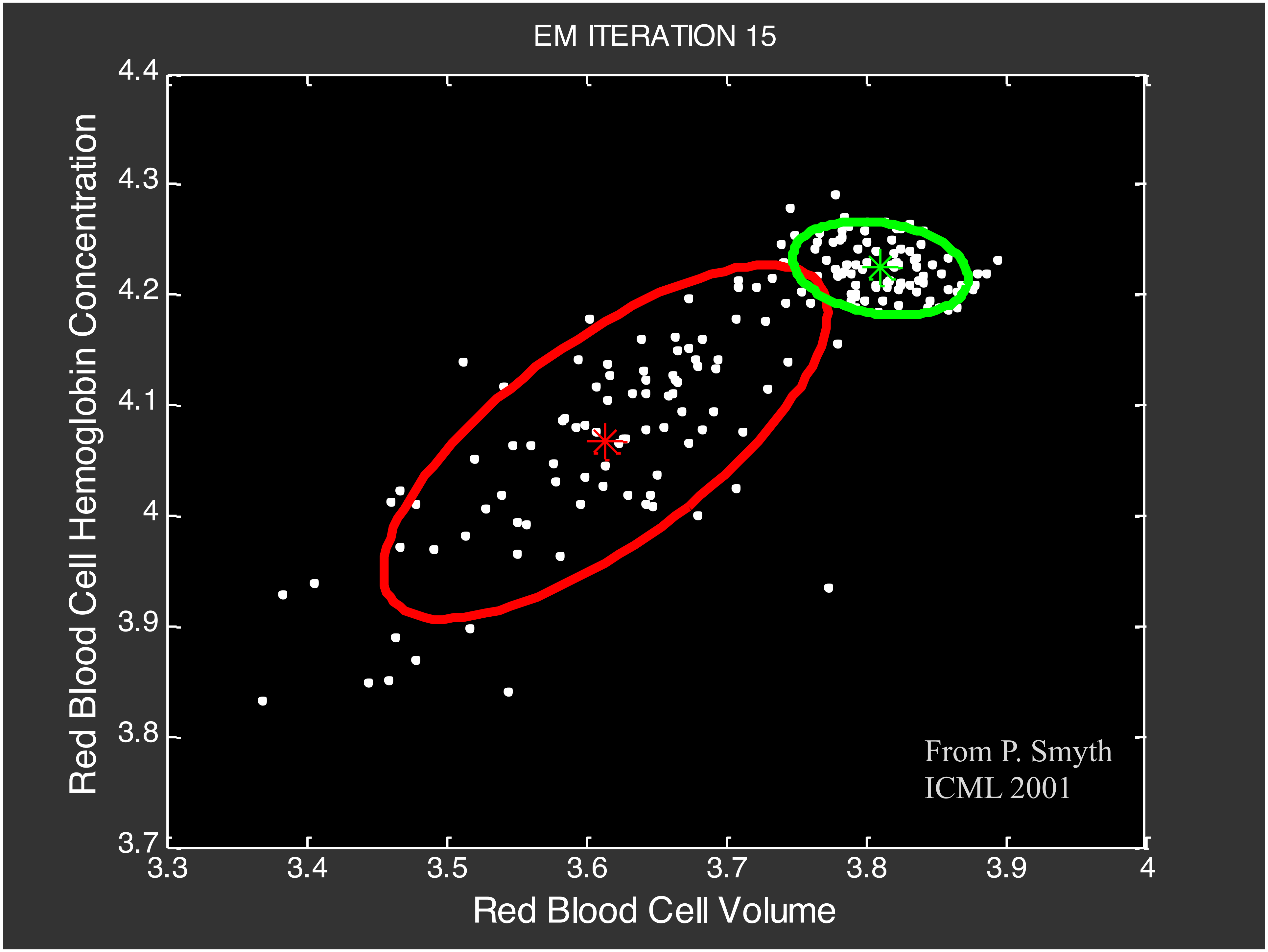


From P. Smyth
ICML 2001

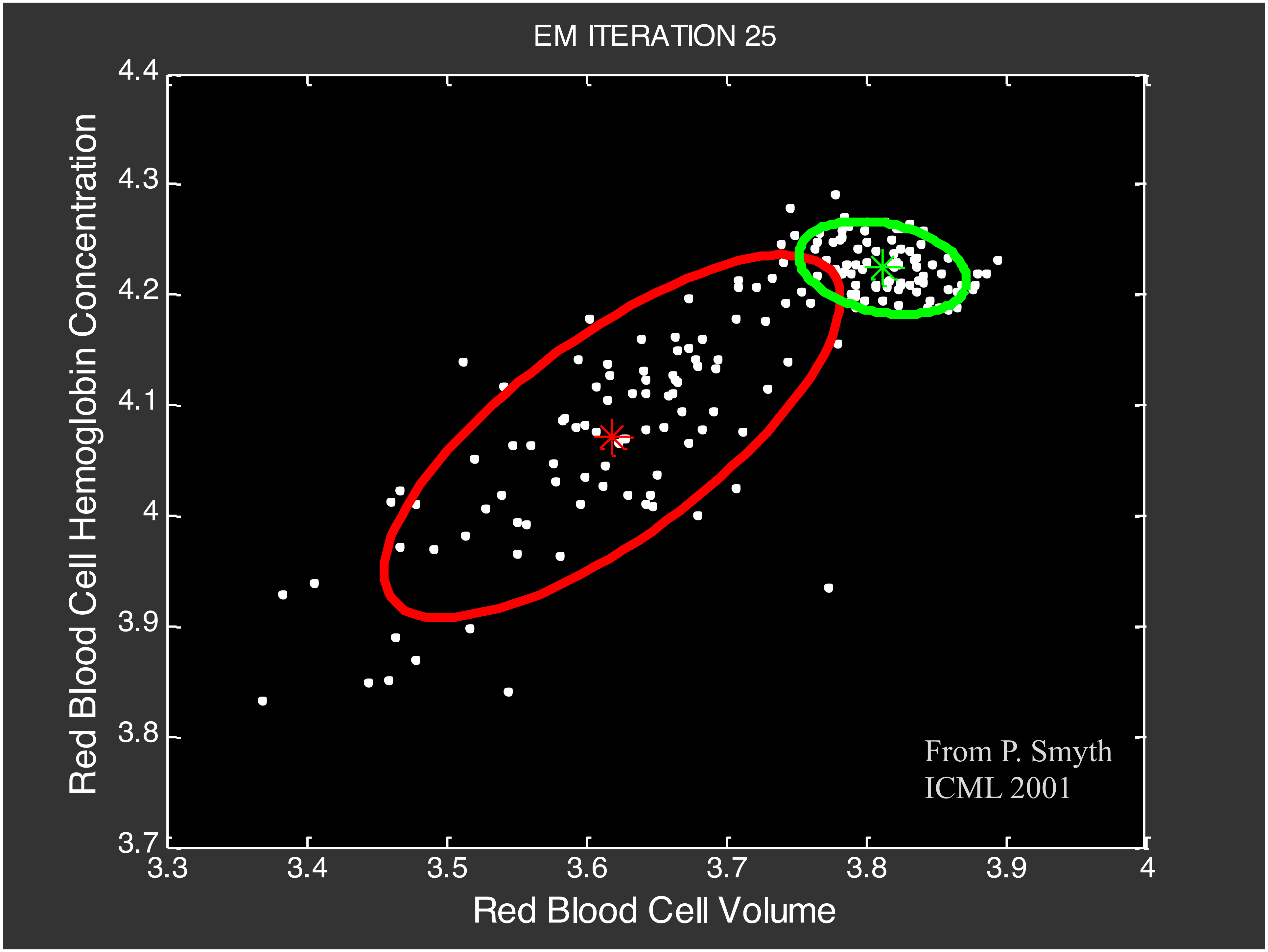

EM ITERATION 3
Red Blood Cell Hemoglobin Concentration
Red Blood Cell Volume
4.4
4.3
4.2
4.1
4
3.9
3.8
3.7
3.3
3.4
3.5
3.6
3.7
3.8
3.9
4
From P. Smyth
ICML 2001


