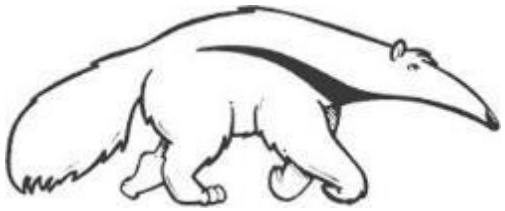
Machine Learning and Data Mining

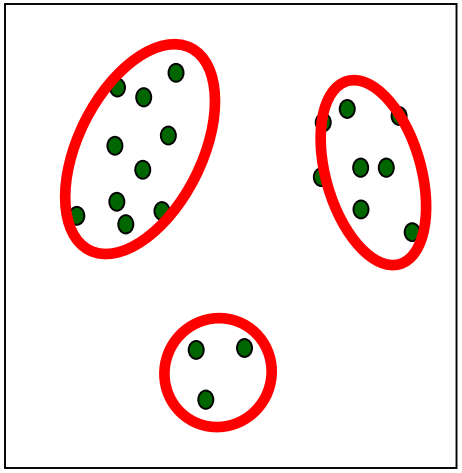
Clustering (1): Basics

Kalev Kask



Unsupervised learning

- Supervised learning
  - Predict target value (“y”) given features (“x”)



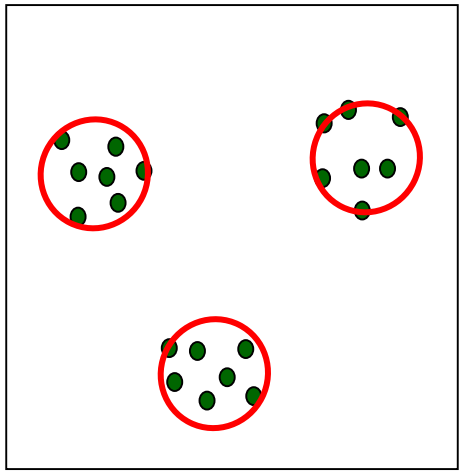
- Unsupervised learning
  - Understand patterns of data (just “x”)
  - Useful for many reasons
    - Data mining (“explain”)
    - Missing data values (“impute”)
    - Representation (feature generation or selection)

- One example: *clustering*
  - Describe data by discrete “groups” with some characteristics

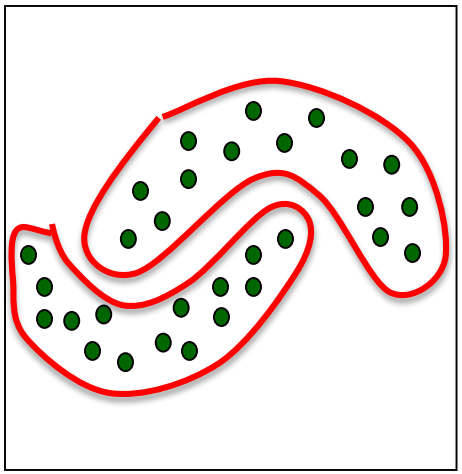
Clustering

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

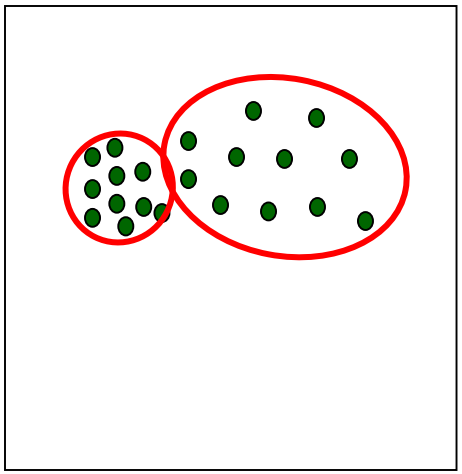
- Examples



Location



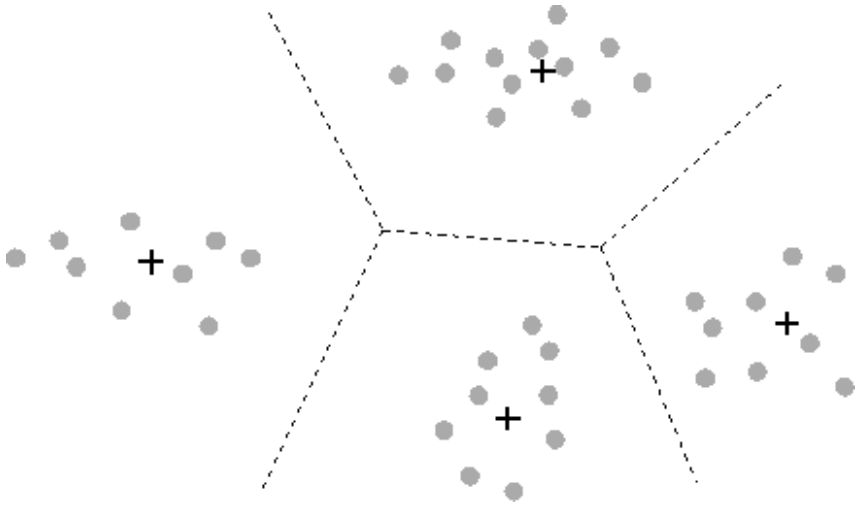
Shape

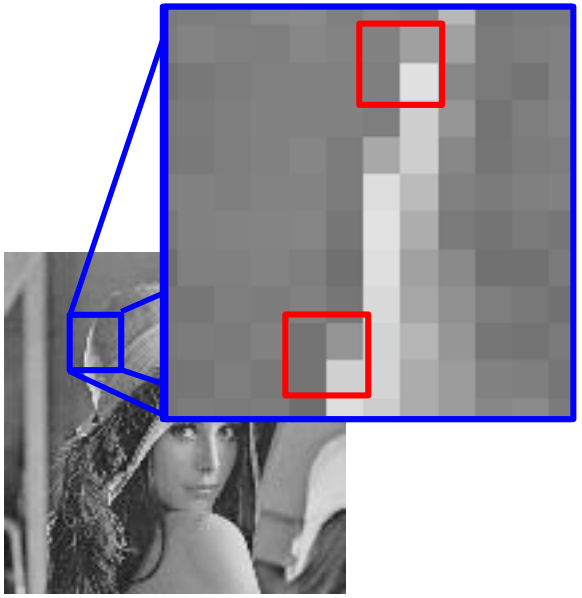


Density

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)

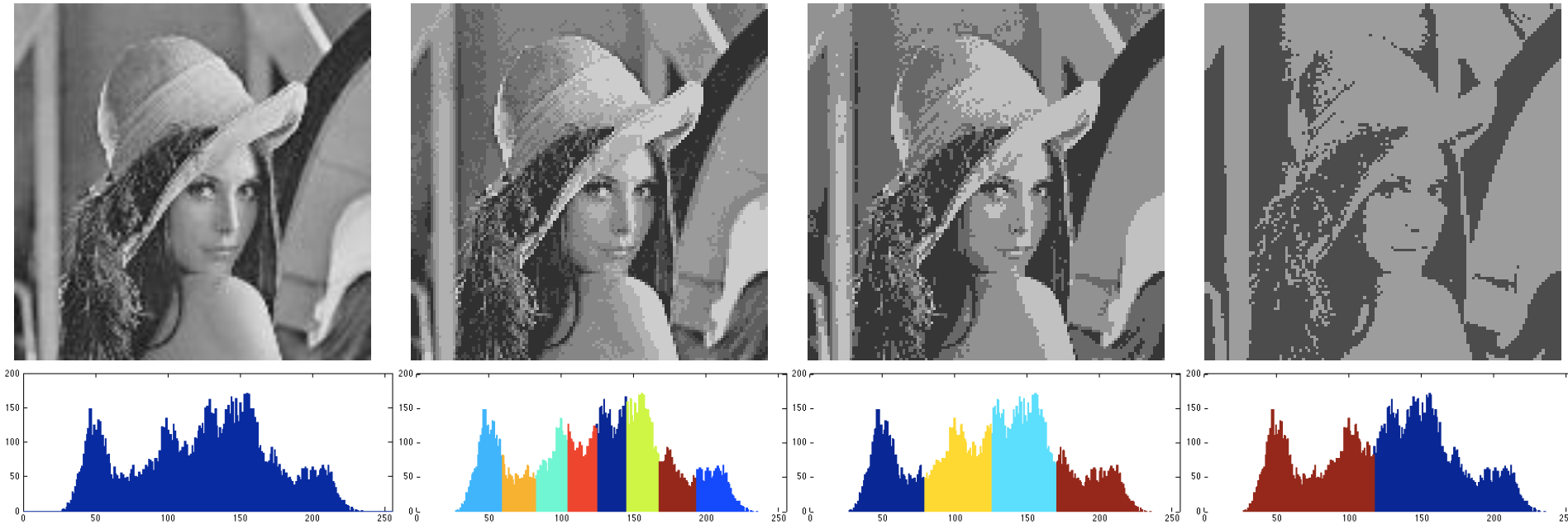




Clustering and Data Compression

- 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)

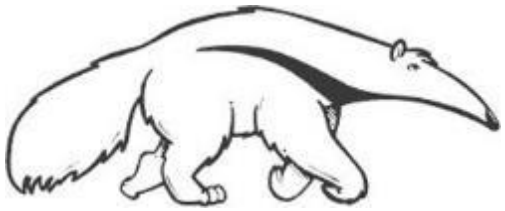
- Example in 1D: cluster pixels’ grayscale values



Machine Learning and Data Mining

Clustering (2):
Hierarchical Agglomerative Clustering

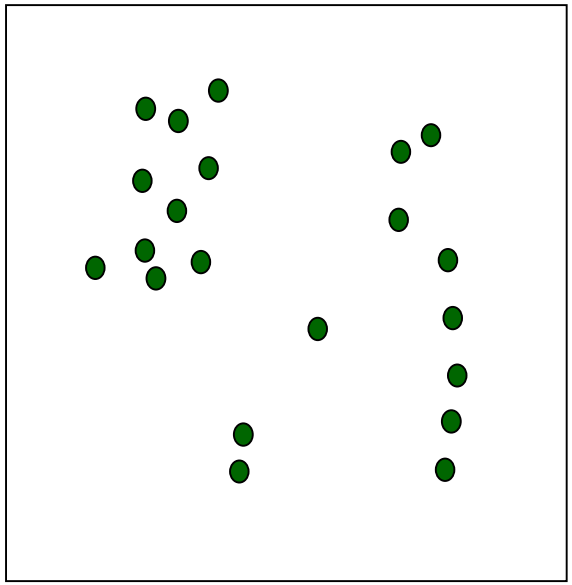
Kalev Kask



Hierarchical Agglomerative Clustering

Initially, every datum is a cluster

Data:



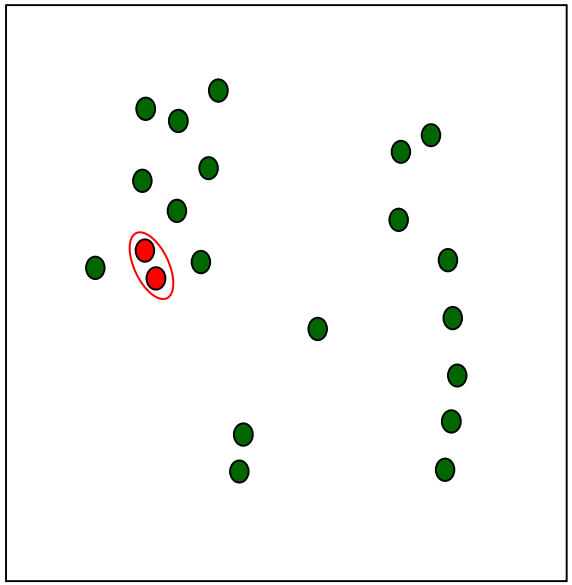
- A simple clustering algorithm
- Define a distance (or dissimilarity) between clusters (we'll return to this)
- Initialize: every example is a cluster
- Iterate:
  - Compute distances between all clusters (store for efficiency)
  - Merge two closest clusters
- Save both clustering and *sequence* of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

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

Iteration 1

Builds up a sequence of clusters (“hierarchical”)

Data:



