THE UNIVERSITY of TENNESSEE KNOXVILLE

Lecture 13: Gaussian Mixture Models and Density Based Clustering

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Clustering: Data Structures

- Hierarchical clustering
- K-means clustering
- Gaussian Mixture Models
- Density-based clustering
- Spectral clustering

Data matrix (two modes)

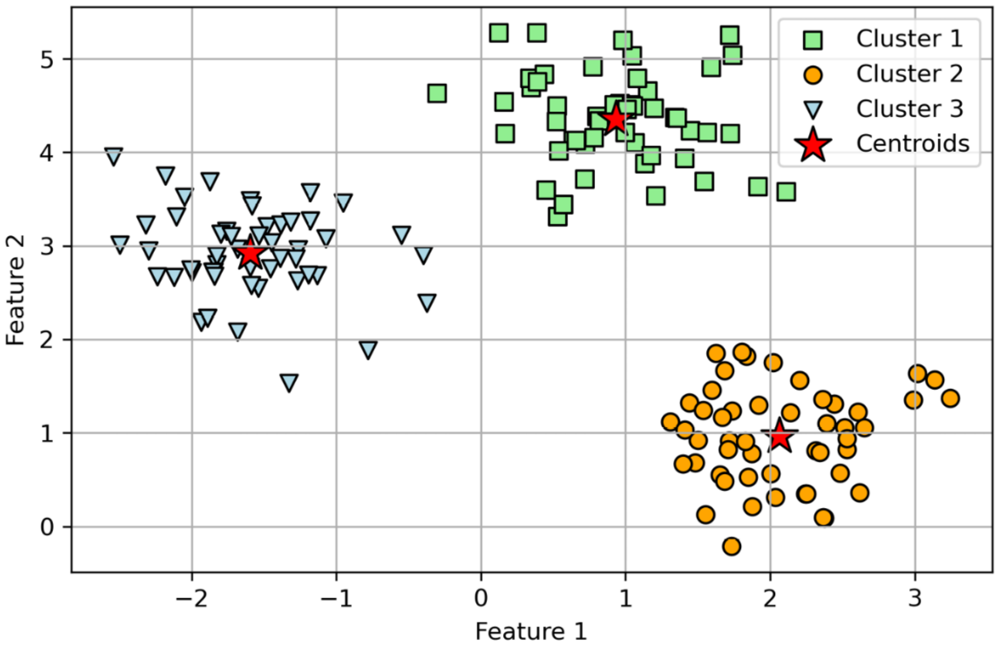
$$\begin{bmatrix} x_{11} & \cdots & x_{1f} & \cdots & x_{1p} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{i1} & \cdots & x_{if} & \cdots & x_{ip} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{n1} & \cdots & x_{nf} & \cdots & x_{np} \end{bmatrix}$$

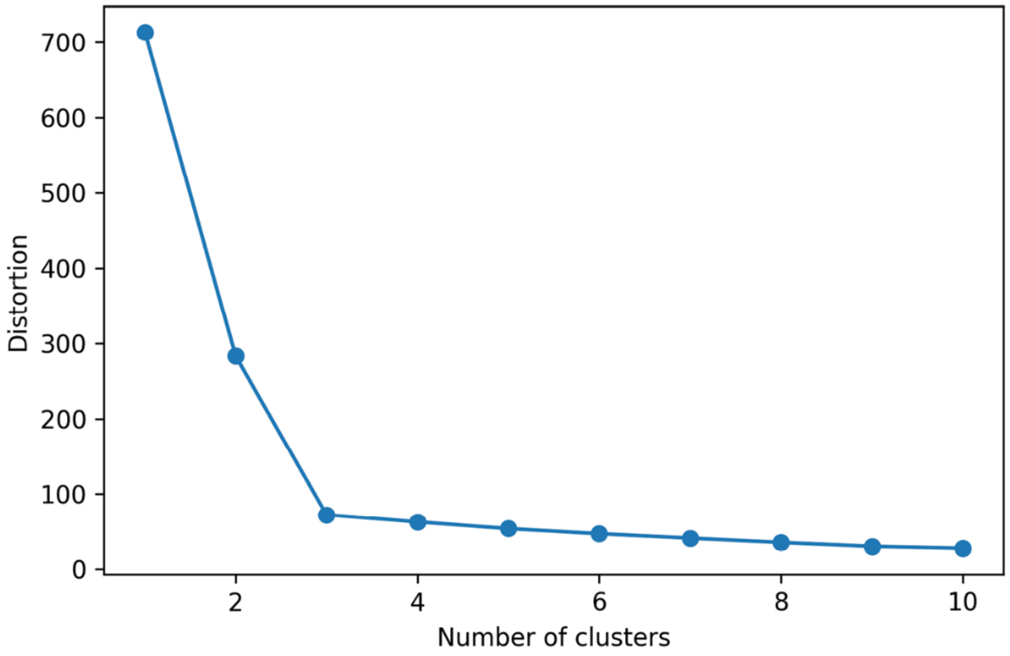
Dissimilarity matrix (one mode)

$$\begin{bmatrix} 0 & & & & \\ d(2,1) & 0 & & & \\ d(3,1) & d(3,2) & 0 & & \\ : & : & : & & \\ d(n,1) & d(n,2) & \cdots & \cdots & 0 \end{bmatrix}$$

From: Han and Kamber, Data Mining: Concepts and Techniques

K-means clustering and elbow methods





Calculate cluster size as a function of number of clusters

Silhouette

We need techniques that find a balance between inter-cluster similarity and intra-cluster dissimilarity

Silhouette:

- Scores any clustering with an arbitrary number of unique clusters. Clustering can come from any clustering algorithm.
- $a(i)$ = average dissimilarity of instance i to all other instances in the cluster to which i is assigned – **Minimize**
  - Dissimilarity could be Euclidian distance, etc.
- $b(i)$ = the smallest average dissimilarity of instance i to all instances in the closest cluster to $b(i)$ – **Maximize**
- $b(i)$ is smallest for the best different cluster that i could be assigned to – the best cluster that you would move i to if needed