EM ITERATION 5
Red Blood Cell Hemoglobin Concentration
Red Blood Cell Volume
3.7
3.8
3.9
4
4.1
4.2
4.3
4.4
3.3
3.4
3.5
3.6
3.7
3.8
3.9
4
From P. Smyth
ICML 2001

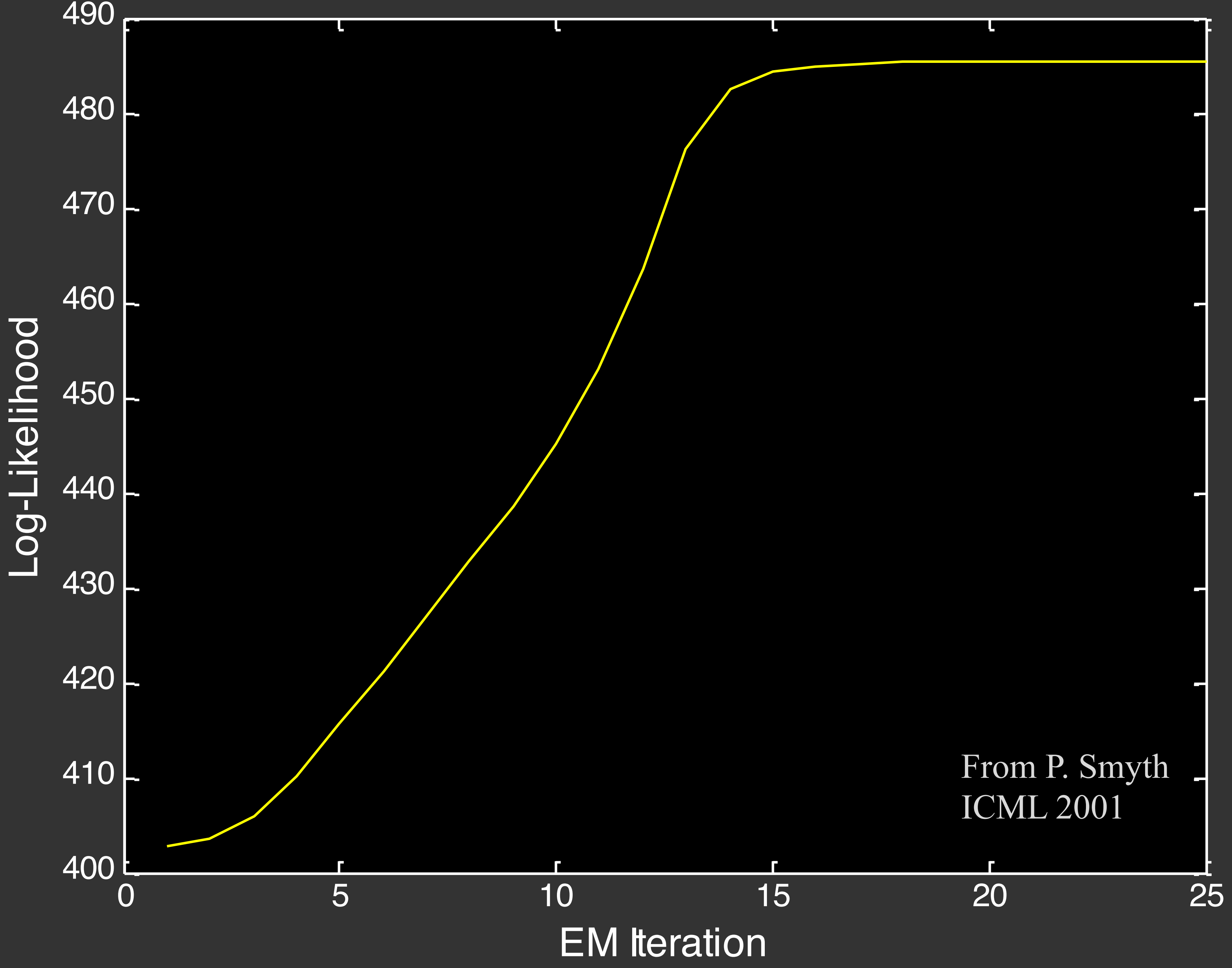

EM ITERATION 10
4.4
4.3
4.2
4.1
4
3.9
3.8
3.7
3.3
3.4
3.5
3.6
3.7
3.8
3.9
4
Red Blood Cell Hemoglobin Concentration
Red Blood Cell Volume
From P. Smyth
ICML 2001



