K-means and Hierarchical Clustering

Schwartz

August 15, 2017

Best. Music. *EVAR*

1. Elliott Smith
2. Sufjan Stevens
3. Iron and Wine
4. Damien Rice

1. Die Antwoord
2. Kendrick Lamar
3. Dan le Sac Vs Scroobius Pip

1. Rufus Wainwright
2. Lyle Lovett
3. Julie Doiron

1. D'Gary
2. Kishi Bashi
3. Christine and the Queens
4. Beirut

1. Rage Against the Machine
2. System of a Down
3. Smashing Pumpkins

1. Beck
2. Cake
3. Beastie Boys

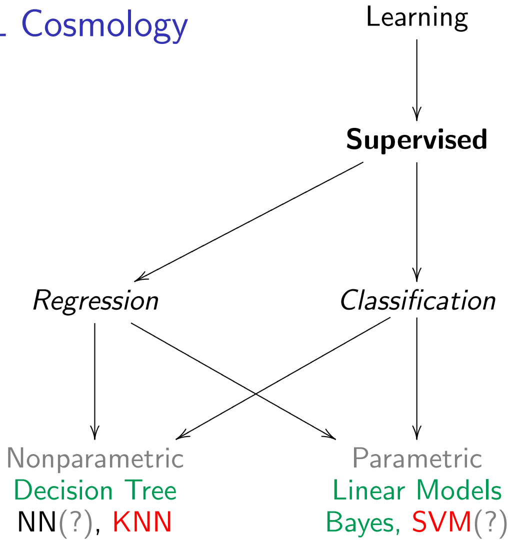
Objectives

- Review *Supervised* versus *Unsupervised*
- K-means (not to be confused with KNN)
  - and the curse of dimensionality
  - *norms* and the curse of dimensionality
  - more about the curse of dimensionality
- Choosing K
  - Elbow, Silhouette, and Gap methods
- Hierarchical clustering
- DBSCAN
- Bayesian mixture models
- Expectation-Maximization (EM) algorithm

ML Cosmology

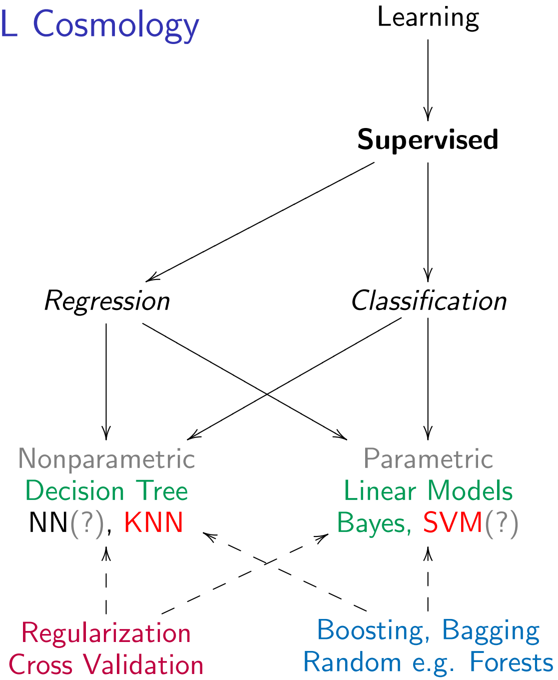
$$
\begin{tikzcd}
& \text{Learning} \arrow[d] \\
& \textbf{Supervised} \arrow[dl] \arrow[d] \\
\textit{Regression} & \textit{Classification}
\end{tikzcd}
$$

ML Cosmology



Continuous?
Categorical

ML Cosmology



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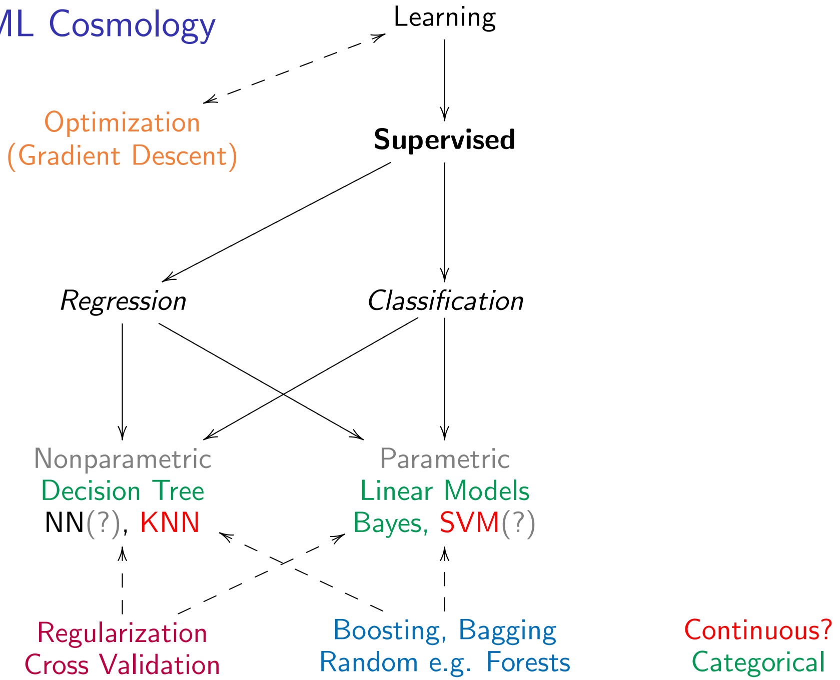