Dendrogram:

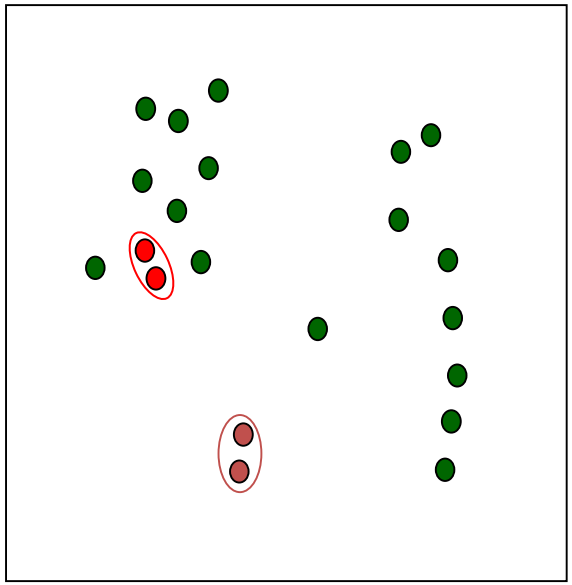
Height of the join indicates dissimilarity

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

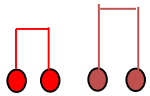
Iteration 2

Builds up a sequence of clusters (“hierarchical”)

Data:



Dendrogram:



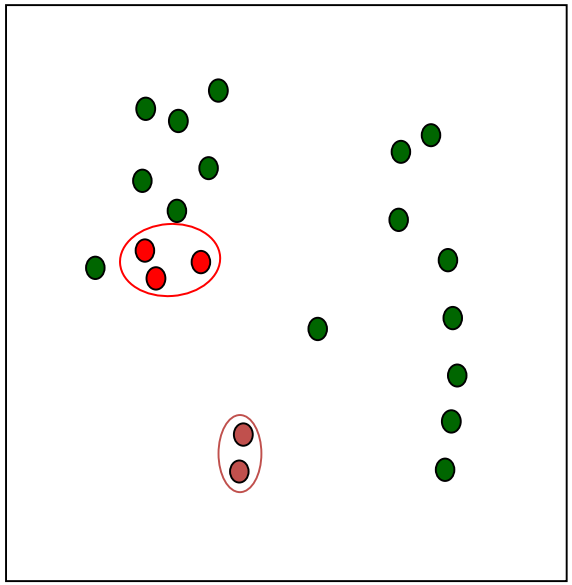
Height of the join indicates dissimilarity

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

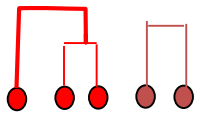
Iteration 3

Builds up a sequence of clusters (“hierarchical”)

Data:



Dendrogram:



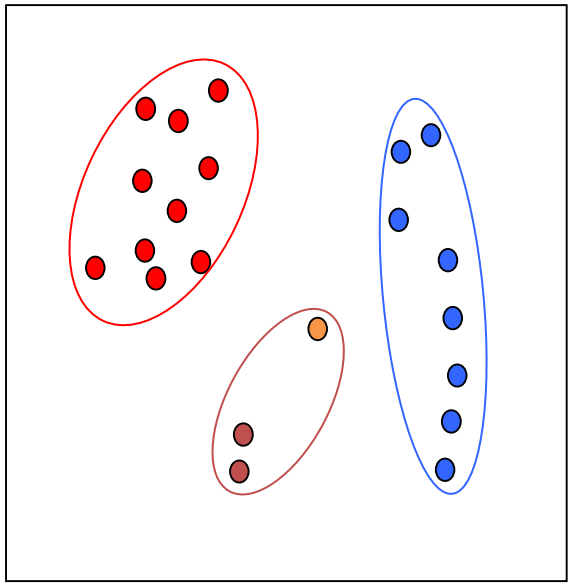
Height of the join indicates dissimilarity

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

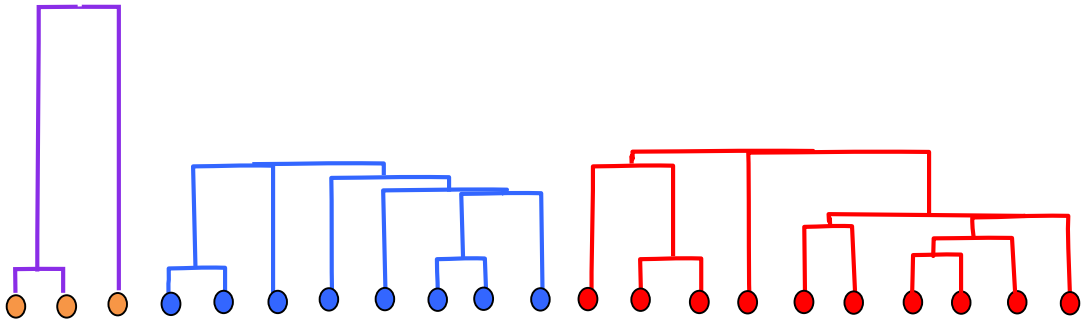
Iteration m-3

Builds up a sequence of clusters (“hierarchical”)

Data:



Dendrogram:



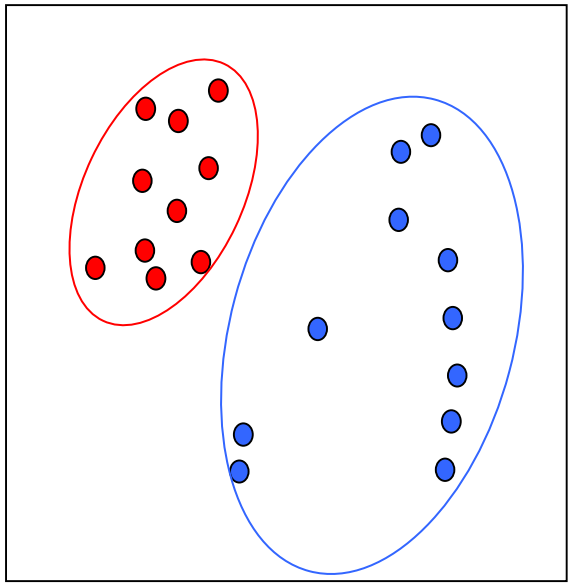
In matlab: “linkage” function (stats toolbox)
In mltools: “agglomerative”

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

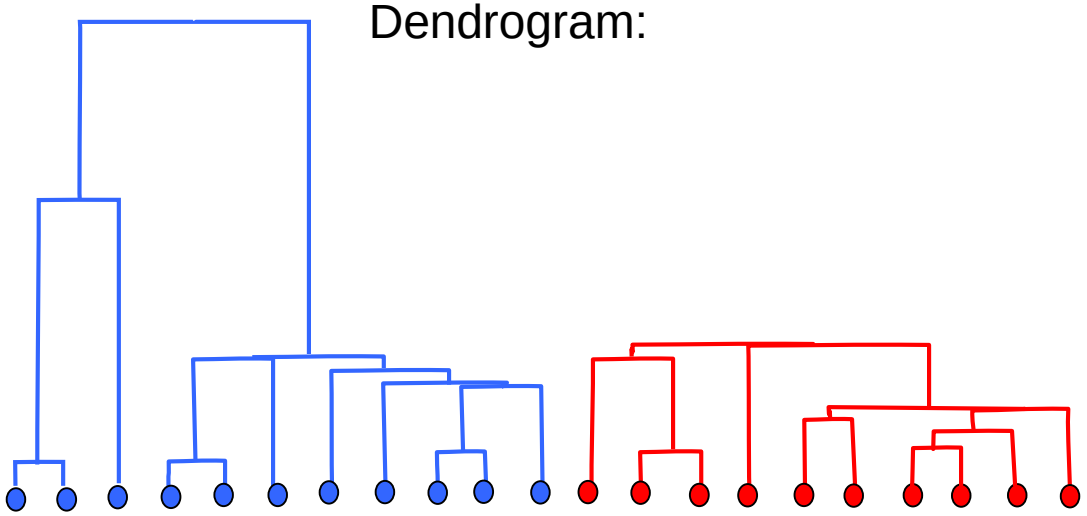
Iteration m-2

Builds up a sequence of clusters (“hierarchical”)

Data:



Dendrogram:



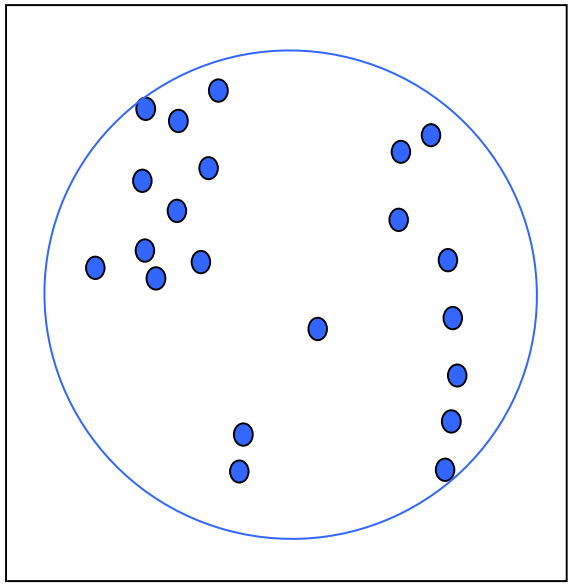
In matlab: “linkage” function (stats toolbox)
In mltools: “agglomerative”

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

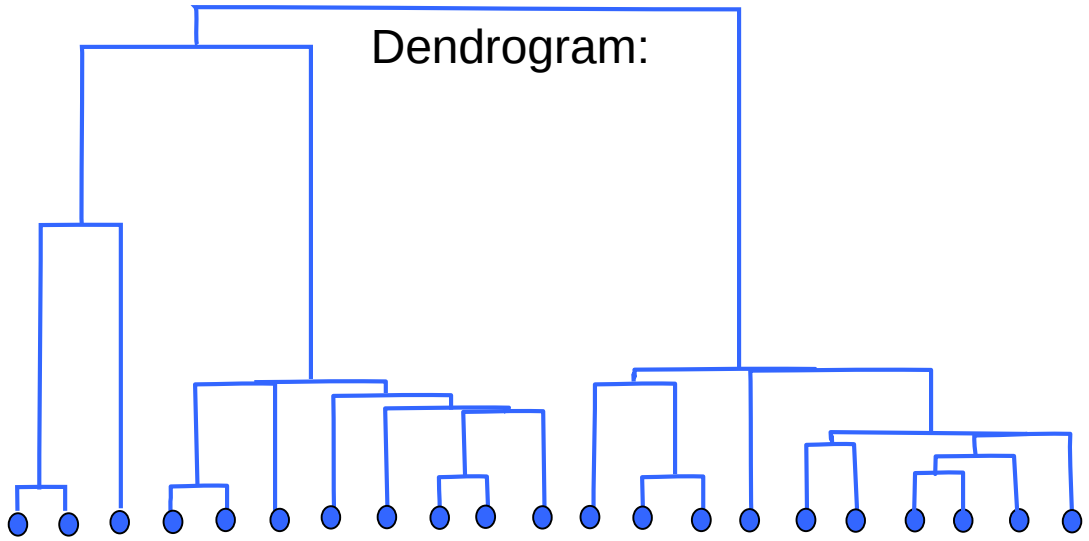
Iteration m-1

Builds up a sequence of clusters (“hierarchical”)

Data:



Dendrogram:



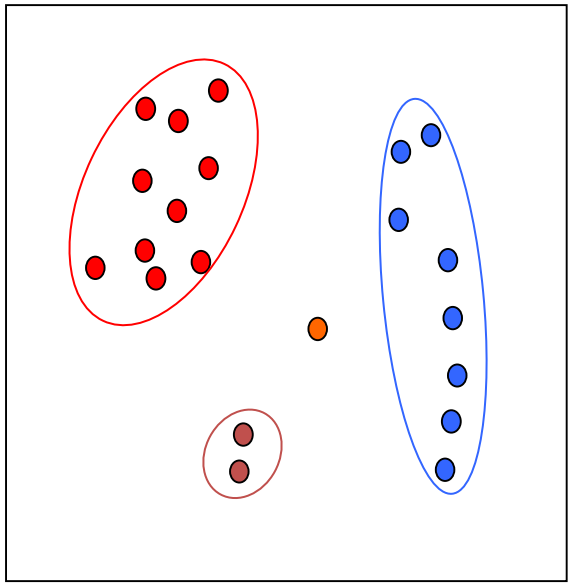
In matlab: “linkage” function (stats toolbox)
In mltools: “agglomerative”