Silhouette

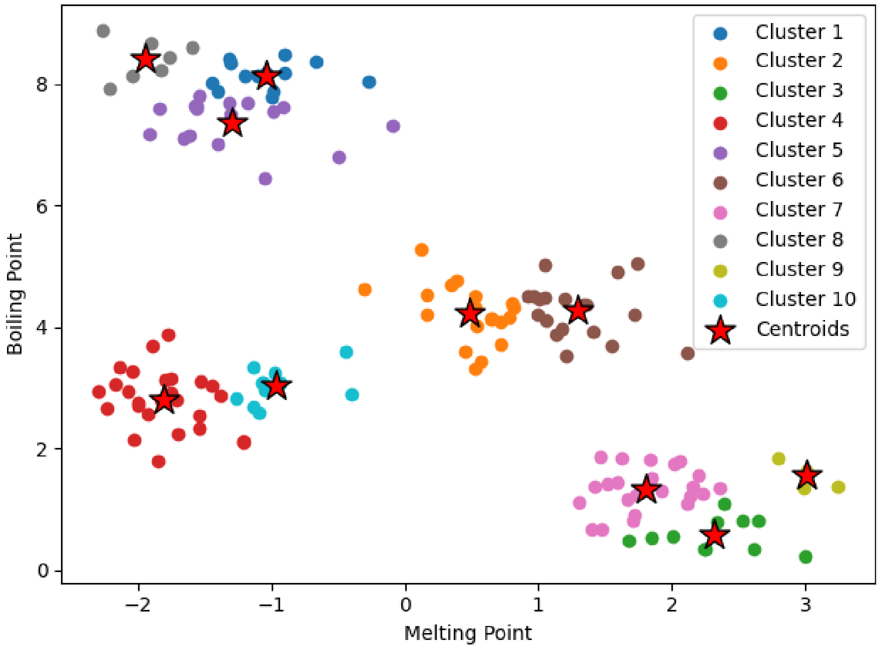
1. Calculate the **cluster cohesion**, $a^{(i)}$, as the average distance between an example, $\boldsymbol{x}^{(i)}$, and all other points in the same cluster.

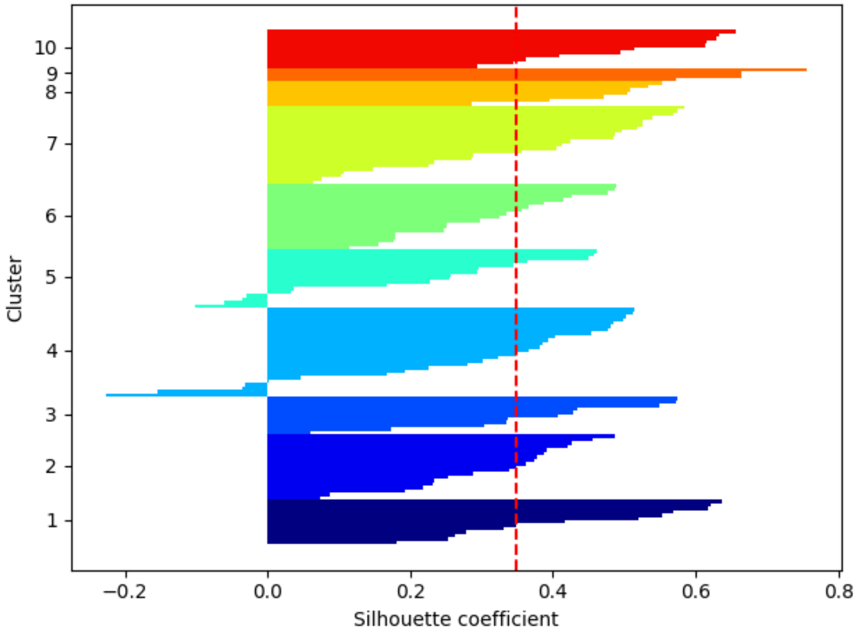
2. Calculate the **cluster separation**, $b^{(i)}$, from the next closest cluster as the average distance between the example, $\boldsymbol{x}^{(i)}$, and all examples in the nearest cluster.

3. Calculate the silhouette, $s^{(i)}$, as the difference between cluster cohesion and separation divided by the greater of the two, as shown here:

$$s^{(i)} = \frac{b^{(i)} - a^{(i)}}{max\{b^{(i)}, a^{(i)}\}}$$

Silhouette





- The quality of a single cluster can be measured by the average silhouette score of its members, (close to 1 is best)
- The quality of a total clustering can be measured by the average silhouette score of all the instances
- To find best clustering, compare total silhouette scores across clusterings with different *k* values and choose the highest

Summary of k-means clustering

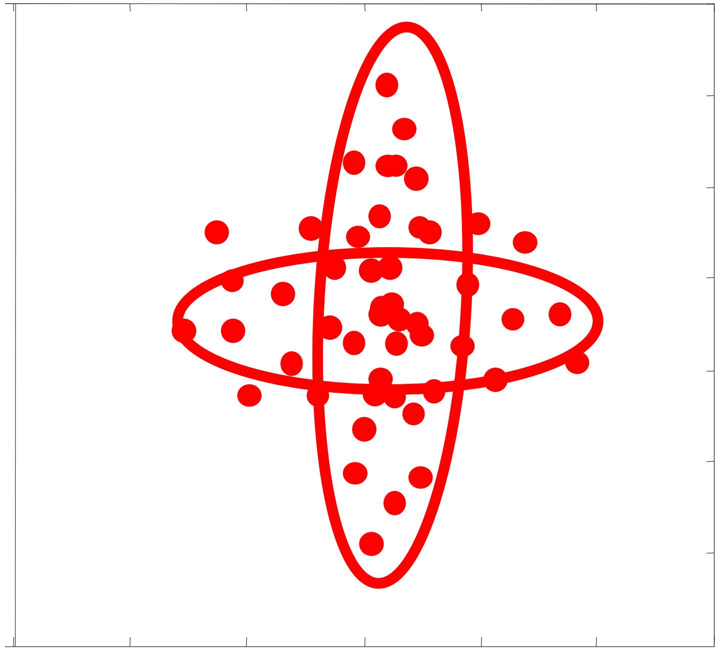
- **Strengths**
  - *Relatively efficient*: $O(tkn)$, where n is number of objects, k is number of clusters, and t is number of iterations. Normally, k, $t << n$.
  - Often terminates at a local optimum

- **Weakness**
  - Applicable only when mean is defined (what about categorical data)?
  - Need to specify k, the number of clusters, in advance
  - Unable to handle noisy data and outliers
  - Not suitable to discover clusters with non-convex shapes
  - Scales matter

Mixture 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?