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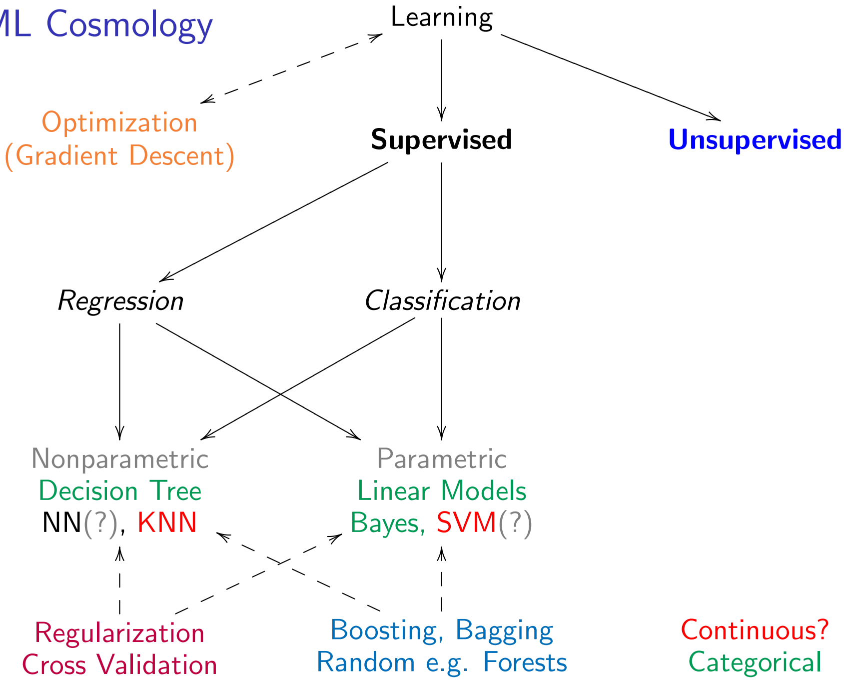

ML Cosmology

Learning

Optimization
(Gradient Descent)

Supervised

Unsupervised

Regression

Classification

K-means
Hierarchical
Clustering, PCA
... and so on ...

Nonparametric
Decision Tree
NN(?), KNN

Parametric
Linear Models
Bayes, SVM(?)

Regularization
Cross Validation

Boosting, Bagging
Random e.g. Forests

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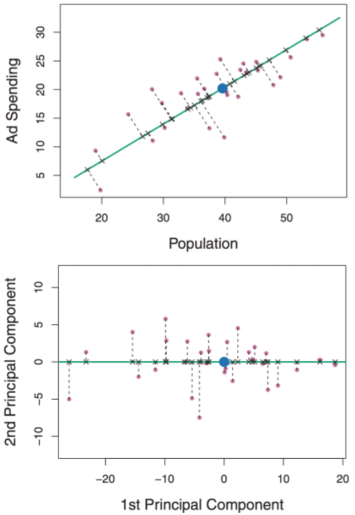
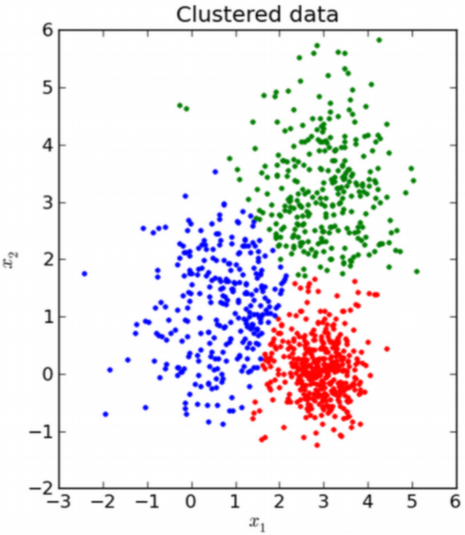
Categorical

Unsupervised learning





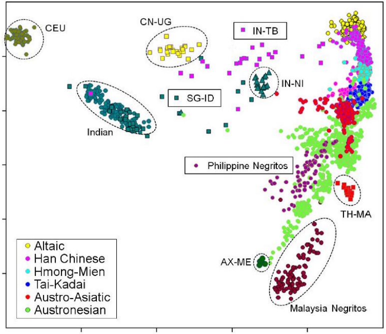
Low dimensional representations of data capturing data variation

Homogeneous subgroups capturing data substructure

Supervised versus Unsupervised

Human Genetic Diversity in Asia

Two-Dimensional Representation



Supervised versus Unsupervised

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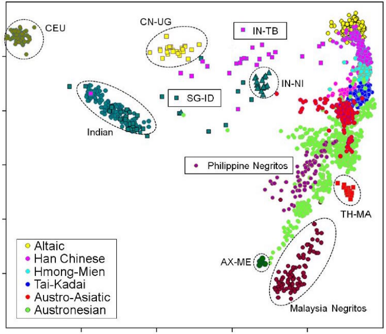

Unsupervised learning provides

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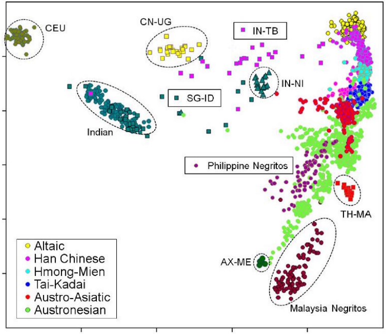