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

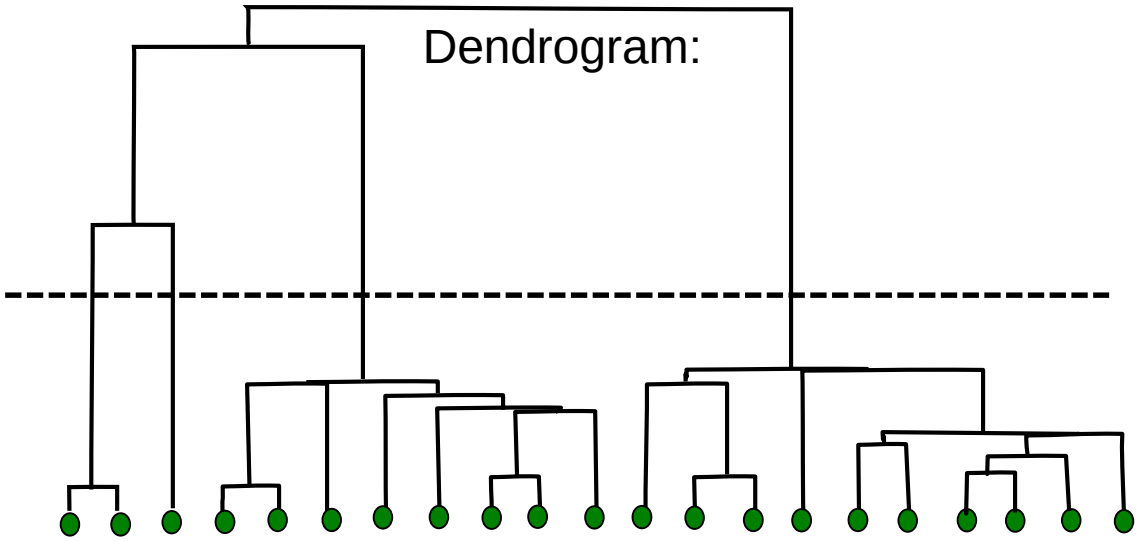
From dendrogram to clusters

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

Data:



Dendrogram:

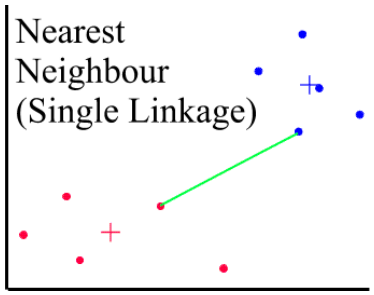


In matlab: "linkage" function (stats toolbox)
In mltools: "agglomerative"

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

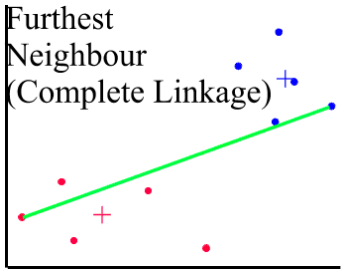
Cluster distances

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



produces minimal spanning tree.

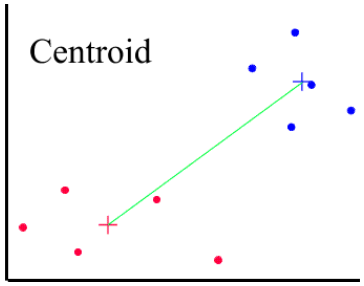
$$D_{\max}(C_i, C_j) = \max_{x \in C_i,\ y \in C_j} |x - y|^2$$



avoids elongated clusters.

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

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



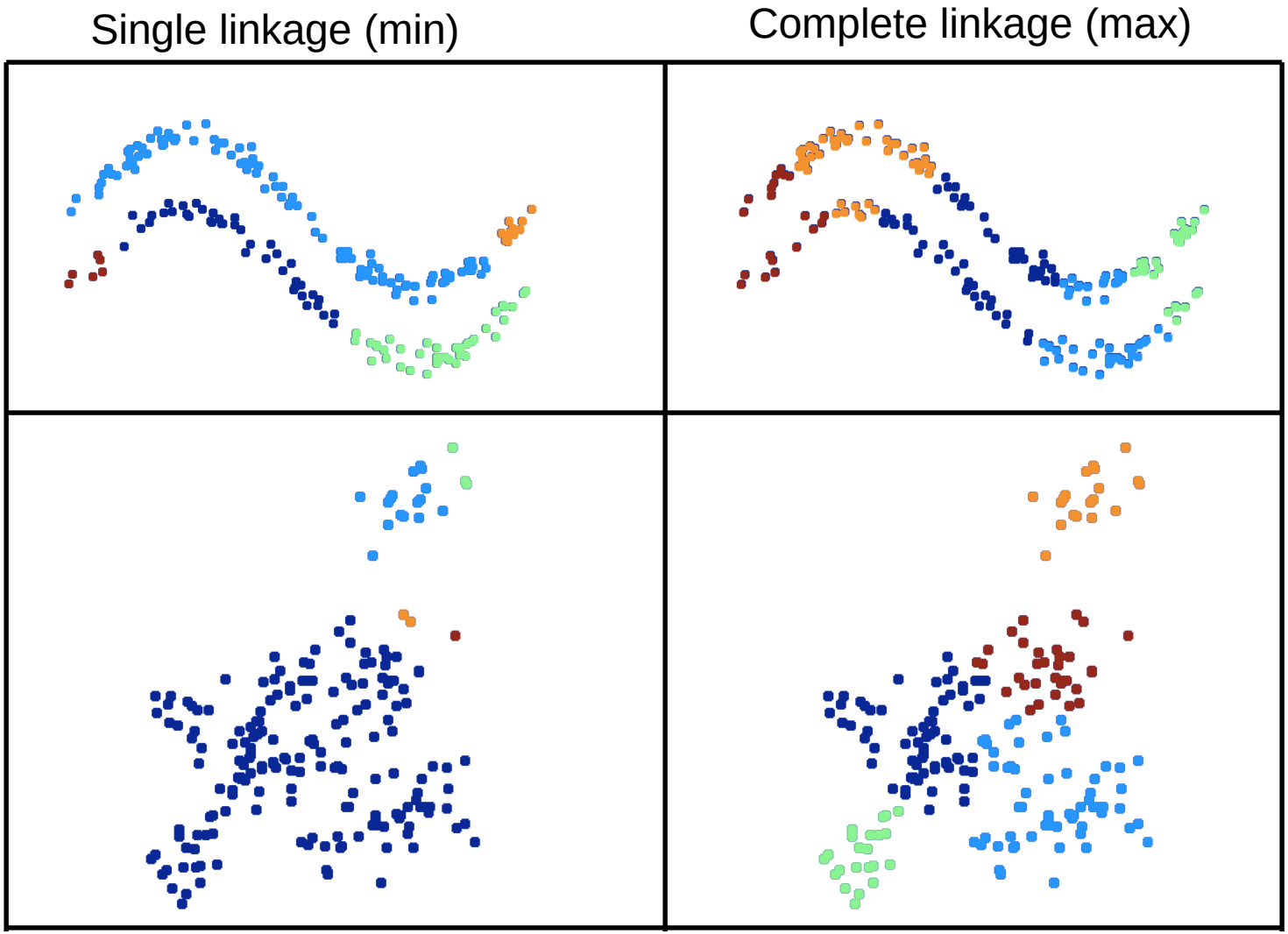
Need:

D(A,C) → D(A+B,C)

D(B,C) →

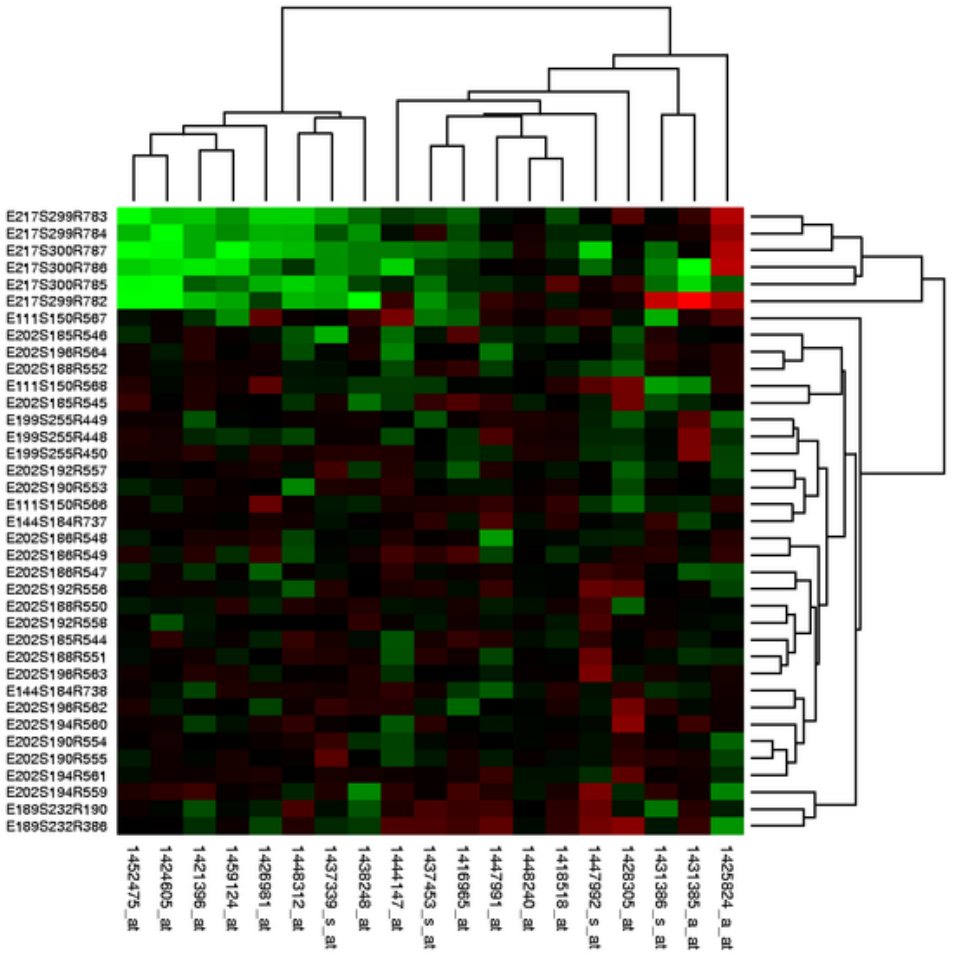
Cluster distances

- 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)