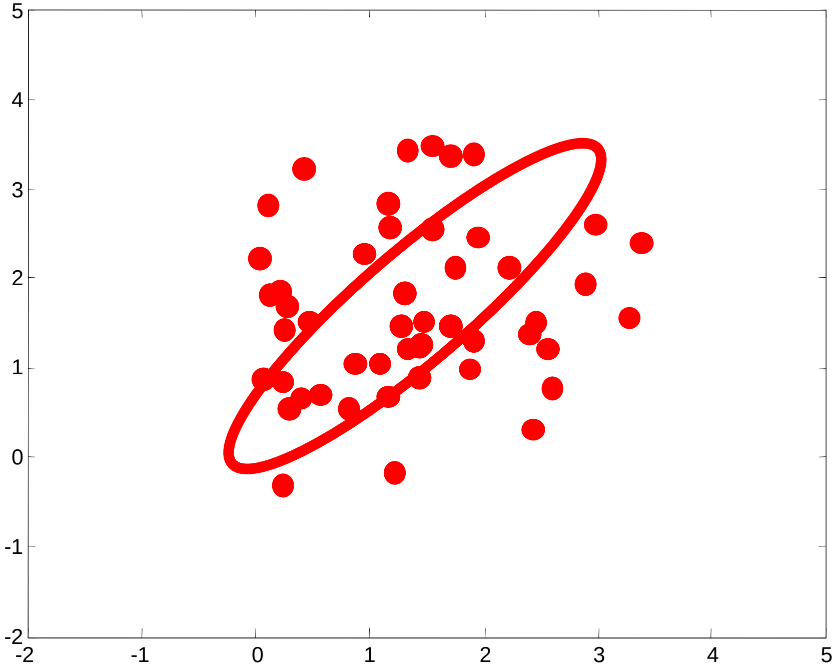
Gaussian mixture models

- Clusters modeled as Gaussian distributions
- EM algorithm: assign data to cluster with some *probability*

(adapted from) Prof. Alexander Ihler

Multivariate Gaussian Model

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



Maximum Likelihood estimates

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

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

We model each cluster using Gaussian distribution

(adapted from) Prof. Alexander Ihler

Expectation Maximization: E-Step

- Initialize parameters of each cluster: 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)