EM ITERATION 15
Red Blood Cell Hemoglobin Concentration
Red Blood Cell Volume
3.3
3.4
3.5
3.6
3.7
3.8
3.9
4
3.7
3.8
3.9
4
4.1
4.2
4.3
4.4
From P. Smyth
ICML 2001


EM ITERATION 25
Red Blood Cell Hemoglobin Concentration
Red Blood Cell Volume
4.4
4.3
4.2
4.1
4
3.9
3.8
3.7
3.3
3.4
3.5
3.6
3.7
3.8
3.9
4
From P. Smyth
ICML 2001

LOG-LIKELIHOOD AS A FUNCTION OF EM ITERATIONS



EM and missing data

- EM is a general framework for partially observed data
  - "Complete data" xi, zi – features and assignments
  - Assignments zi are missing (unobserved)

- EM corresponds to
  - Computing the distribution over all zi given the parameters
  - Maximizing the "expected complete" log likelihood
  - GMMs = plug in "soft assignments", but not always so easy

- Alternatives: Stochastic EM, Hard EM
  - Instead of expectations, just sample the zi or choose best (often easier)
  - Called "imputing" the values of z
  - Hard EM: similar to EM, but less "smooth", more local minima
  - Stochastic EM: similar to EM, but with extra randomness
    - Not obvious when it has converged

Summary

- Gaussian mixture models
  - Flexible class of probability distributions
  - Explain variation with hidden groupings or clusters of data
  - Latent "membership" $z^{(i)}$
  - Feature values $x^{(i)}$ are Gaussian given $z^{(i)}$
- Expectation-Maximization
  - Compute soft membership probabilities, "responsibility" r_{ic}
  - Update mixture component parameters given soft memberships
  - Ascent on log-likelihood: convergent, but local optima
- Selecting the number of clusters
  - Penalized likelihood or validation data likelihood

Gibbs sampling for clustering

- Another technique for inferring uncertain cluster assignments
  - K-means: take the best assignment
  - EM: assign “partially”
  - Stochastic EM: sample assignment
  - All: choose best cluster descriptions given assignments
- Gibbs sampling (“Markov chain Monte Carlo”)
  - Assign randomly, probability equal to EM’s weight
  - *Sample* a cluster description given assignment
  - Requires a probability model over cluster parameters
- This doesn’t really find the “best” clustering
  - It eventually samples almost all “good” clusterings
  - Converges “in probability”, randomness helps us explore configurations
  - Also tells us about uncertainty of clustering
  - Disadvantage: not obvious when “done”

“Infinite” mixture models

- How many clusters are there?

- Gibbs sampling has an interesting solution
  - Write a distribution over k, the # of clusters
  - Sample k also

- Can do our sampling sequentially
  - Draw each zi given all the others
  - Instead of sampling cluster parameters, marginalize them
  - Defines a distribution over groupings of data
- Now, for each zi, sample
  - Join an existing cluster? Or, join a new cluster?
- What are these probabilities?
  - “Dirichlet process” mixture models

Parametric and Nonparametric Models

- Every model has some parameters
  - "The stuff you have to store to make your prediction"
  - Logistic regression: weights
  - Decision tree: feature to split, value at each level
  - Gaussian mixture model: means, covariances, sizes
- Parametric vs Nonparametric models
  - Parametric: fixed # of parameters
  - Nonparametric: # of parameters grows with more data
- What type are
  - Logistic regression?
  - Nearest neighbor prediction?
  - Decision trees?
  - Decision trees of depth < 3?
  - Gaussian mixture model?

Summary

- Clustering algorithms
  - Agglomerative clustering
  - K-means
  - Expectation-Maximization

Open questions for each application:

- What does it mean to be “close” or “similar”?
  - Depends on your particular problem…
- “Local” versus “global” notions of simliarity
  - Former is easy, but we usually want the latter…
- Is it better to “understand” the data itself (unsupervised learning), to focus just on the final task (supervised learning), or both?
- Do we need a generative model? Out-of-sample assignments?