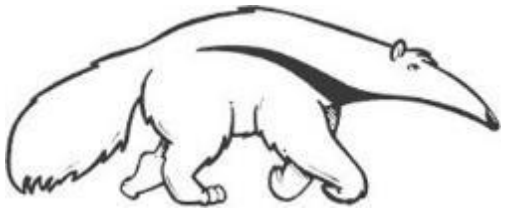
Summary

- 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

Machine Learning and Data Mining

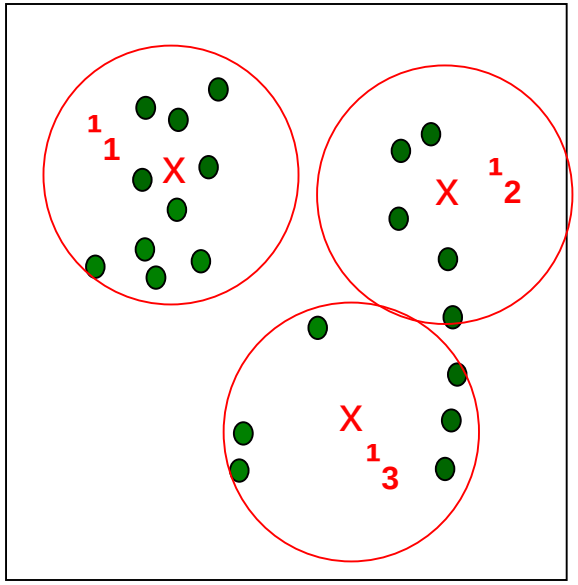
Clustering (3):
k-Means Clustering

Kalev Kask



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

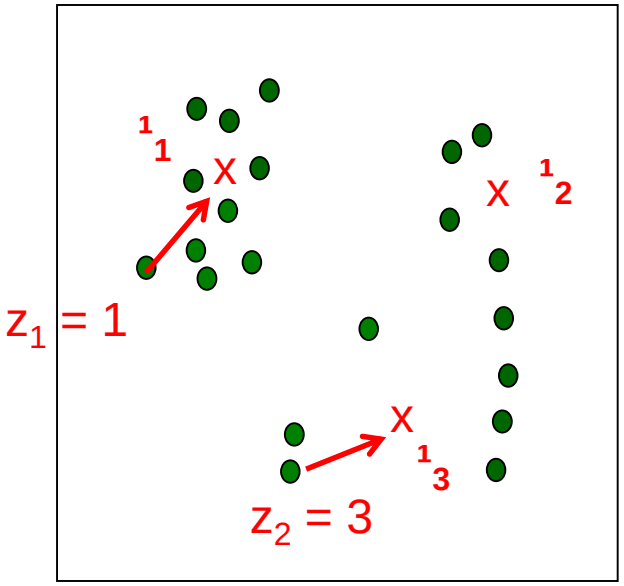
Each cluster c "described" by a center ^1_c

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 i^{th} example: z_i 2 1..K

Matlab: "kmeans" (stats toolbox)

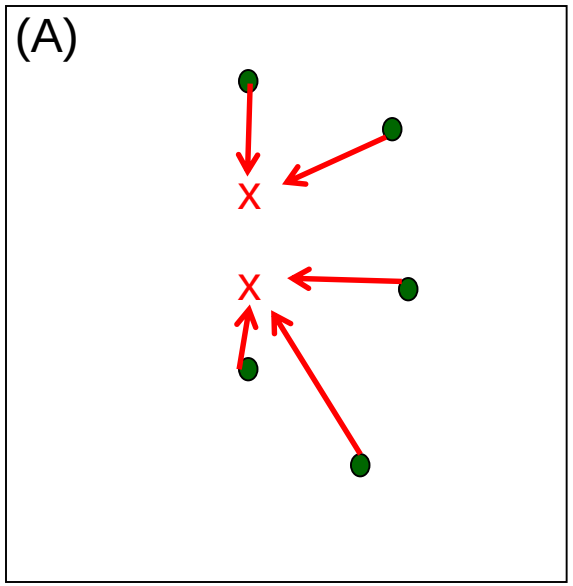
K-Means Clustering

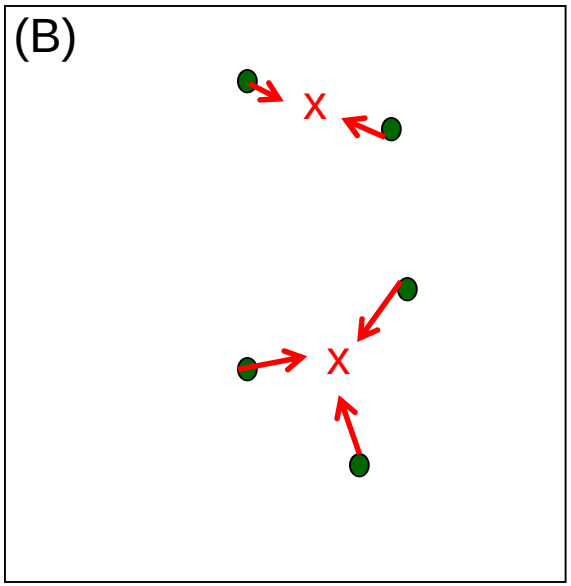
- Iterate until convergence:
  - (A) For each datum, find the closest cluster

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

  - (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

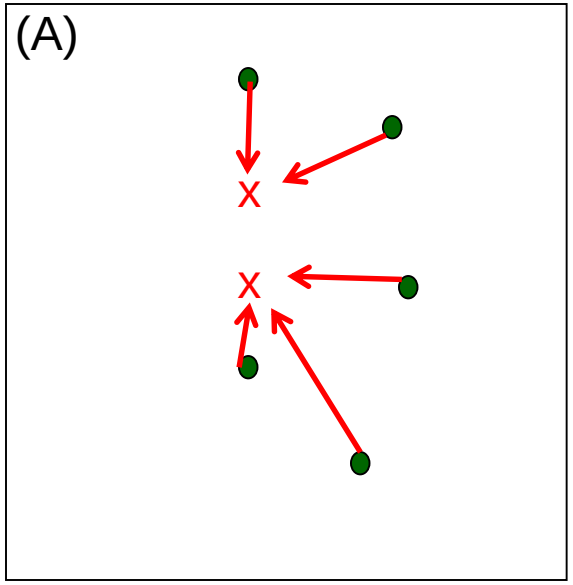
- Optimizing the cost function:

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

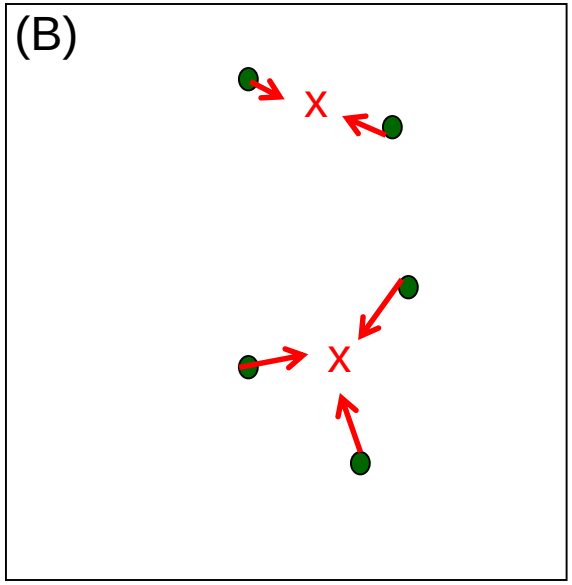
- Coordinate descent:

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 $^1{}_c$



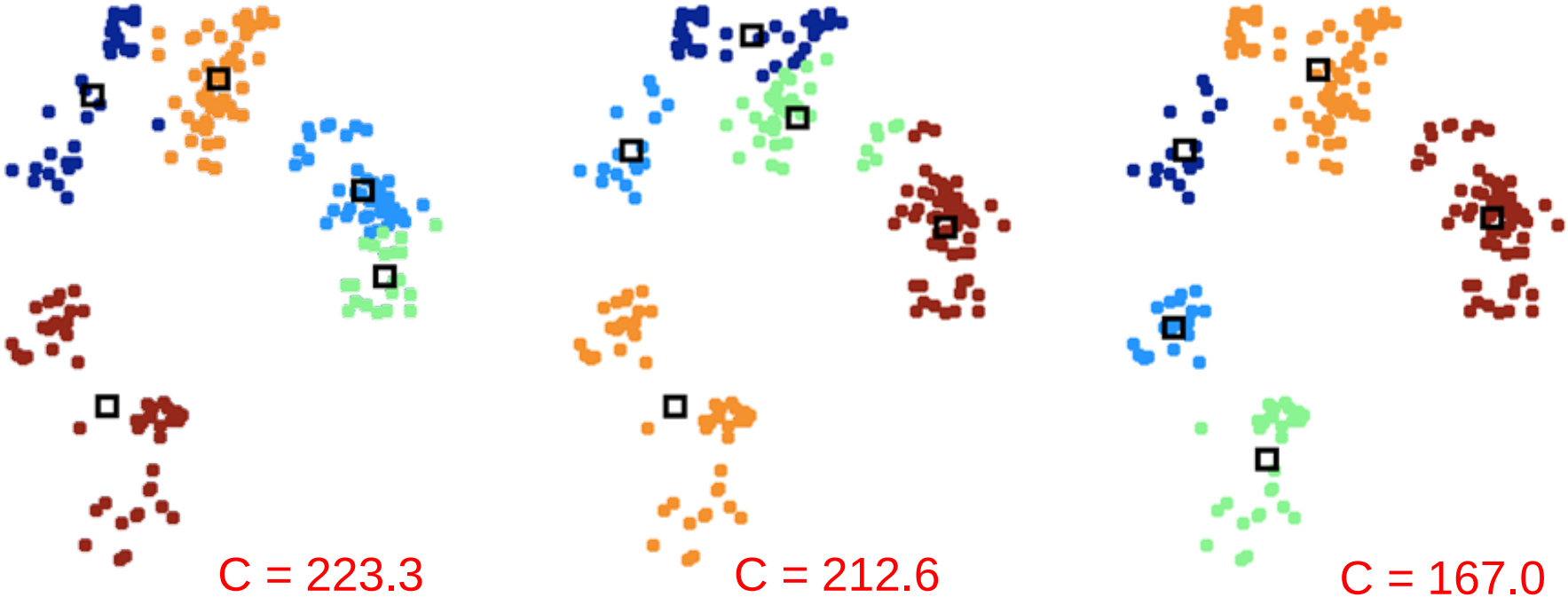
Over the cluster centers:
Cluster c only depends on x_i with z_i=c
Minimized by selecting the mean



Initialization

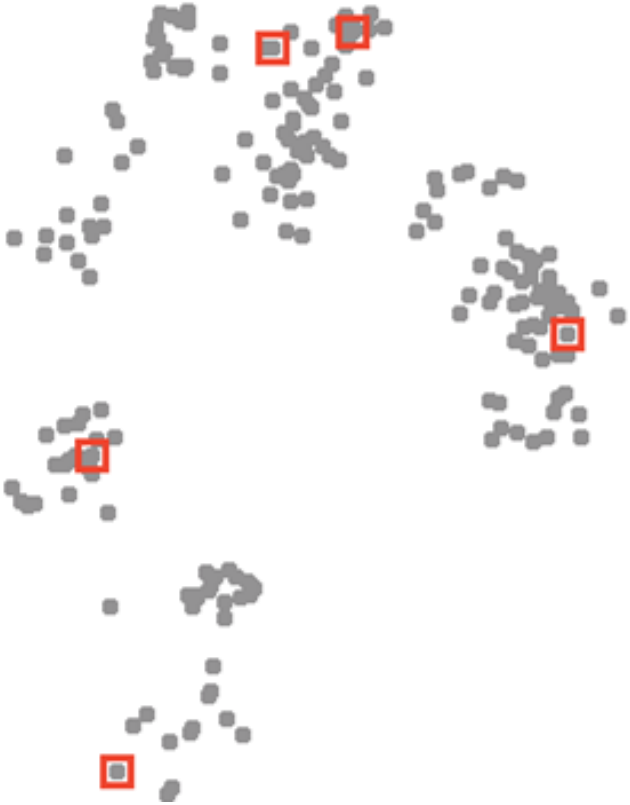
- Multiple local optima, depending on initialization