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

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

(adapted from) Prof. Alexander Ihler

Expectation Maximization: M-Step

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

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

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

Total responsibility allocated to cluster c

$$\pi_c = \frac{N_c}{N}$$

Fraction of total assigned to cluster c

$$\mu_c = \frac{1}{N_c} \sum_i r_{ic} x_i$$

Weighted mean of assigned data

$$\Sigma_c = \frac{1}{N_c} \sum_i r_{ic} (x_i - \mu_c)^T (x_i - \mu_c)$$

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

(adapted from) Prof. Alexander Ihler

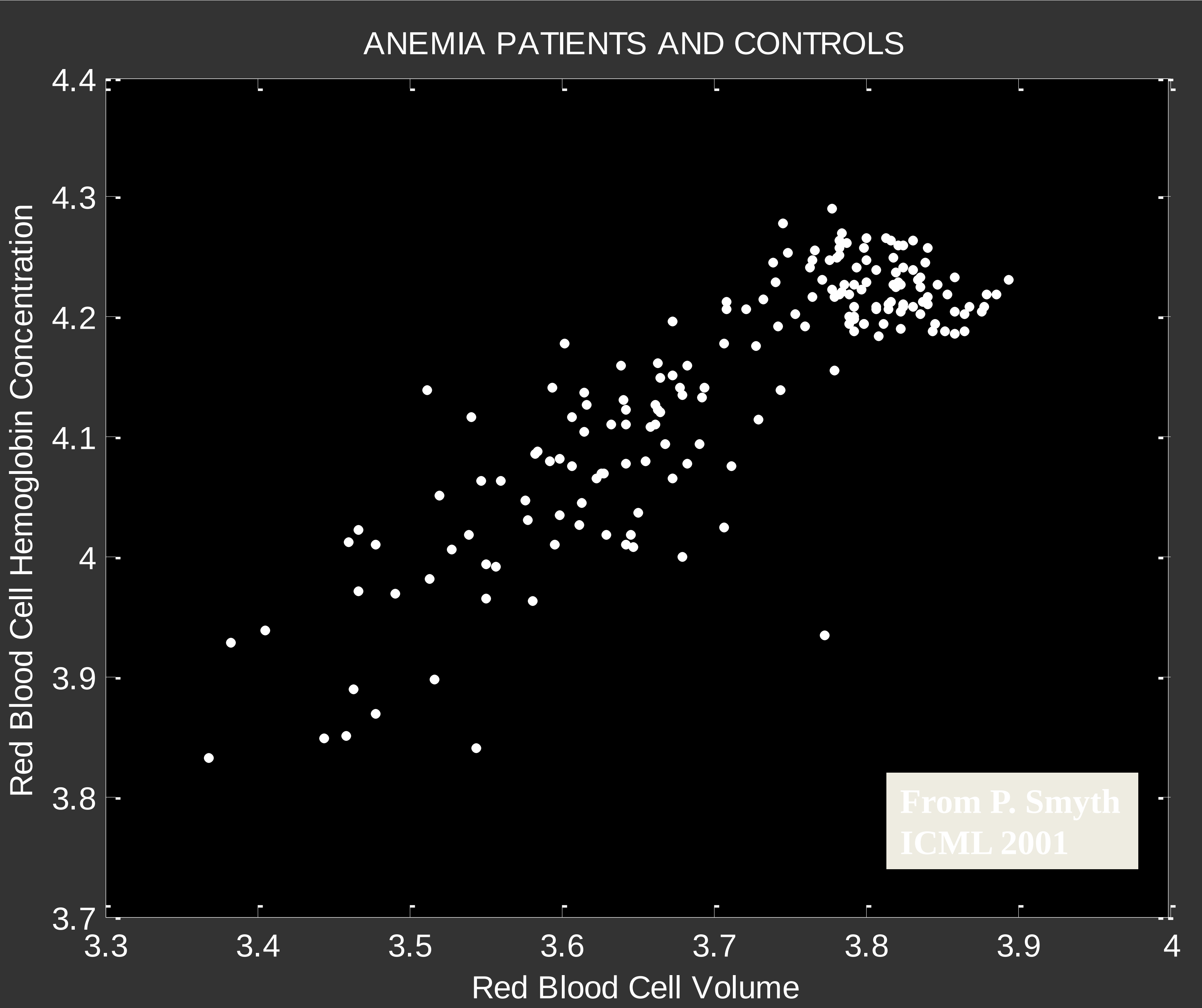
Expectation Maximization

- Each step increases the log-likelihood of our model

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

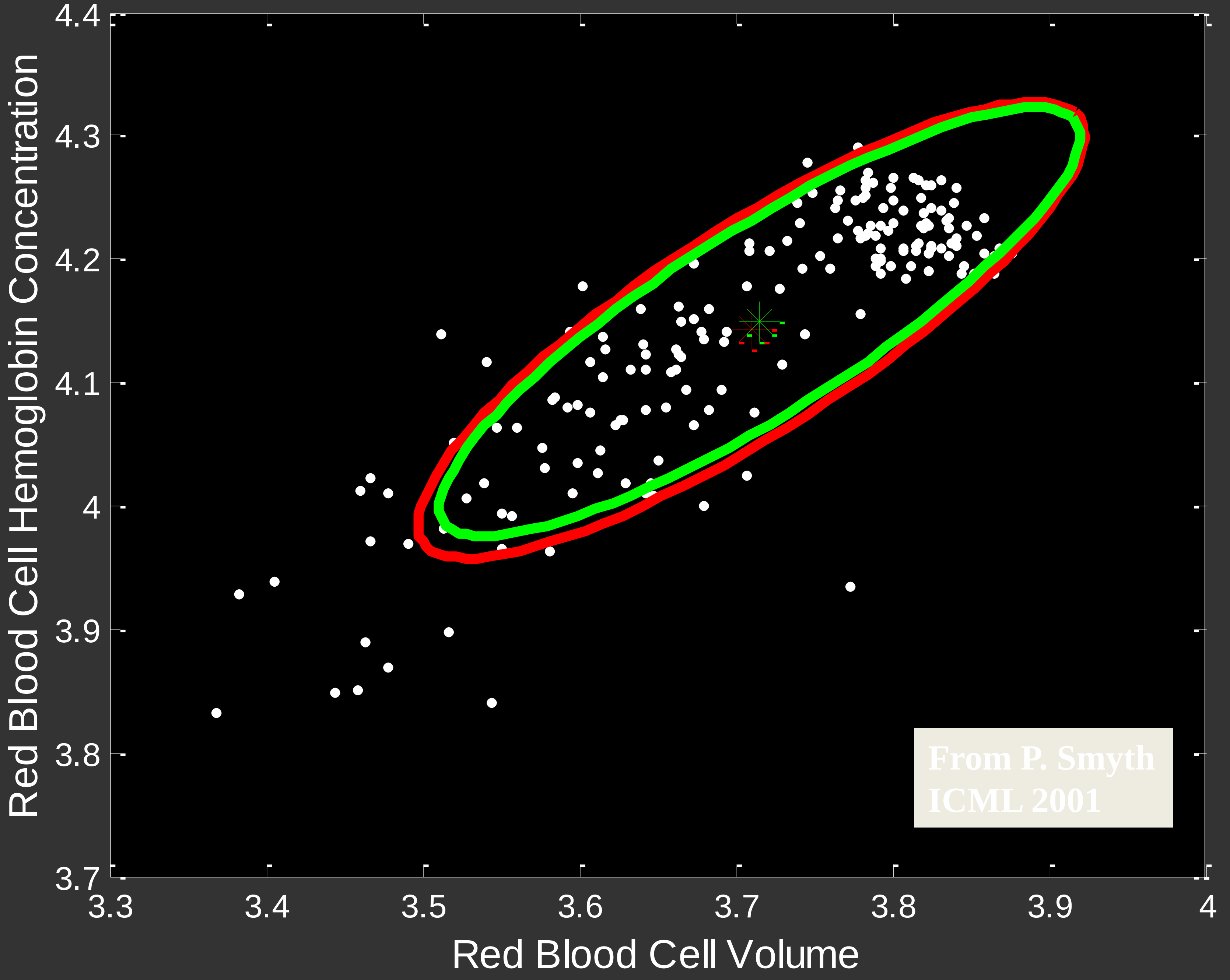
- Iterate until convergence
  – Convergence guaranteed – another ascent method

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



From P. Smyth
ICML 2001

EM ITERATION 1



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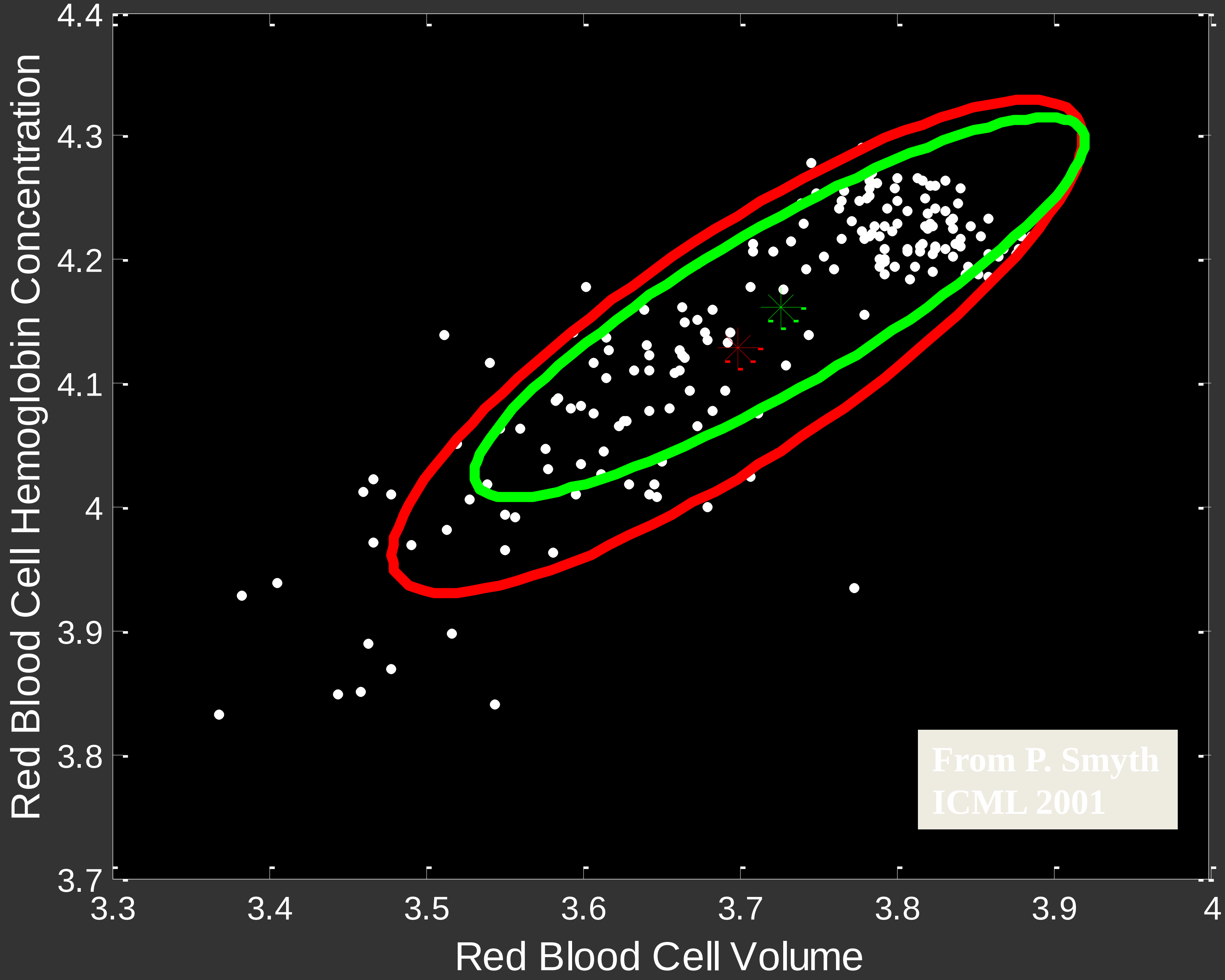
EM ITERATION 3