Unsupervised learning provides

- exploratory data analysis (EDA) to look at/uncover feature structure

Supervised versus Unsupervised

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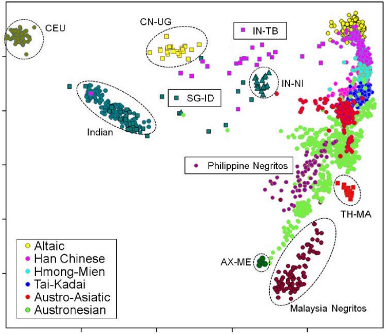

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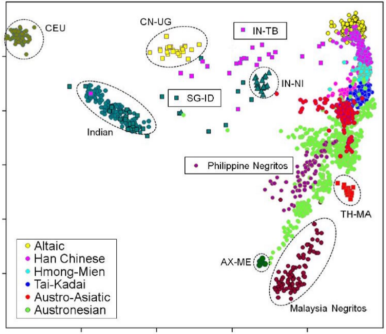

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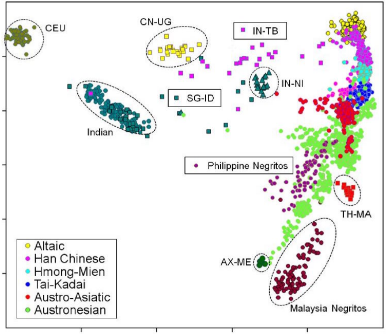

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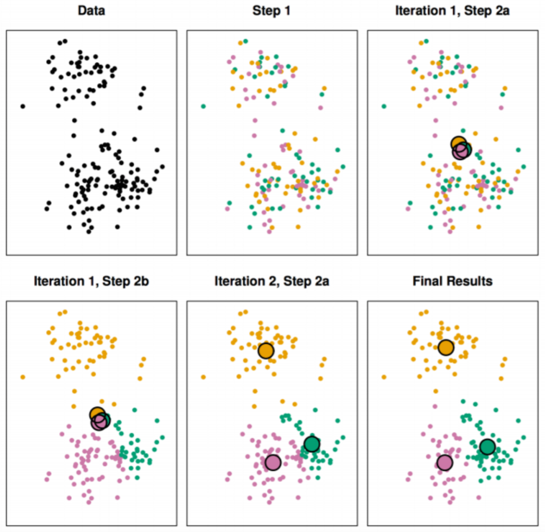
"Labels" are sometimes used to facilitate these objectives but unlike supervised learning, unsupervised learning is not necessarily immediately concerned with predicting outcomes (labels, targets, Y, dependent/endogenous variables)

K-Means

1. Choose *number of clusters*, K
2. Randomly assign data to each cluster k
3. Compute the centroid for each cluster k
4. Assign data to the cluster with the closest centroid
5. Return to step 3, unless the centroids have stabilized



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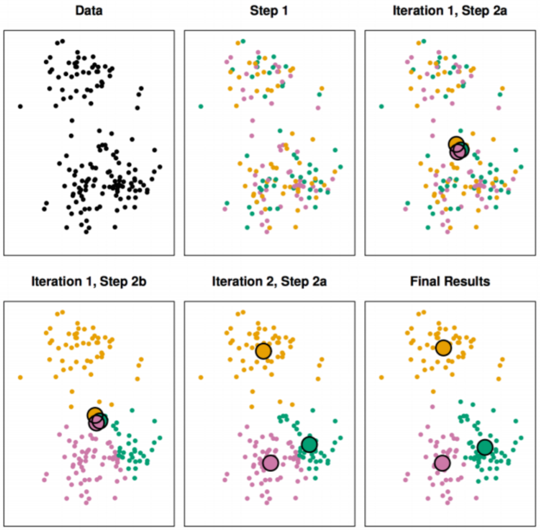
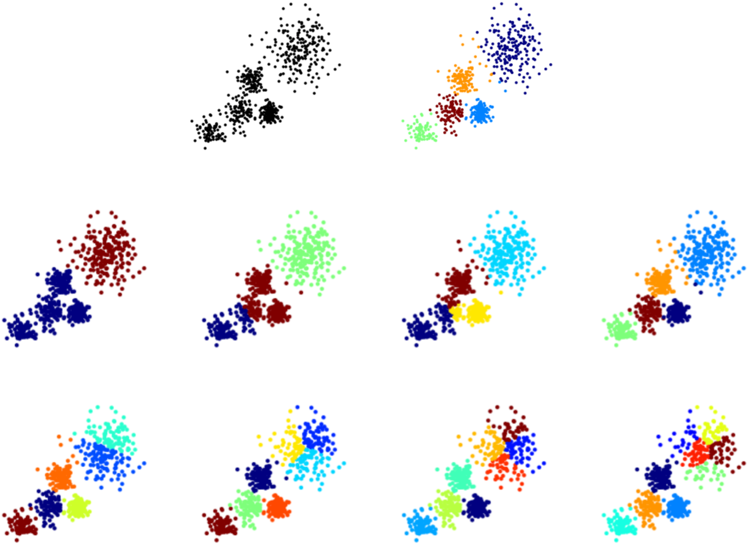


Other init. ideas?

K?