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



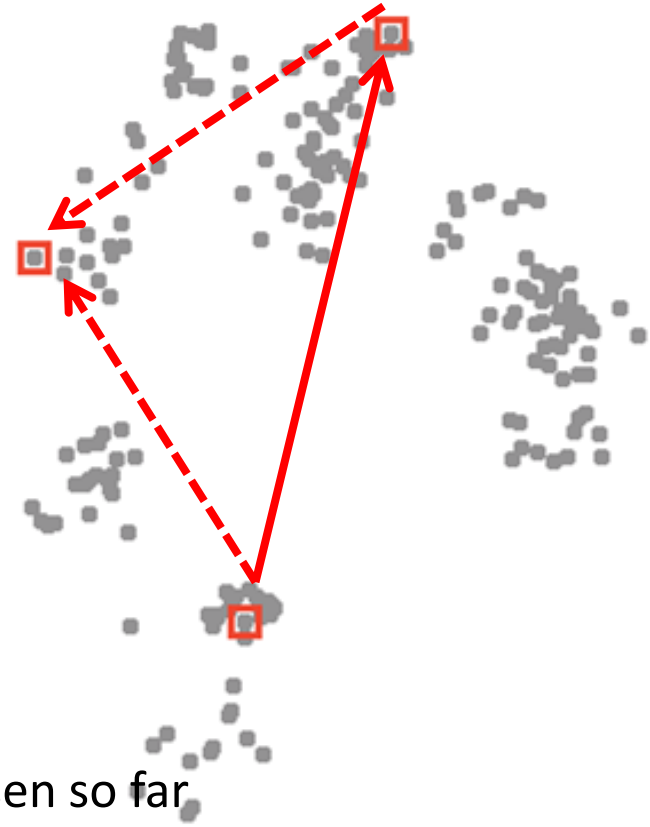
Initialization methods

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

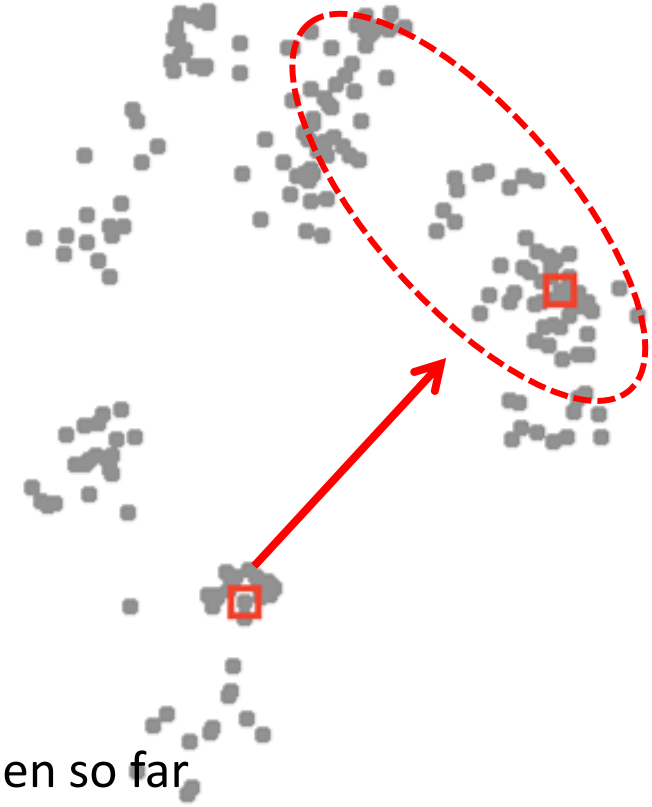


Initialization methods

- 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) / squared distance from x to current centers
  - Likely to put a cluster far away, in a region with lots of data