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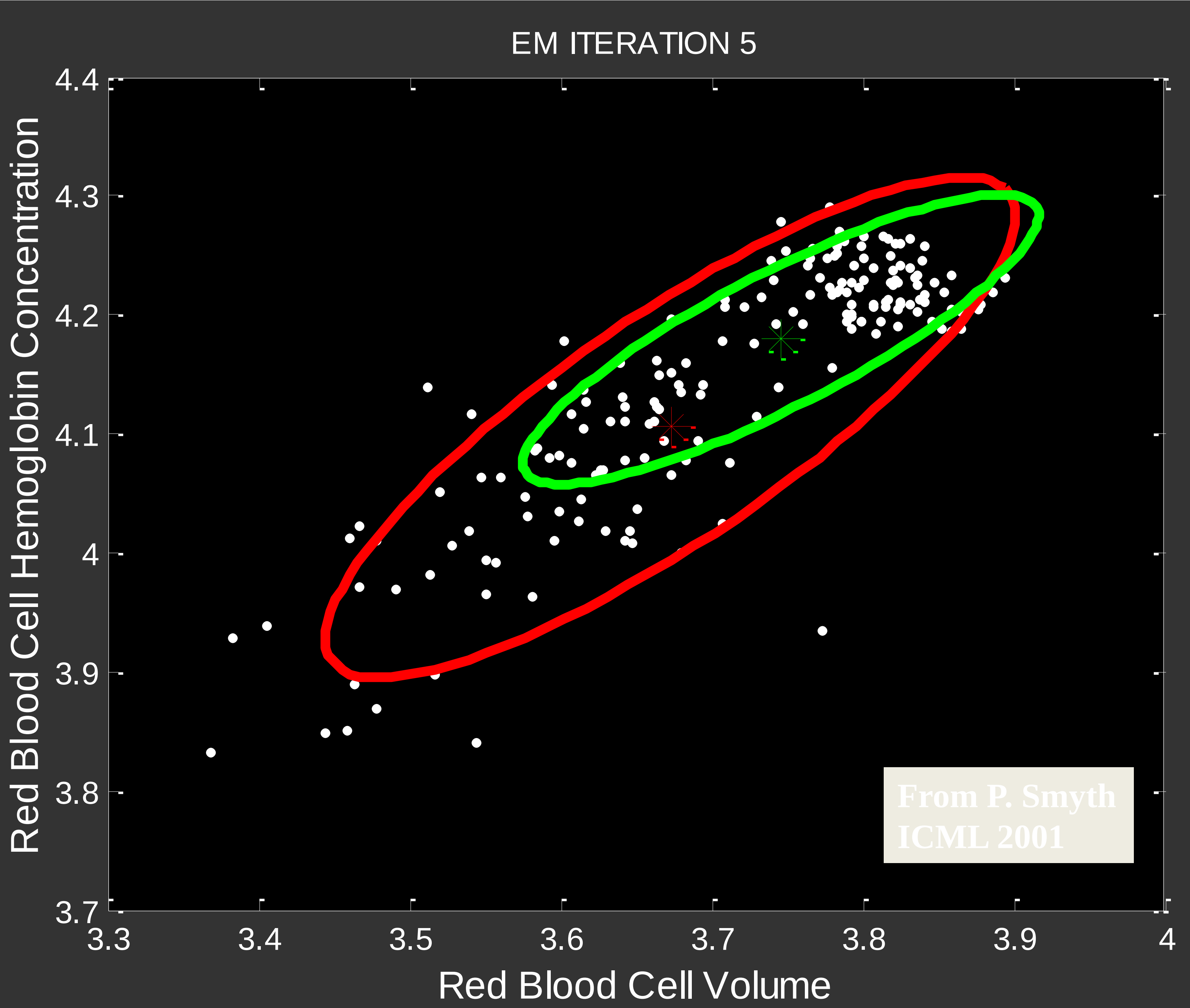

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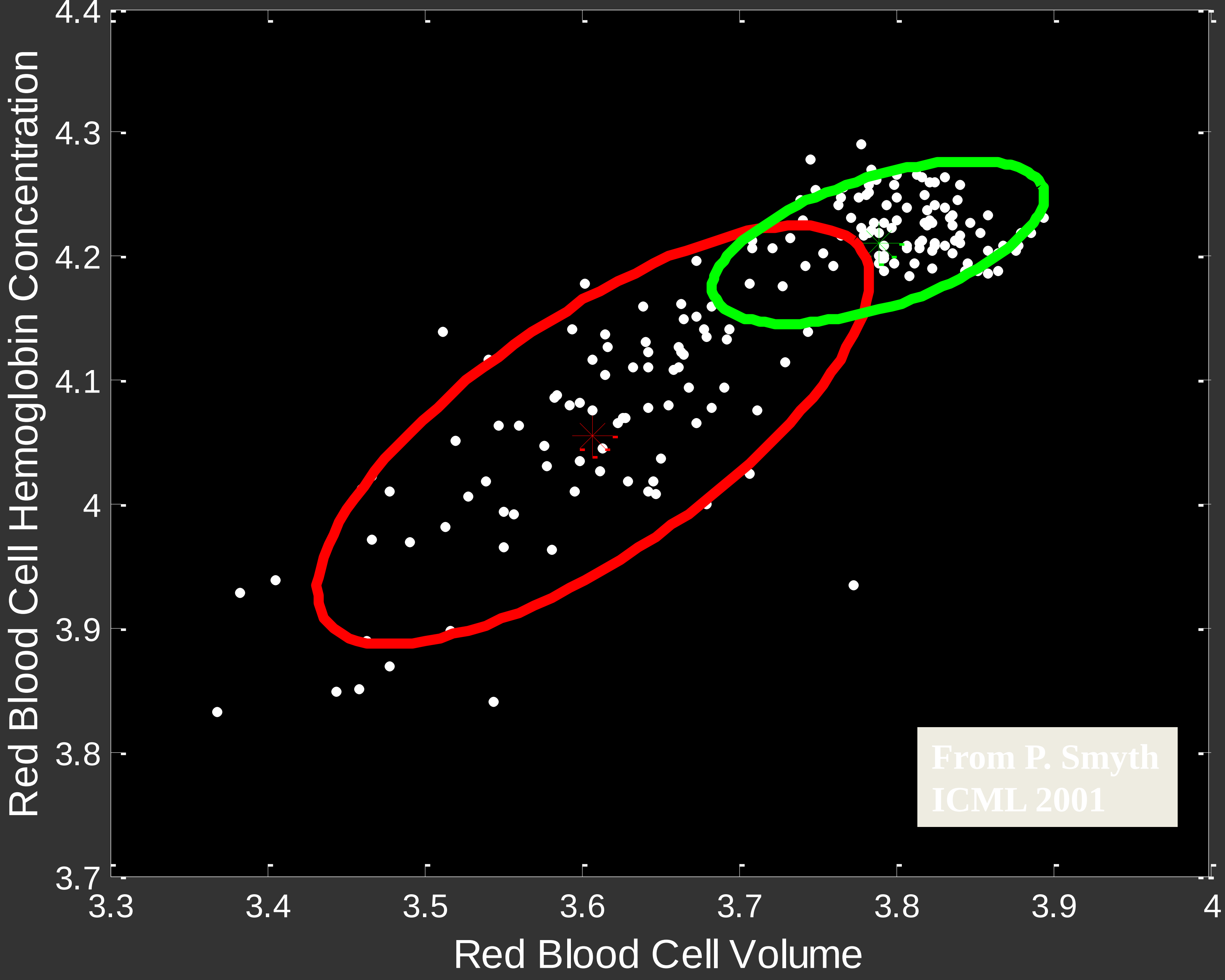
EM ITERATION 10