Elbow and Silhouette methods

For some clustering

$C_K(i) \mapsto \{1, 2, \cdots K\}$

clustering fit can be measured as

$$W(C_K) = \frac{1}{K} \sum_{C_K(i)=C_K(j)=k} ||x_i - x_j||^2$$

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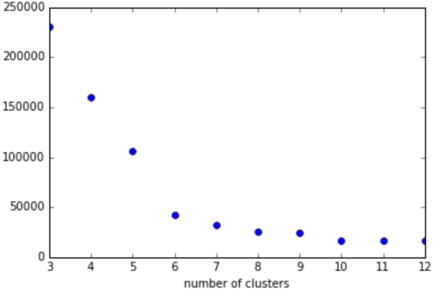
Select based on diminishing returns



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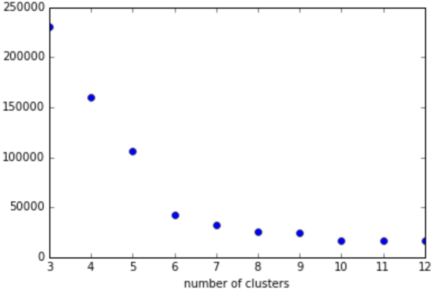

$\bar{\Delta}_i^k$: x_i's dissimilarity in cluster k

$\bar{\Delta}_i^{k'}$: x_i's dissimilarity to cluster k'

(x_i in, & closest to clusters k, k')

$$Silhouette(i) = \frac{\bar{\Delta}_i^{k'} - \bar{\Delta}_i^k}{\max(\bar{\Delta}_i^{k'}, \bar{\Delta}_i^k)}$$

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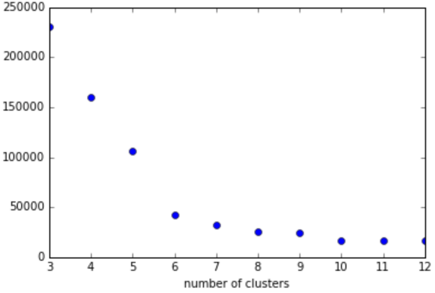
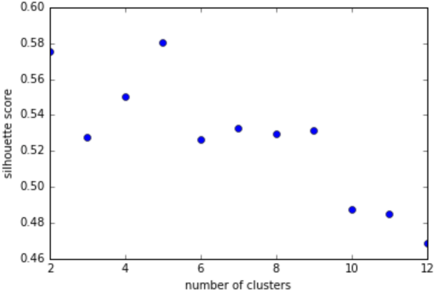


Compare average silhouette scores



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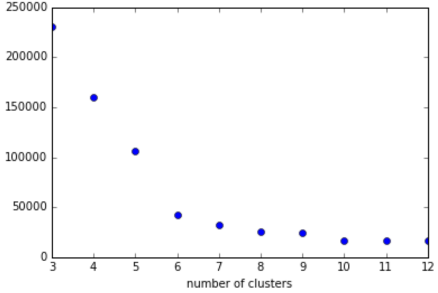
Interpret silhouette scores?

Select based on diminishing returns



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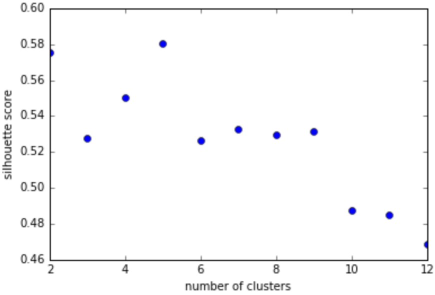

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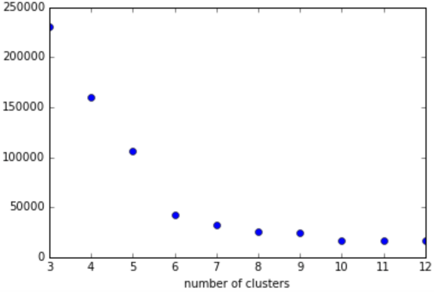
Does the scaling of the x matter?

Select based on diminishing returns



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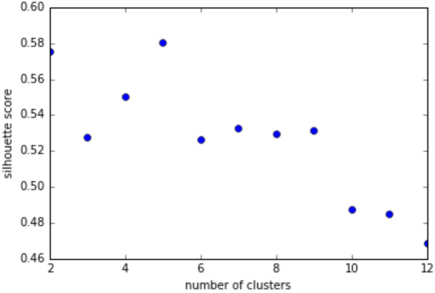

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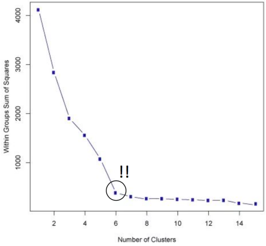

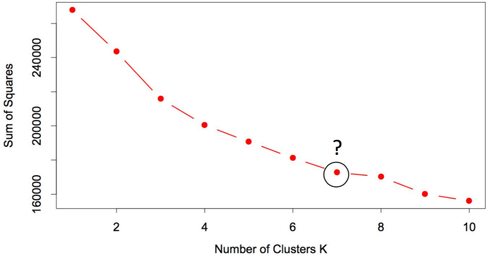

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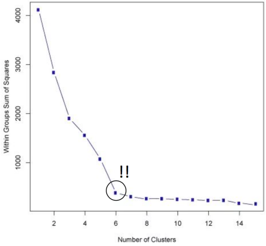