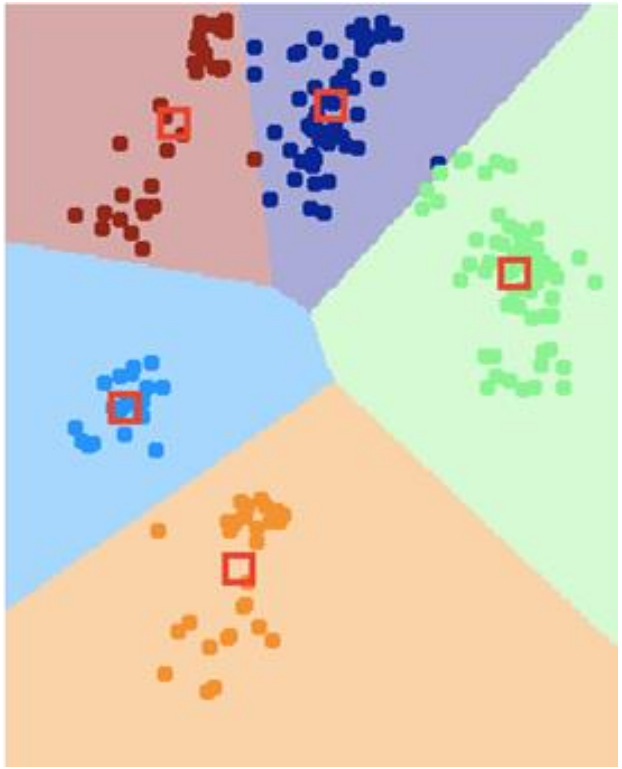
Out-of-sample points

- 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);
```



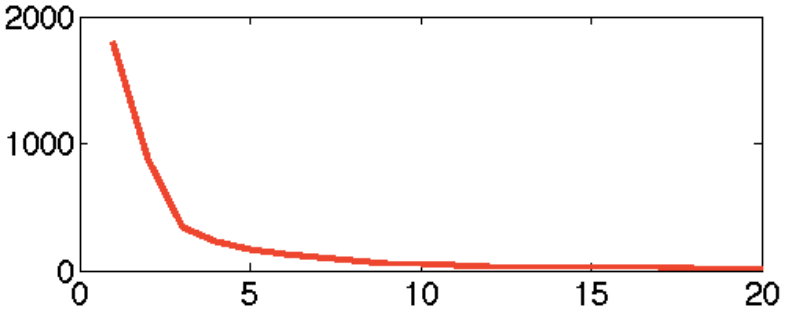
Choosing the number of clusters

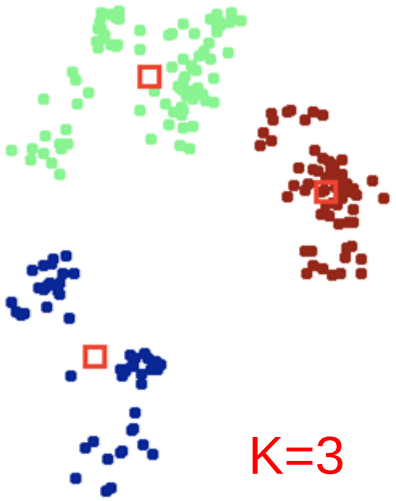
- With cost function

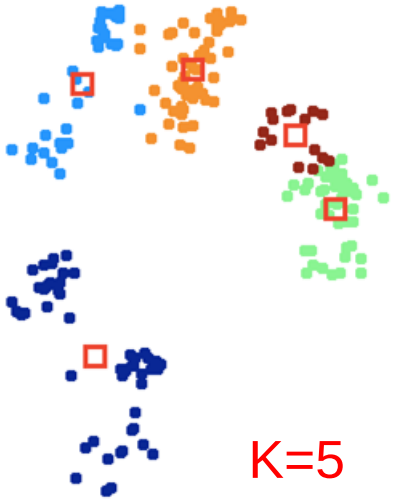
$$C(\underline{z}, \underline{\mu}) = \sum_i \| x_i - \mu_{z_i} \|^2$$

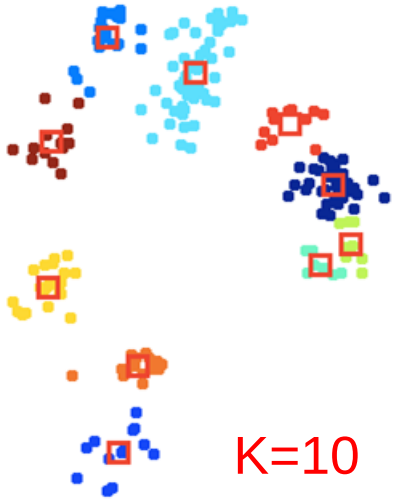
what is the optimal value of k?

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




K=3


K=5

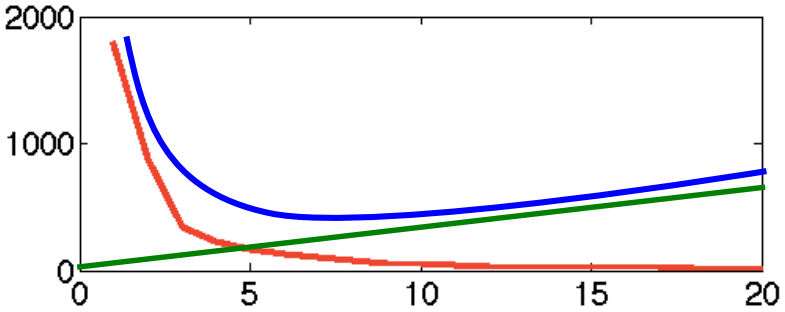

K=10

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…

- 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)

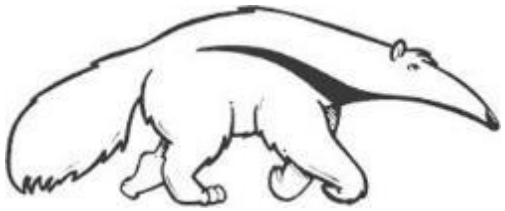
Summary

- 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.)

Machine Learning and Data Mining

Clustering (4):
Gaussian Mixtures & EM

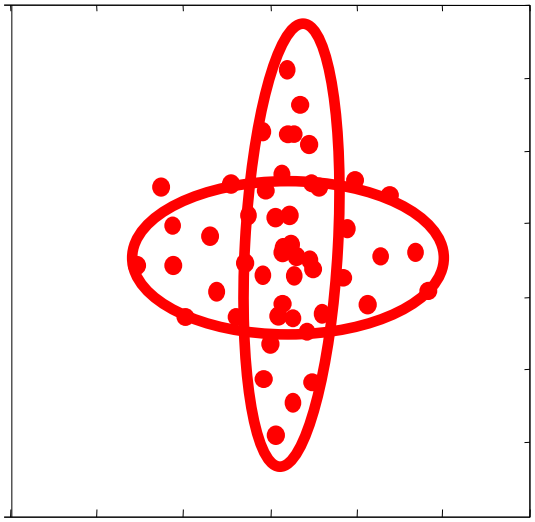
Kalev Kask



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?

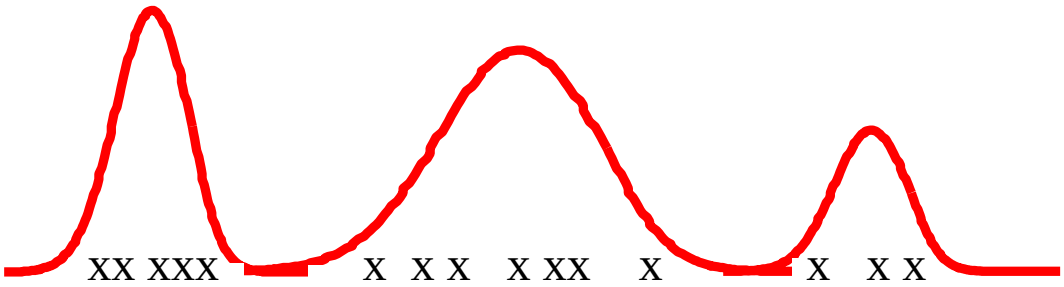
- Gaussian mixture models
  - Clusters modeled as Gaussians
    - Not just by their mean
  - EM algorithm: assign data to cluster with some *probability*
  - Gives probability model of x! ("generative")



Mixtures of Gaussians

- Start with parameters describing each cluster
- Mean ^1_c , variance $^3\!/_{4c}$, "size" $^1\!/_{4c}$
- 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:

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

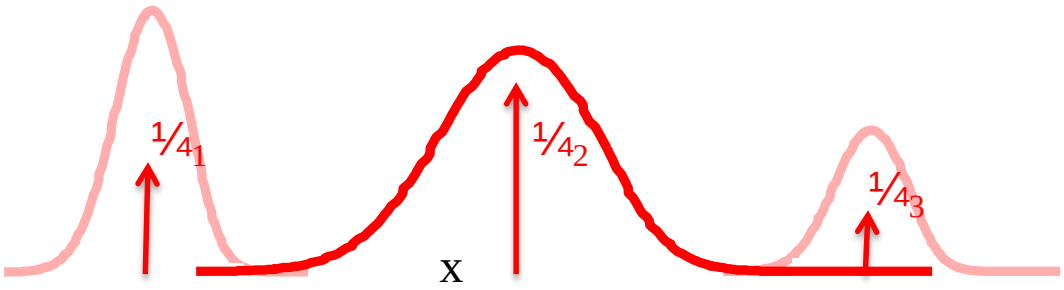
Select a mixture component with probability π