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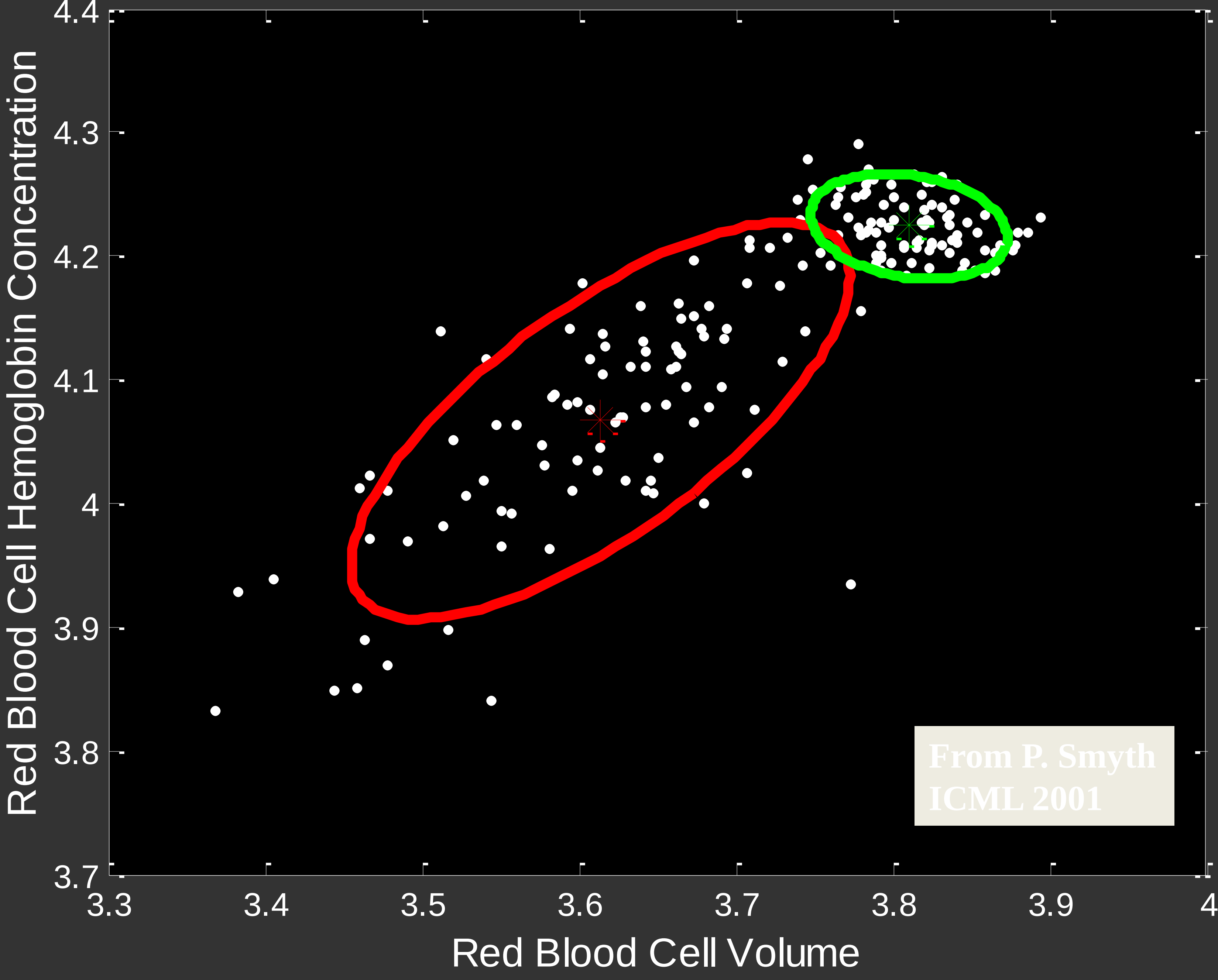
EM ITERATION 15