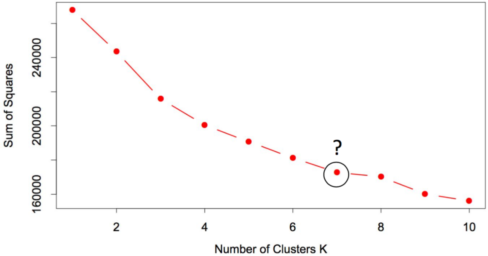

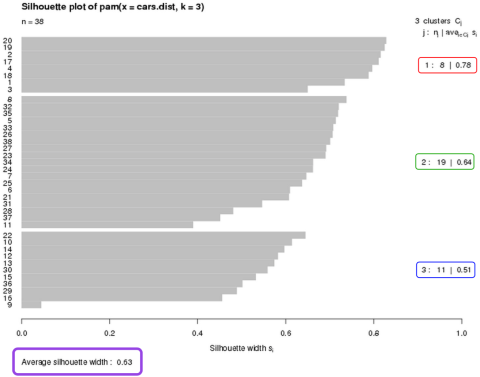

<u>Guidelines for Overall Avg Silhouette</u>

Range	Interpretation
0.71 – 1.0	Strong structure found
0.51 – 0.7	Reasonable structure
0.26 – 0.5	Structure weak/artificial
< 0.25	No substantial structure