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

Sample from that component's Gaussian

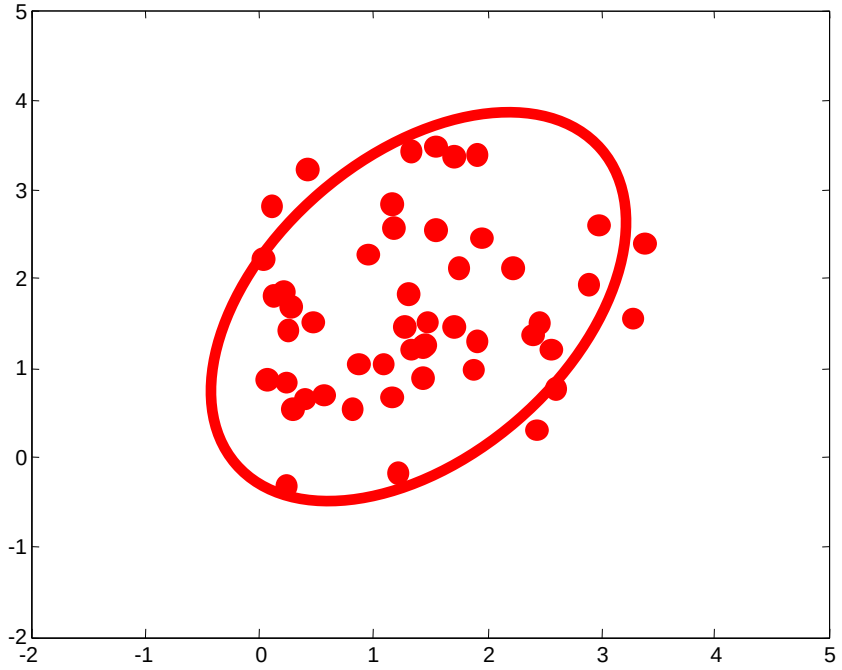
"Latent assignment" z:
we observe x, but z is hidden

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

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

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

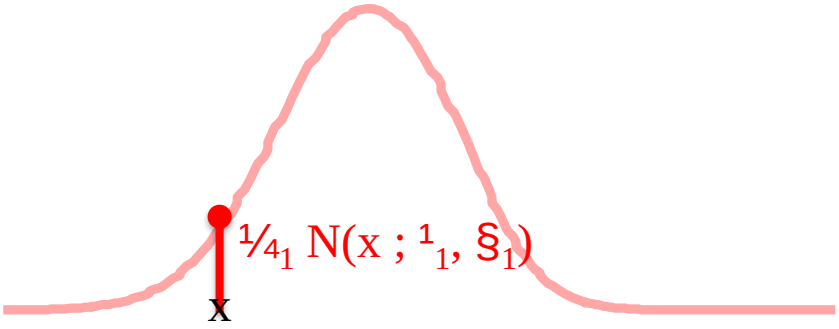
We'll model each cluster using one of these Gaussian "bells"…

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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- E-step ("Expectation")
  - For each datum (example) x_i,
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    - Normalize to sum to one (over clusters c)

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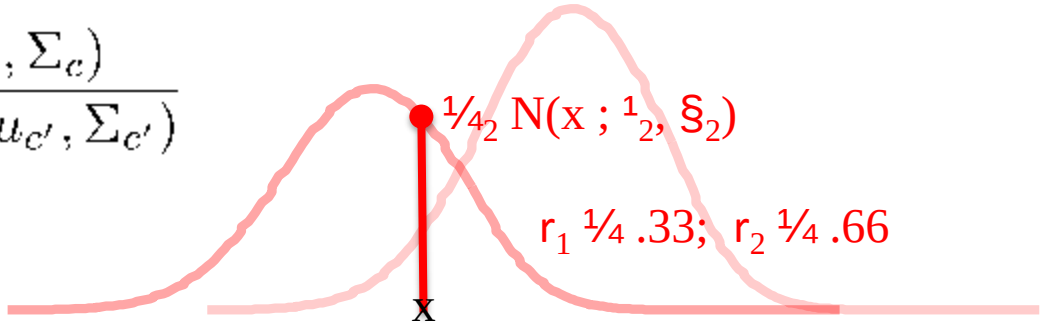


  - If x_i is very likely under the c^{th} Gaussian, it gets high weight
  - Denominator just makes r's sum to one

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

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

Weighted mean of assigned data

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

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

Expectation-Maximization

- Each step increases the log-likelihood of our model

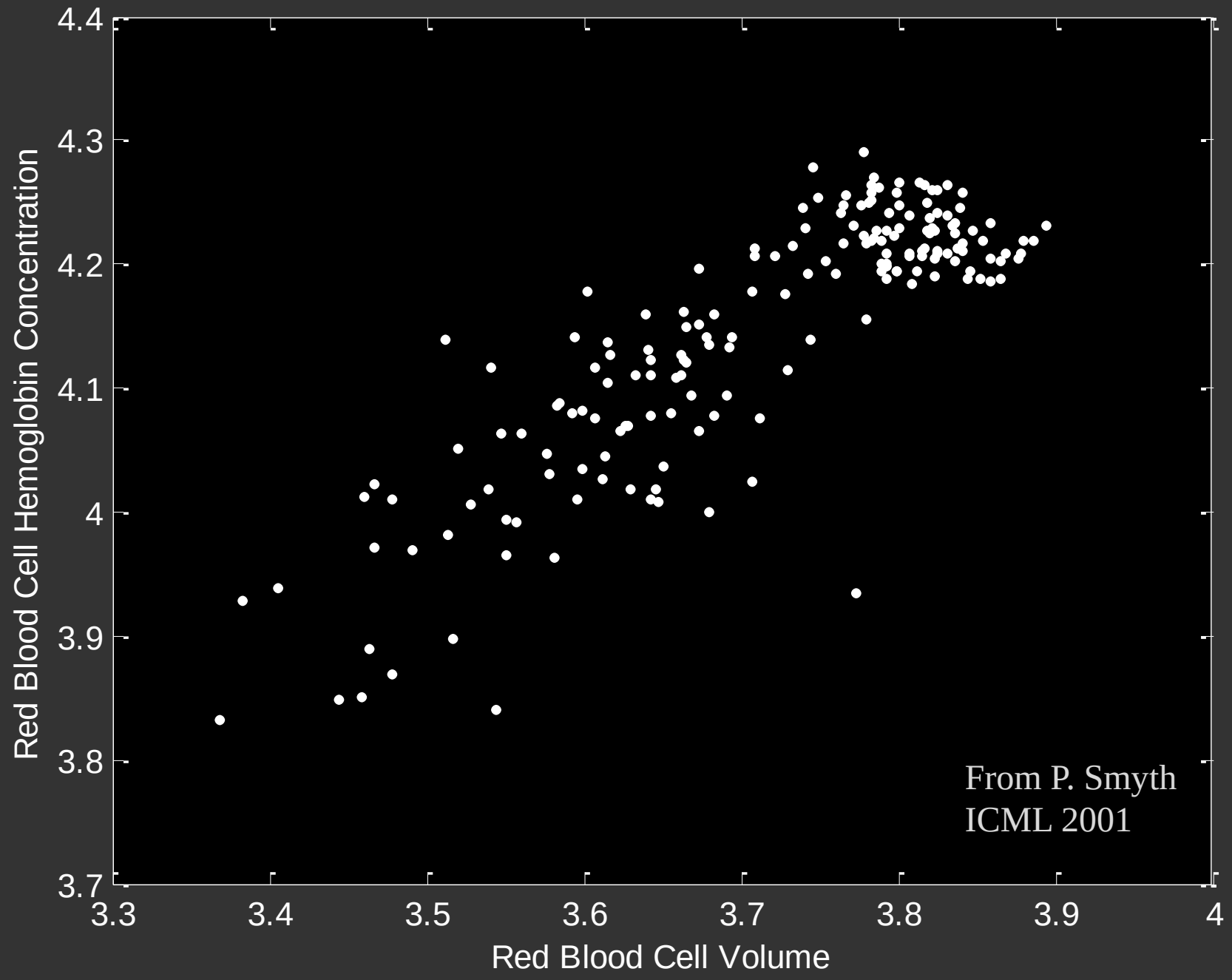
$$\log p(\underline{X}) = \sum_i \log \left[\sum_c \pi_c \, \mathcal{N}(x_i \; ; \; \mu_c, \Sigma_c) \right]$$

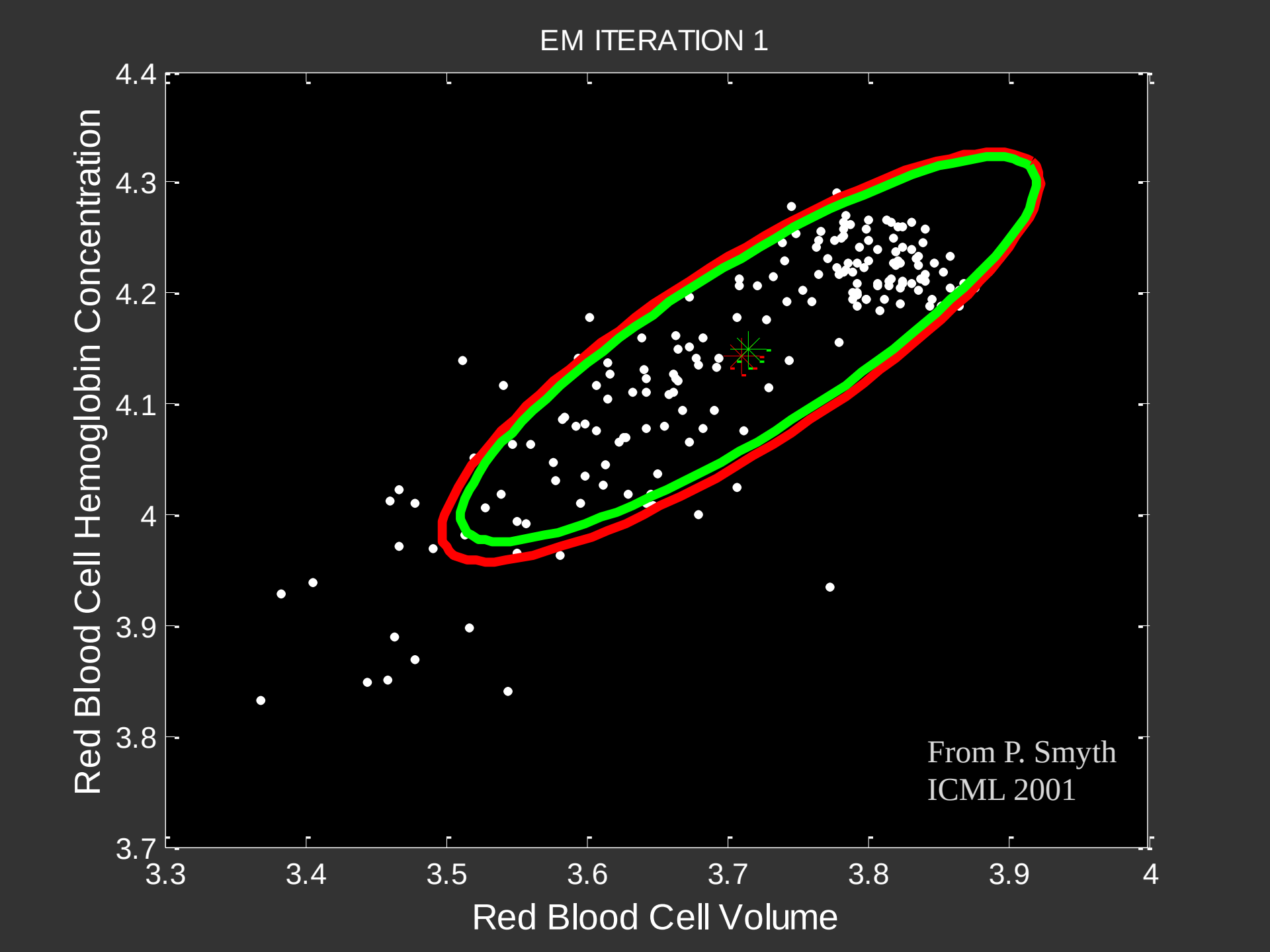
(we won't derive this here, though)

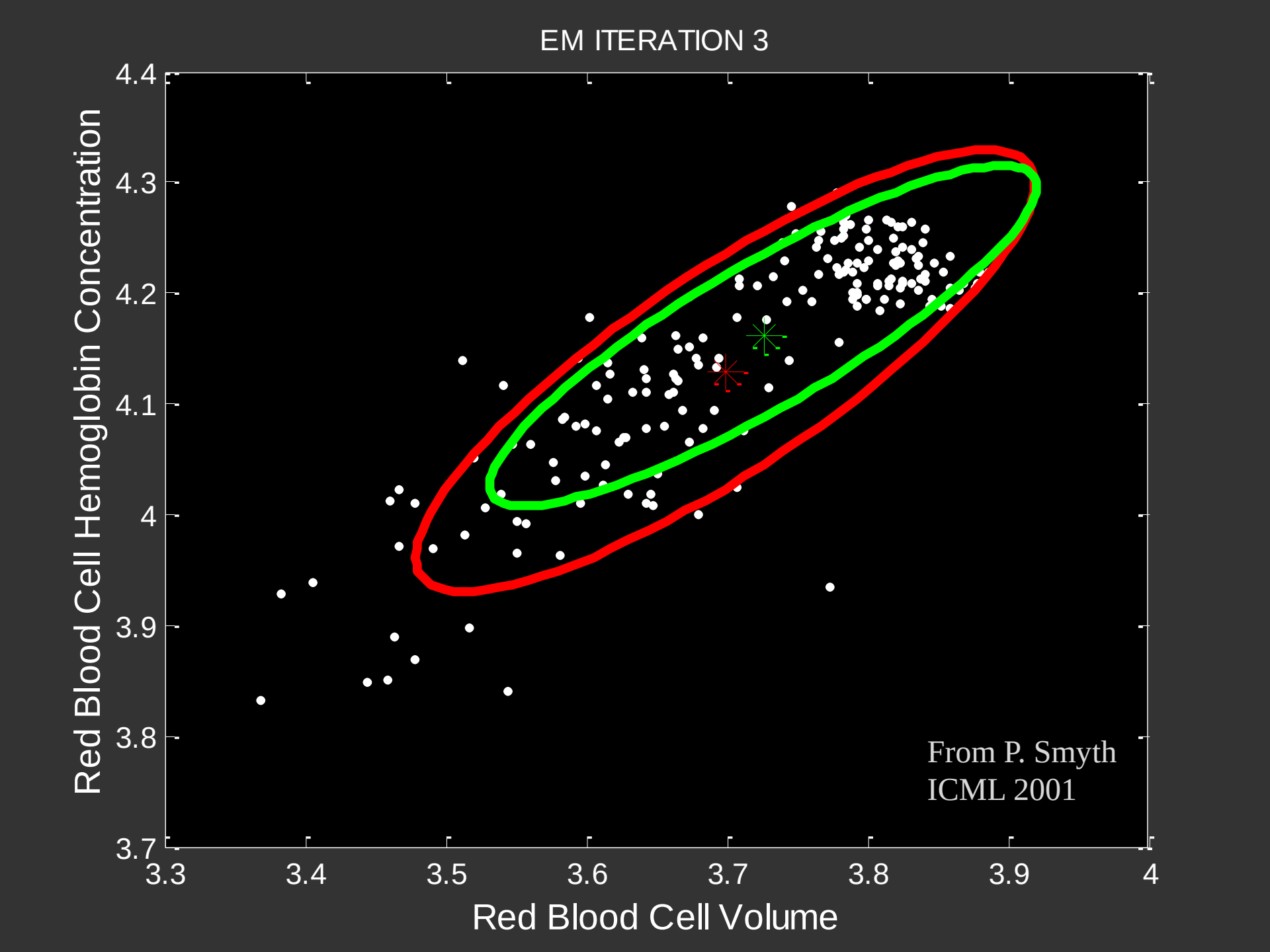
- Iterate until convergence