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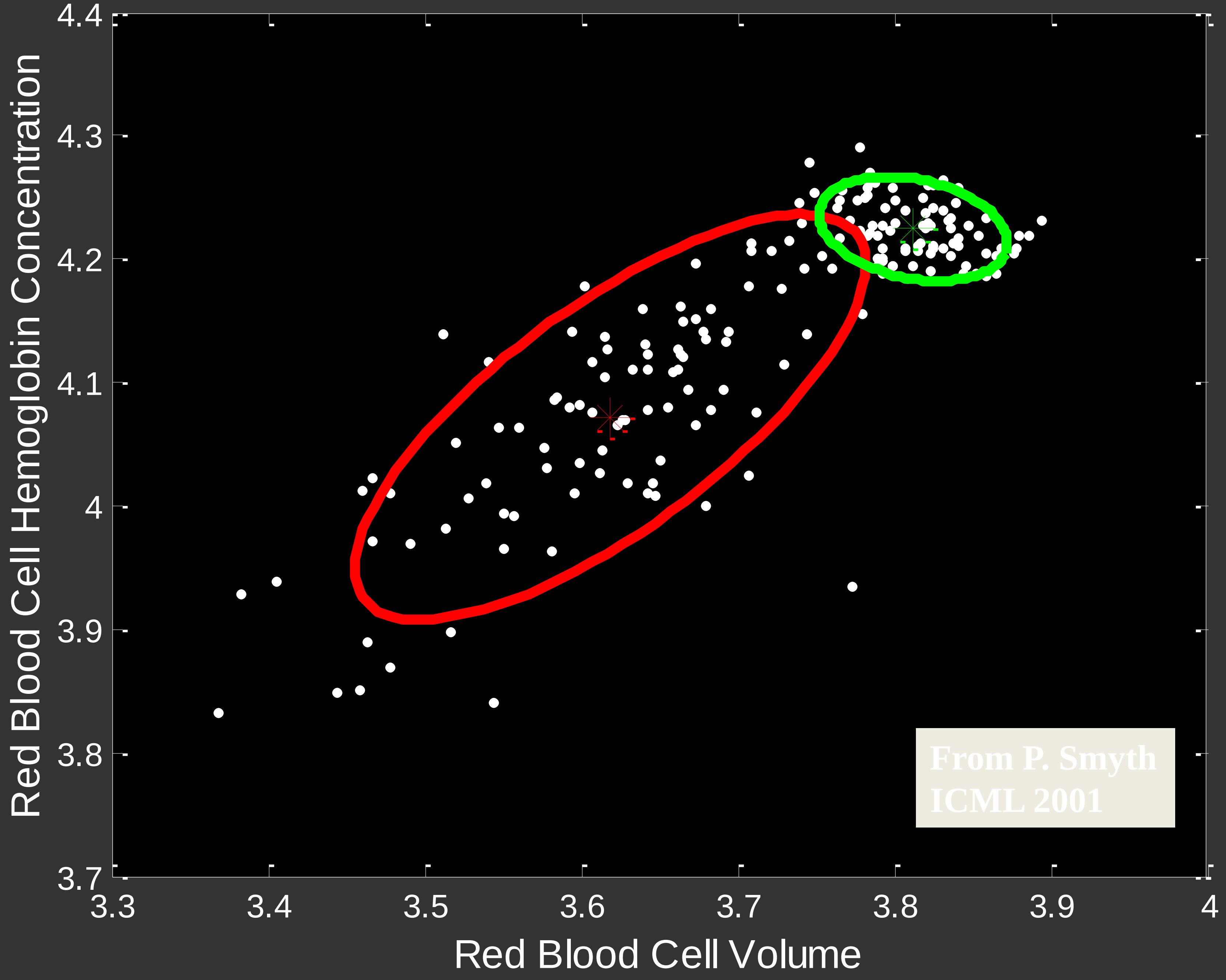
EM ITERATION 25



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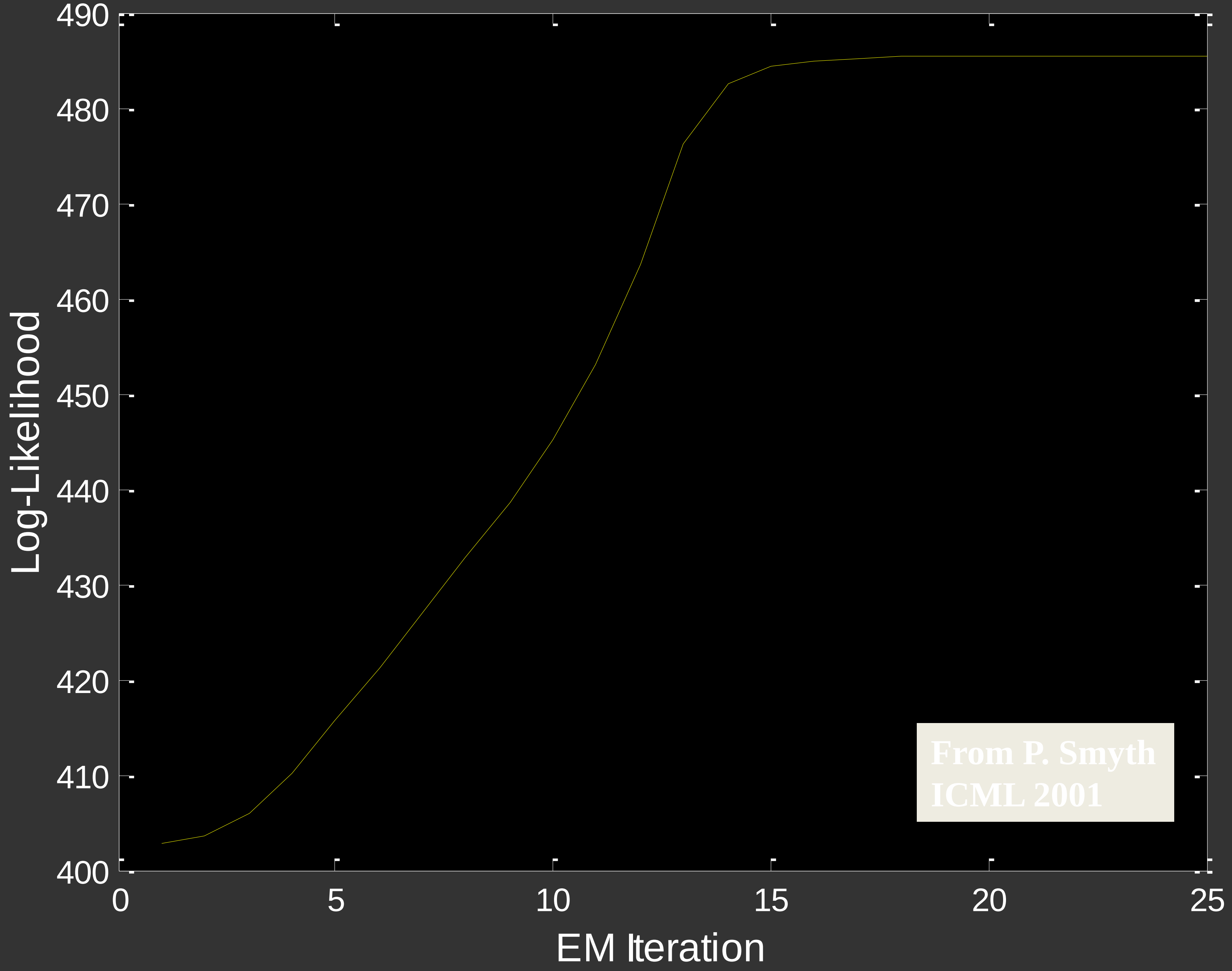
LOG-LIKELIHOOD AS A FUNCTION OF EM ITERATIONS