The *permutation test*

- Students enrolling for a popular class get ids $i = 1, \cdots n$. As the class quickly fills, another section of the class is opened and students for that class are given ids $i = n + 1, \cdots 2n$.

```
id = np.array([ 1,  2,  3,  4,  5,  6,  7,  8,  9, 10, 11, 12, 13, 14, 15, 16, 17,
               18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34,
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- The classes have the same tests...
  How could we test which class is doing better?

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score = np.array([59, 92, 93, 83, 92, 61, 84, 92, 70, 93, 76, 70, 84, 61, 75, 91, 73,
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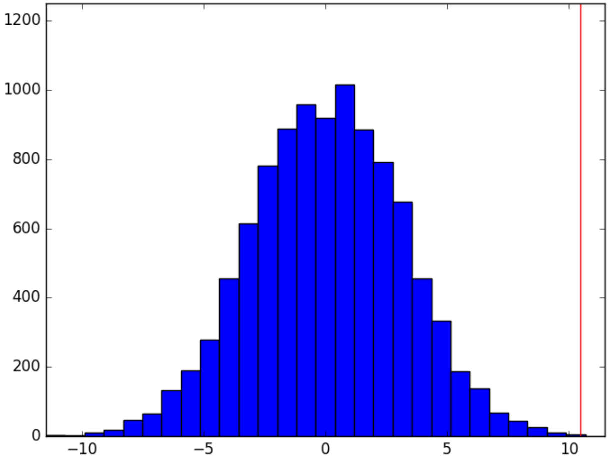
1. Repeatedly permute the index and recalculating the test statistic each time
2. These samples approximate the test statistic distribution under the null
3. Compare the test statistic to this null distribution
   to suggest how "strange" the actual observed test statistic is if the null is true

The *permutation test* *(This is my **favorite** test, btw)*

1. Permute the ids (i.e., believe the null is true: ids don't matter)
2. Recalculate the test statistic each time (under null)
3. See how strange your observed statistic is compared to nulls



The *permutation test* and the *null distribution*

- What was needed in the permutation test was really the distribution of the test statistic under the null hypothesis

The *permutation test* and the *null distribution*

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The *permutation test* and the *null distribution*

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- We can test against *ANY* null distribution we wish to propose

The Gap statistic

Then choose the smallest K such that $\text{Gap}(K) \geq \text{Gap}(K+1) - s_{K+1}$

412 *R. Tibshirani, G. Walther and T. Hastie*

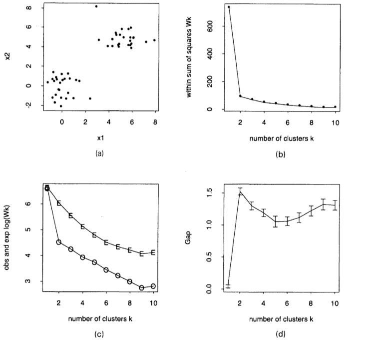

Fig. 1. Results for the two-cluster example: (a) data; (b) within sum of squares function W_k; (c) functions $\log(W_k)$ (O) and $\hat{E}^*_n\{\log(W_k)\}$ (E); (d) gap curve