  - Convergence guaranteed – another ascent method
  - Local optima: initialization often important

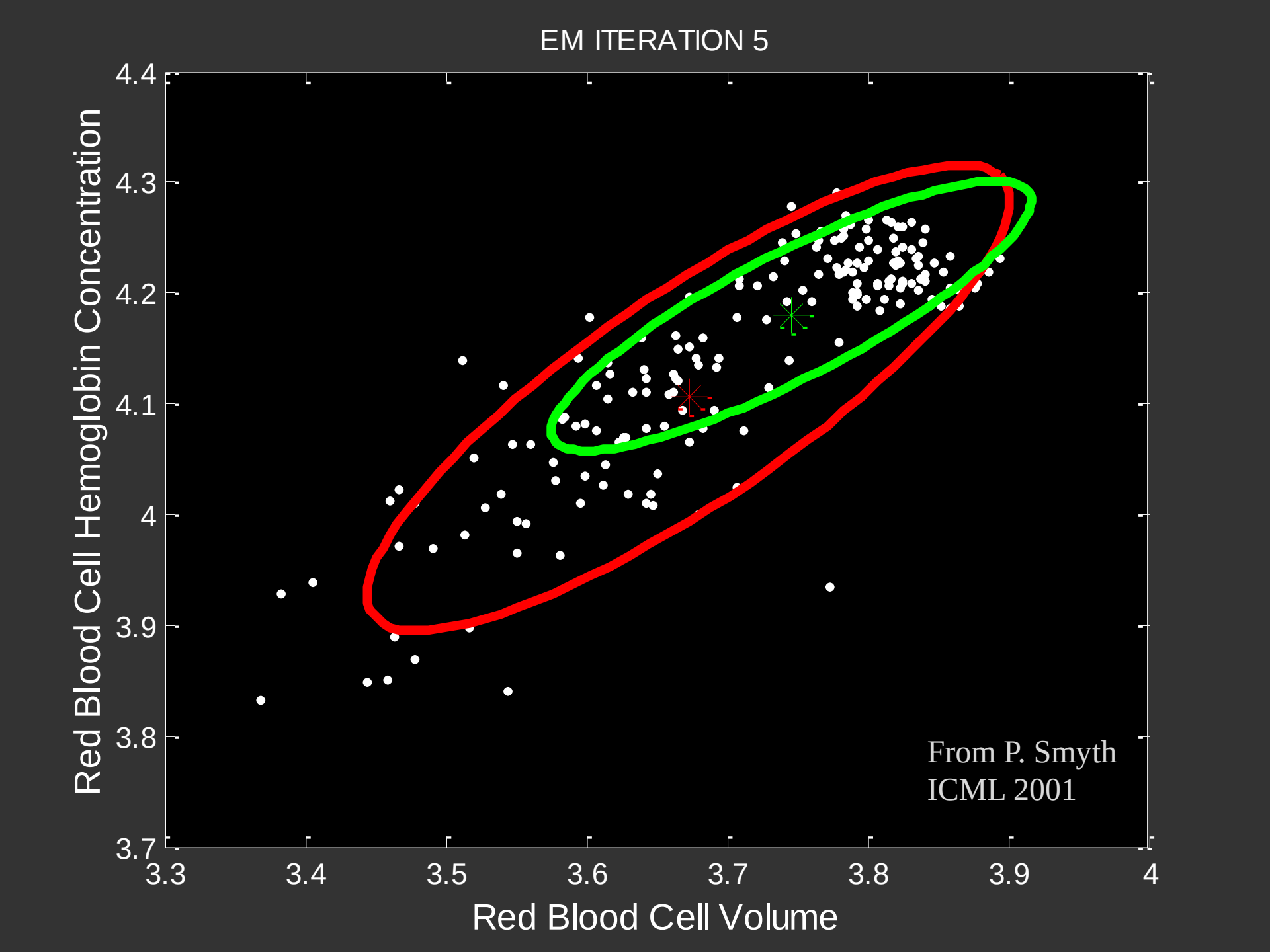
- What should we do
  - If we want to choose a single cluster for an "answer"?
  - With new data we didn't see during training?

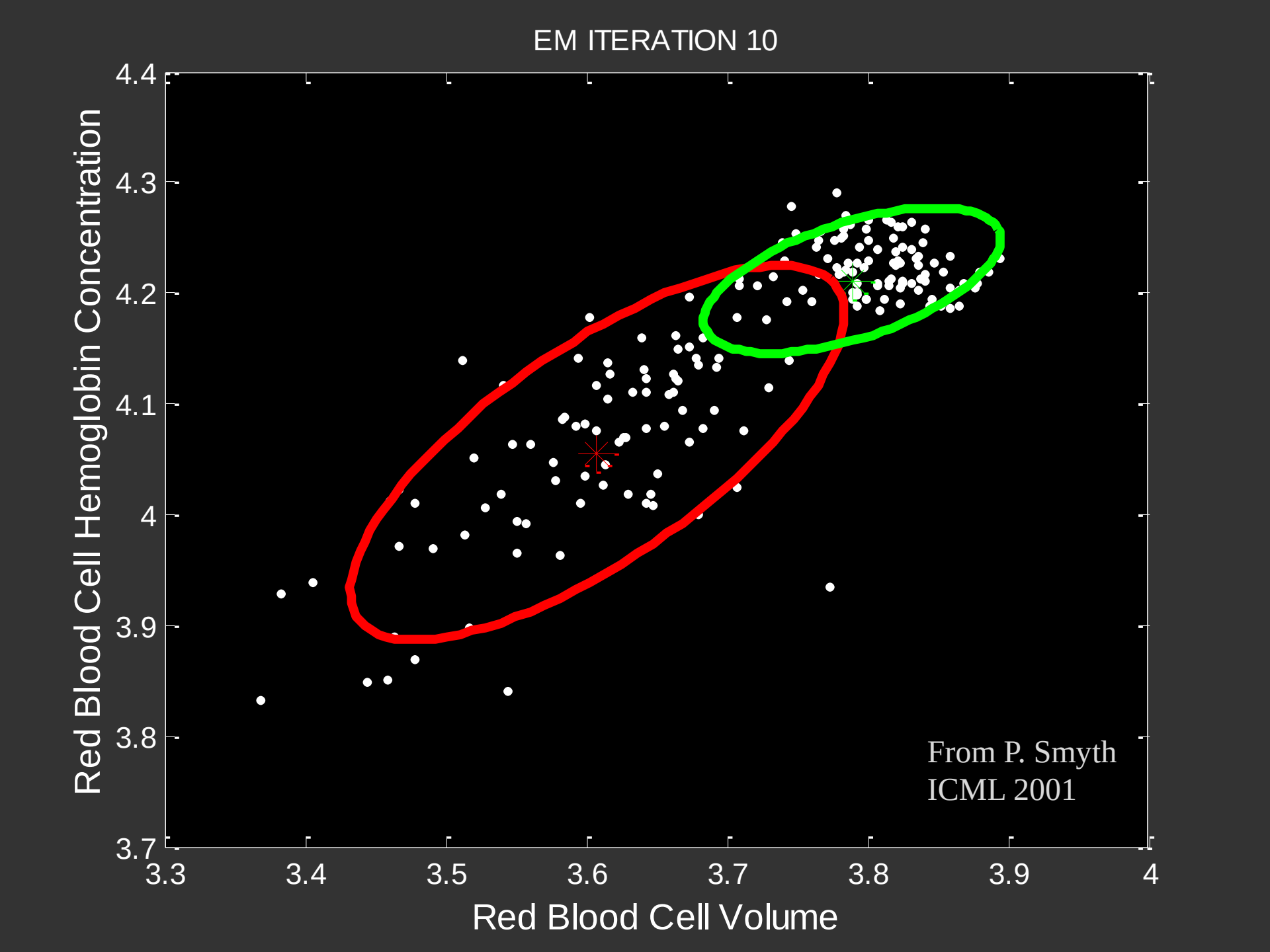
- Choosing the number of clusters
  - Can use penalized likelihood of training data (like k-means
  - True probability model: can use log-likelihood of test data, log p(x')

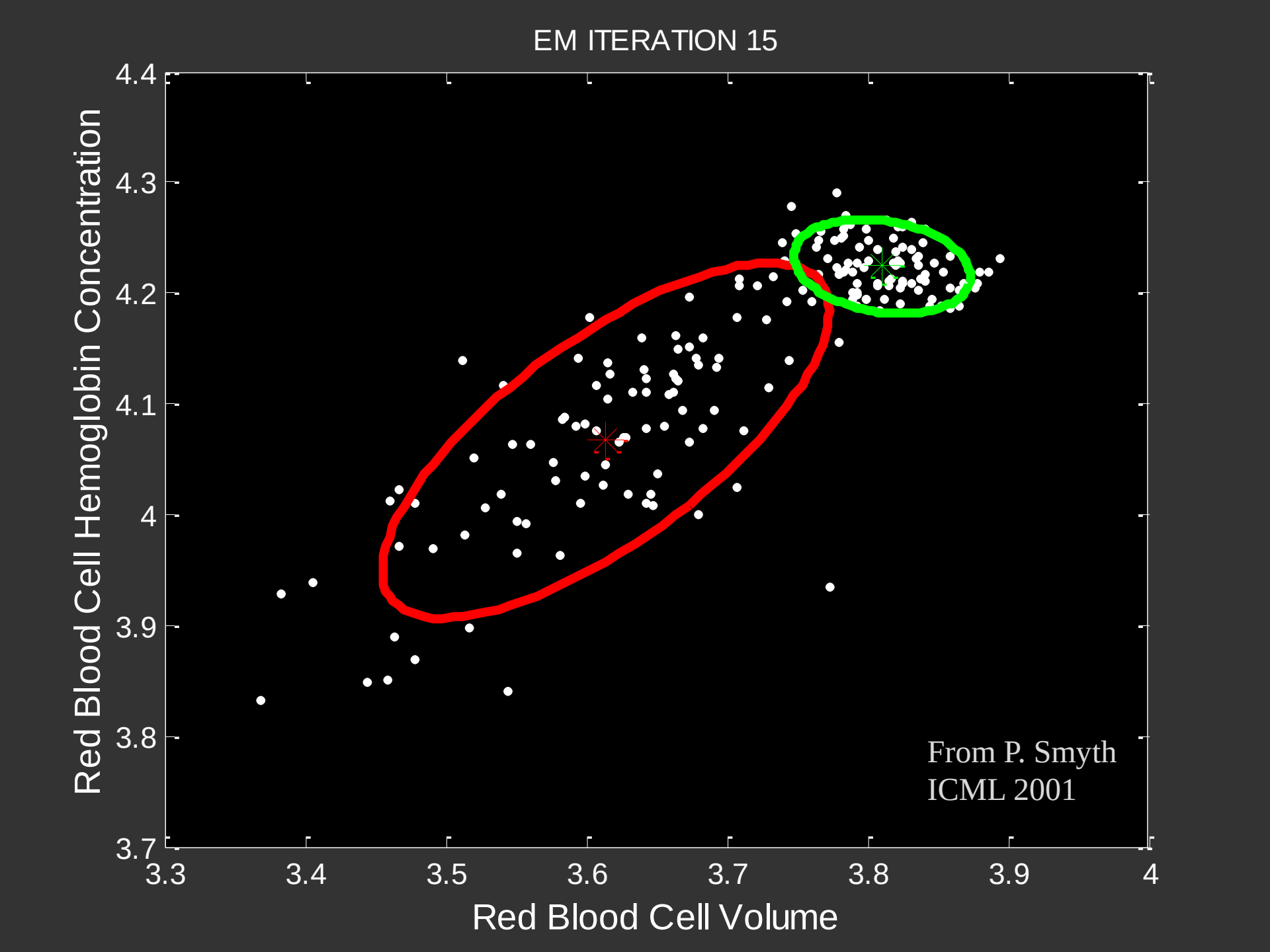

ANEMIA PATIENTS AND CONTROLS
Red Blood Cell Hemoglobin Concentration
Red Blood Cell Volume
4.4
4.3
4.2
4.1
4
3.9
3.8
3.7
3.3
3.4
3.5
3.6
3.7
3.8
3.9
4
From P. Smyth
ICML 2001

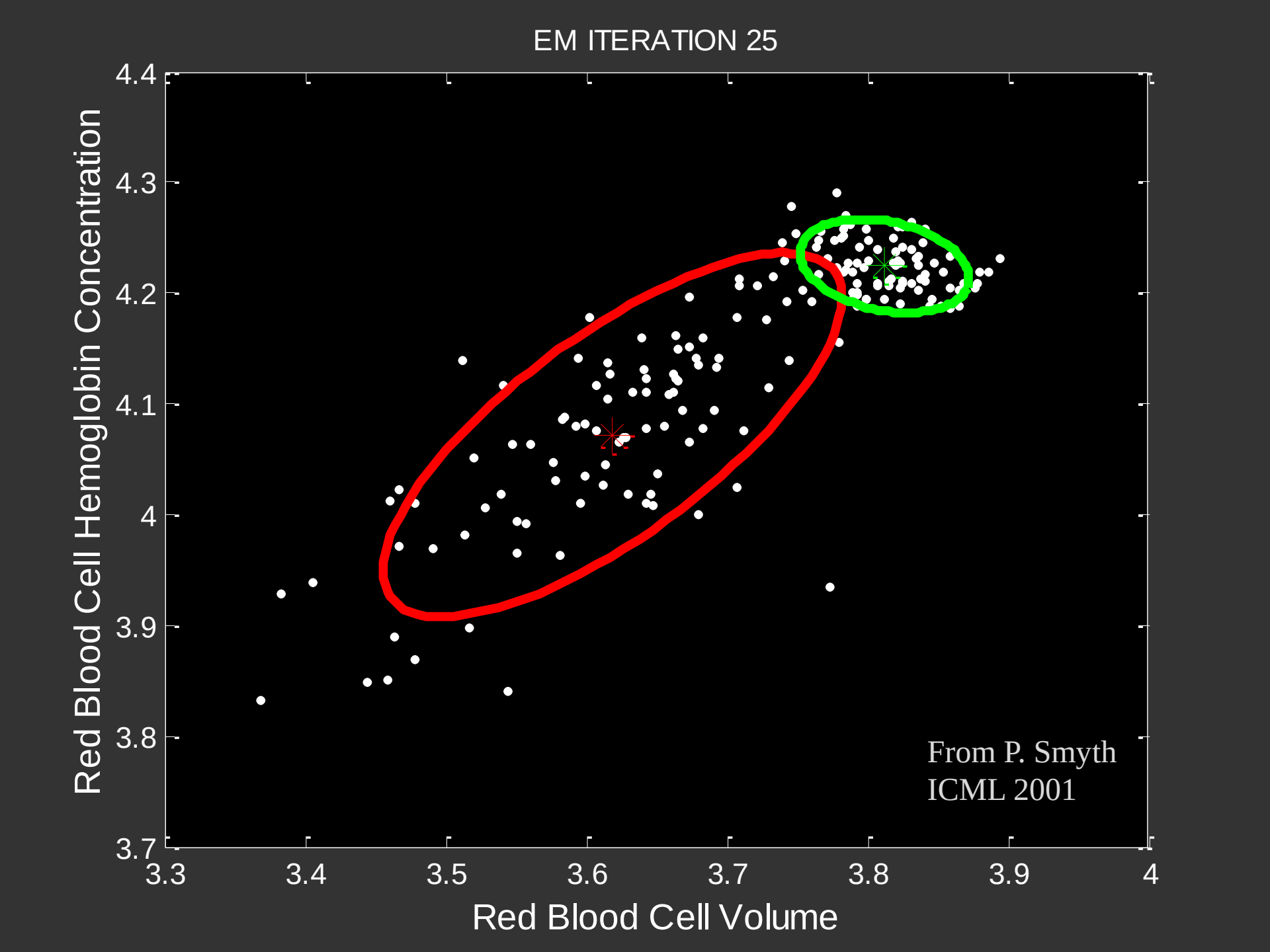

EM ITERATION 1
Red Blood Cell Hemoglobin Concentration
Red Blood Cell Volume
4.4
4.3
4.2
4.1
4
3.9
3.8
3.7
3.3
3.4
3.5
3.6
3.7
3.8
3.9
4
From P. Smyth
ICML 2001

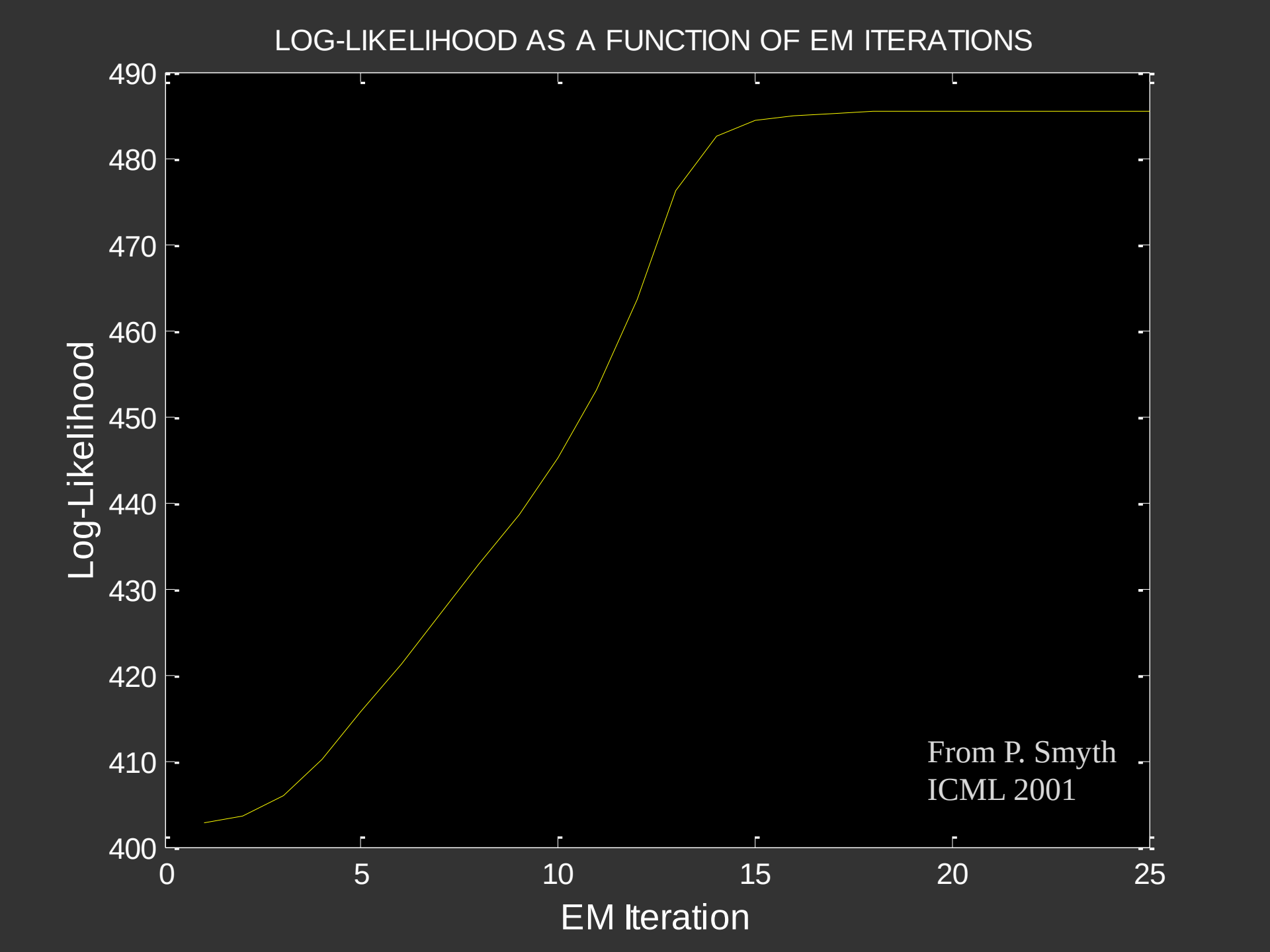

EM ITERATION 3
Red Blood Cell Hemoglobin Concentration
Red Blood Cell Volume
4.4
4.3
4.2
4.1
4
3.9
3.8
3.7
3.3
3.4
3.5
3.6
3.7
3.8
3.9
4
From P. Smyth
ICML 2001


EM ITERATION 5
Red Blood Cell Hemoglobin Concentration
Red Blood Cell Volume
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 10
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 15
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 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
Log-Likelihood
EM Iteration
490
480
470
460
450
440
430
420
410
400
0
5
10
15
20
25
From P. Smyth
ICML 2001

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?