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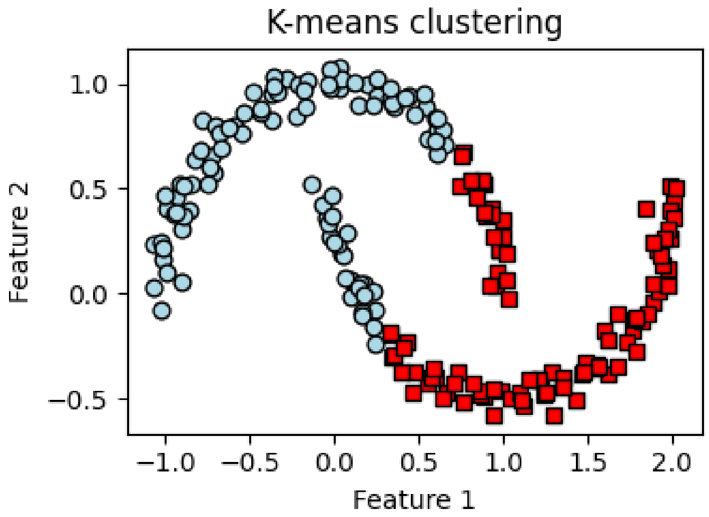
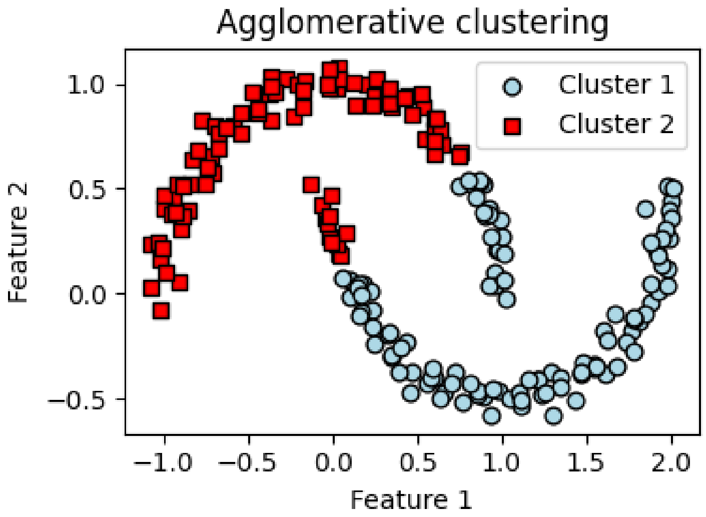
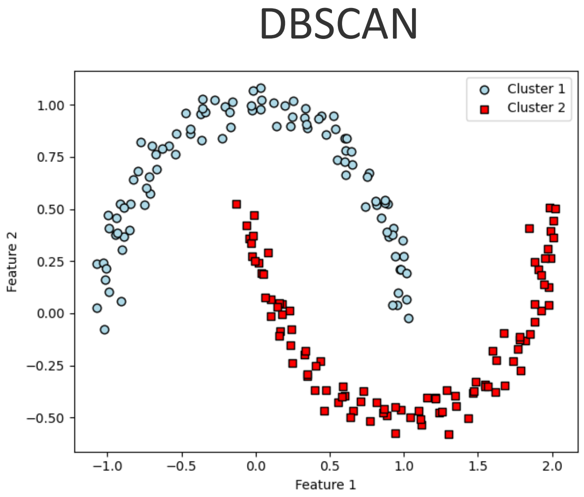
Density Based Clustering


K-means clustering


Agglomerative clustering

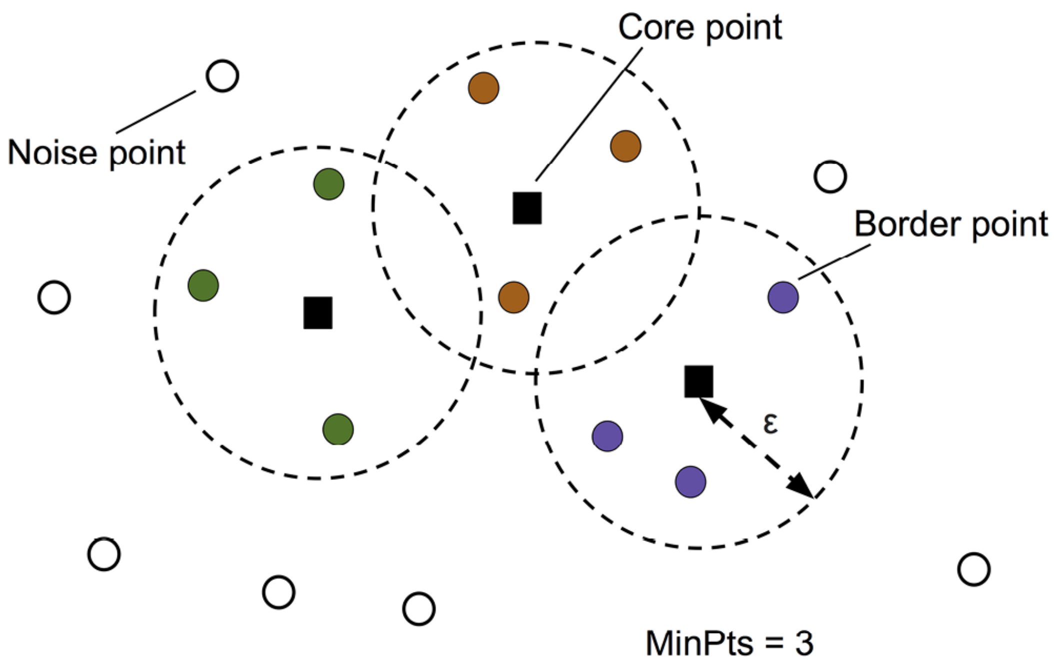

DBSCAN

- Relies on a *density-based* notion of cluster: A *cluster* is defined as a maximal set of density-connected points
- Discovers clusters of arbitrary shape in spatial databases with noise

Density Based Clustering

- Two parameters**:**
  - ***Eps***: Maximum radius of the neighbourhood
  - ***MinPts***: Minimum number of points in an Eps-neighbourhood of that point
- $N_{Eps}(p)$: $\{q \text{ belongs to } D \mid dist(p,q) <= Eps\}$
- Directly density-reachable**:** A point ***p*** is directly density-reachable from a point ***q*** wrt. ***Eps***, ***MinPts*** if
  - ***p*** belongs to $N_{Eps}(q)$
  - core point condition: $|N_{Eps}(q)| >= MinPts$

Density Based Clustering



- Arbitrary select a point ***p***
- Retrieve all points density-reachable from ***p*** wrt ***Eps*** and ***MinPts***.
- If ***p*** is a core point, a cluster is formed.
- If ***p*** is a border point, no points are density-reachable from ***p*** and DBSCAN visits the next point of the database.
- Continue the process until all of the points have been processed.

Summary

- In clustering, clusters are inferred from the data without human input (unsupervised learning)

- However, in practice, it is very domain specific:
  - Definition of distance in data space
  - Representation of data
  - Defining distance between clusters
  - Number of clusters
  - And so on.

- Practice, practice, practice!