416 *R. Tibshirani, G. Walther and T. Hastie*

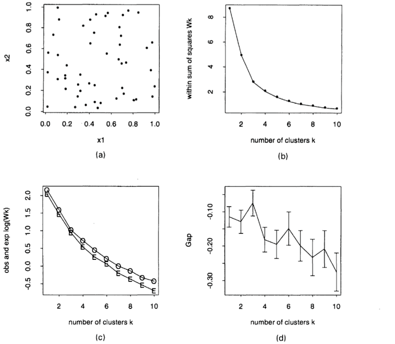

Fig. 2. Results for the uniform data example: (a) data; (b) within sum of squares function W_k; (c) functions $\log(W_k)$ (O) and $\hat{E}^*_n\{\log(W_k)\}$ (E); (d) gap curve

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For M null distribution samples, calculate

$$\text{Gap}(K) = \bar{l} - \log W^{(*)}(C_K) \quad \text{and} \quad s_K = \sqrt{\frac{1}{R}\sum_{j=1}^{M}\left(\log W^{(r)}(C_K) - \bar{l}\right)^2}$$

$$\text{where } W^{(r)}(C_K) = \sum_{C_K(i)=C_K(j)=k} ||x_i^{(r)} - x_j^{(r)}||^2 \quad \text{and} \quad \bar{l} = \frac{1}{R}\sum_{r=1}^{R}\log W^{(r)}(C_K)$$

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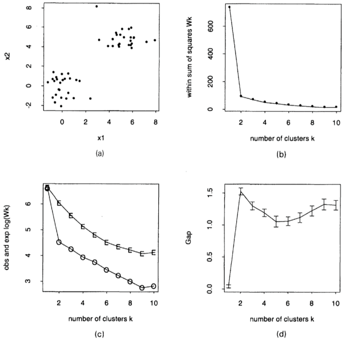

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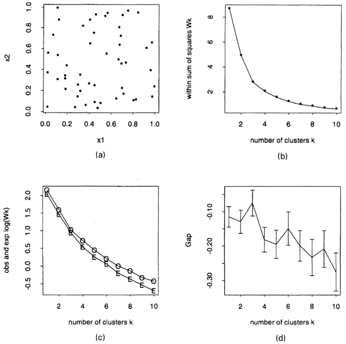

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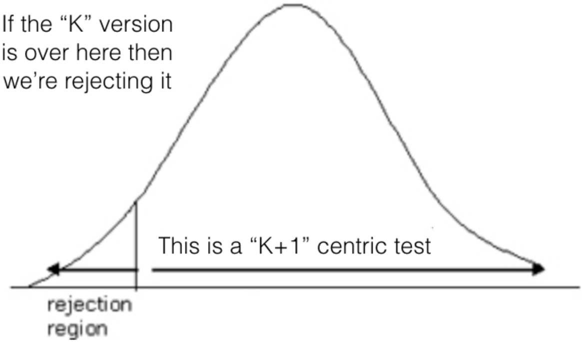

The Curse of Dimensionality

Just as nearest neighbors breaks down in high dimensional space...
Distance based clustering breaks down in high dimensional space...

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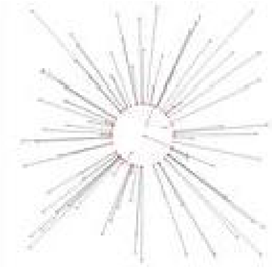
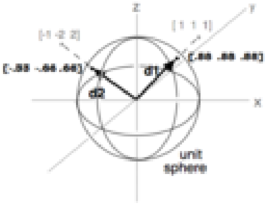
However, when we normalize a vector (e.g., turn bag-of-words into probabilities, or make it a unit vector) we project all vectors onto a *manifold* where "locality" and "neighborhoods" make sense again.



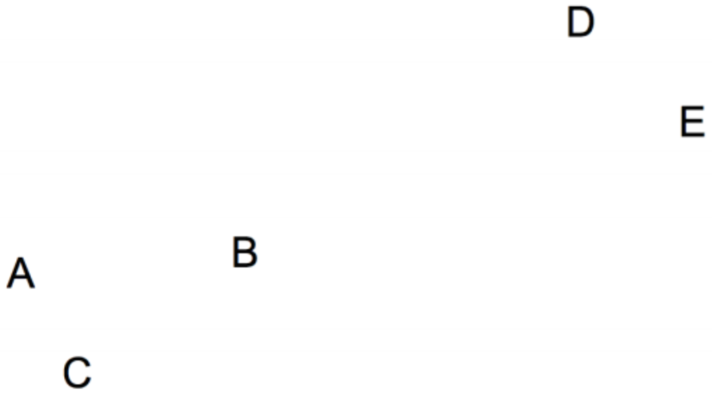


The Curse of Dimensionality

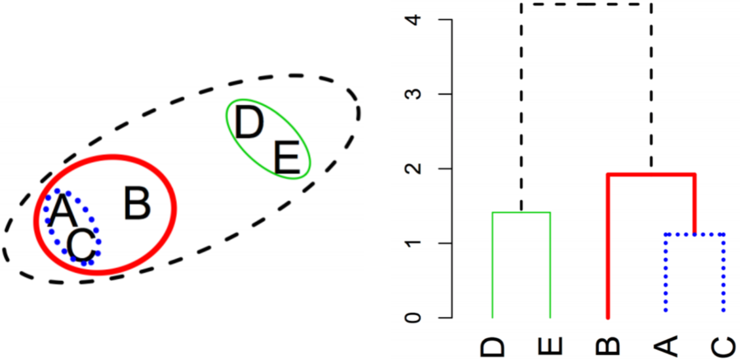
So who is effected by *The Curse of Dimensionality* and *why (not)?*

Hint: *Overfitting* and
The Curse of Dimensionality are
slightly different things...

Challenge

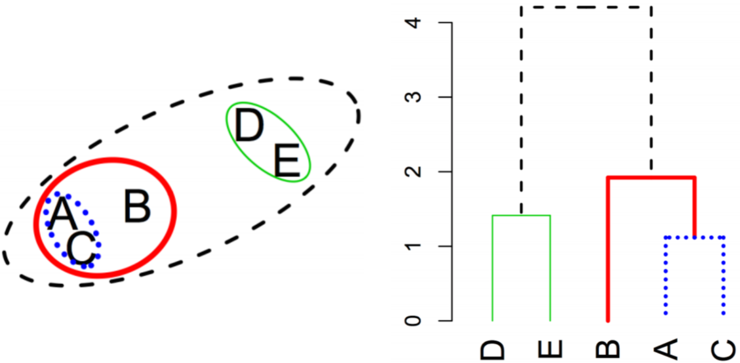


Hierarchical clustering



1. Assign each point to it's own cluster

Hierarchical clustering



1. Assign each point to it's own cluster
2. Computer pairwise cluster distances

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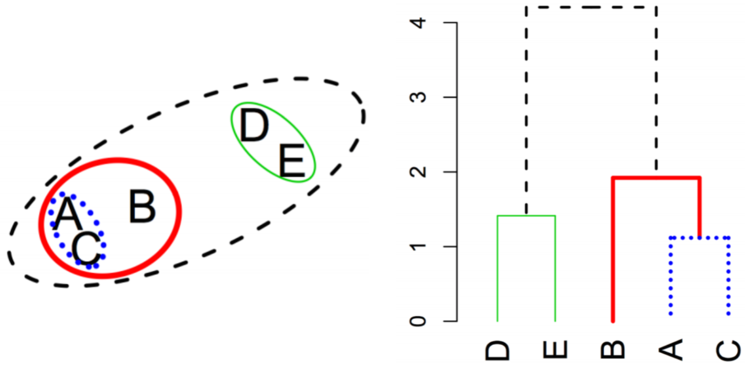

1. Assign each point to it's own cluster
2. Computer pairwise cluster distances
3. Merge *closest two* clusters

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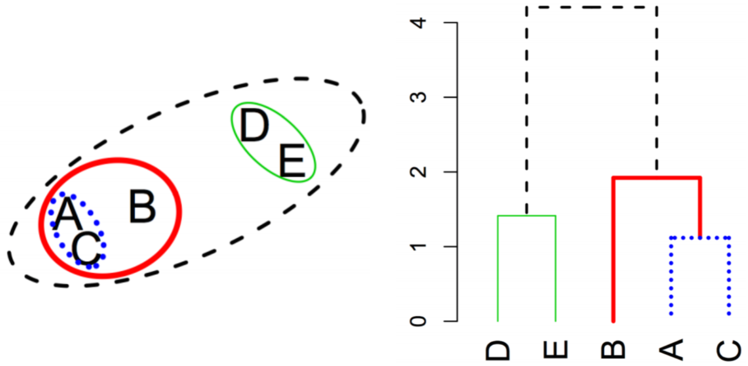

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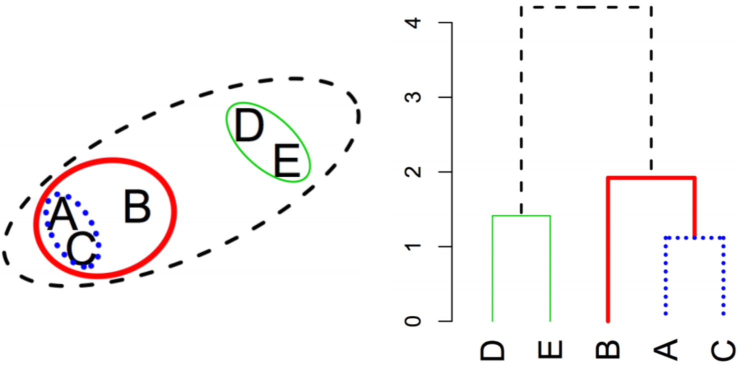

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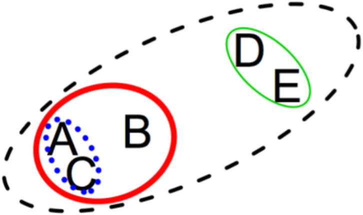
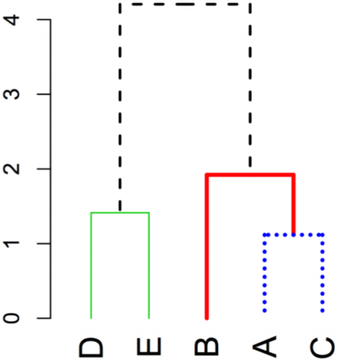
- Single: minimum pairwise point dissimilarity
- Complete: maximum pairwise point dissimilarity
- Average: average pairwise point dissimilarity
- Centroid: centroid dissimilarity

Hierarchical clustering





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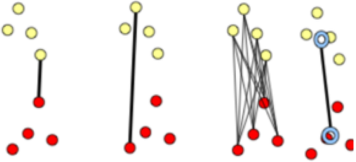

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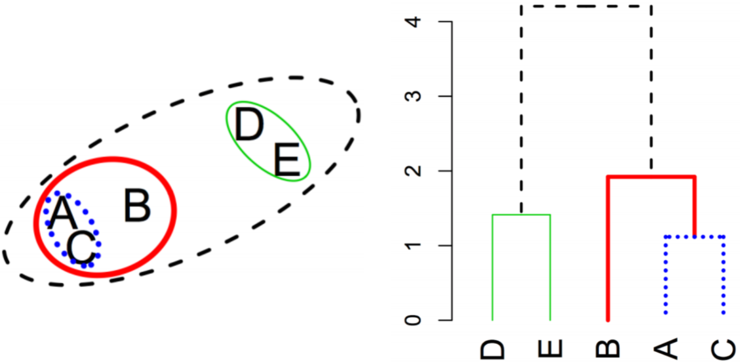

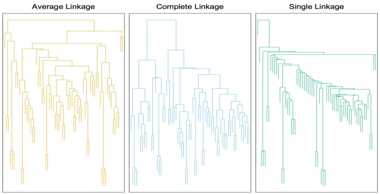

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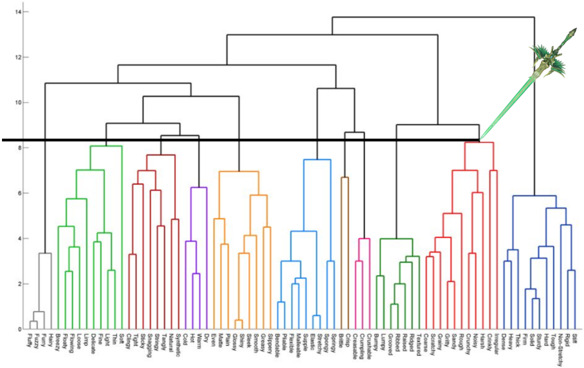
Hierarchical clustering

Clusterings are created based on distance between proposed merges

And then the number of clusters can be chosen *just like* K-means...



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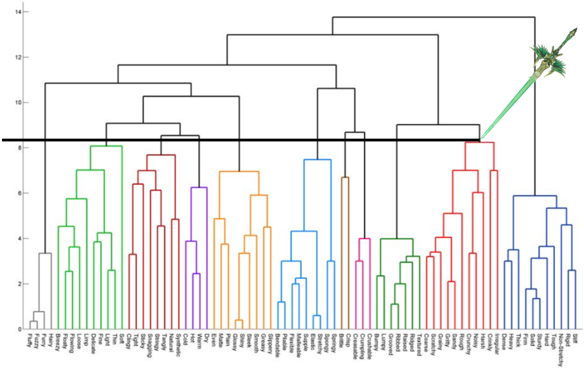
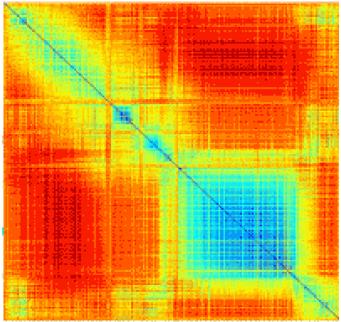
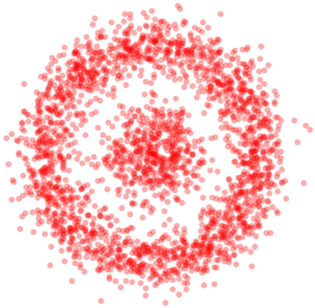




This is super cool, but
unlike K-means, hierarchical clustering requires all pairwise comparisons so it doesn't scale gracefully with increasing data...

DBSCAN



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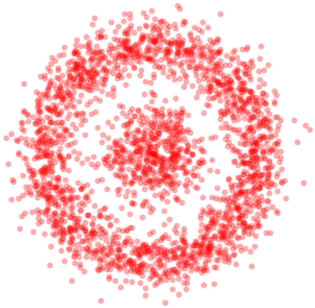

- Specify connection distance ϵ and minimum number of points for core m

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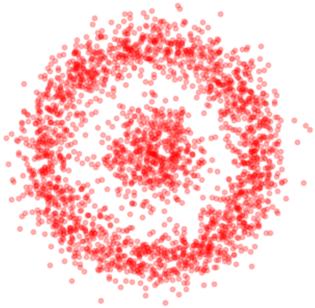

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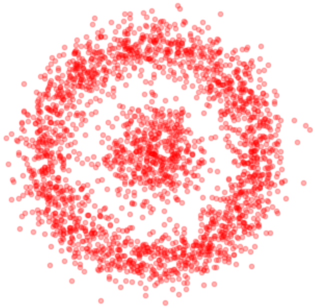

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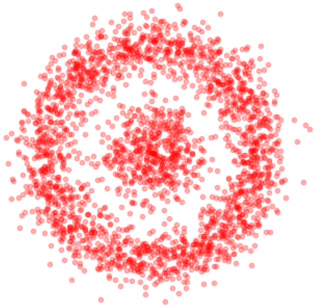

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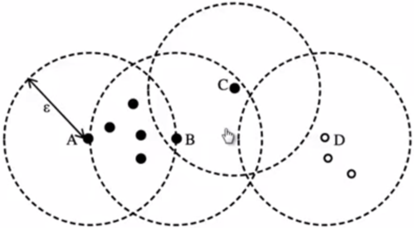

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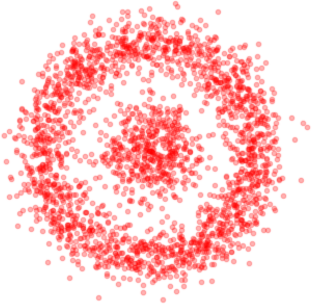

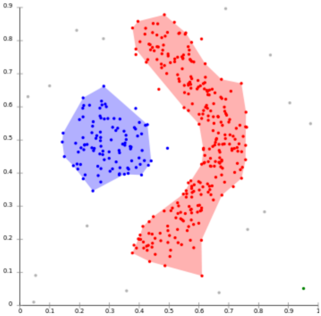

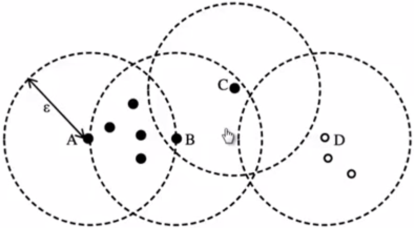

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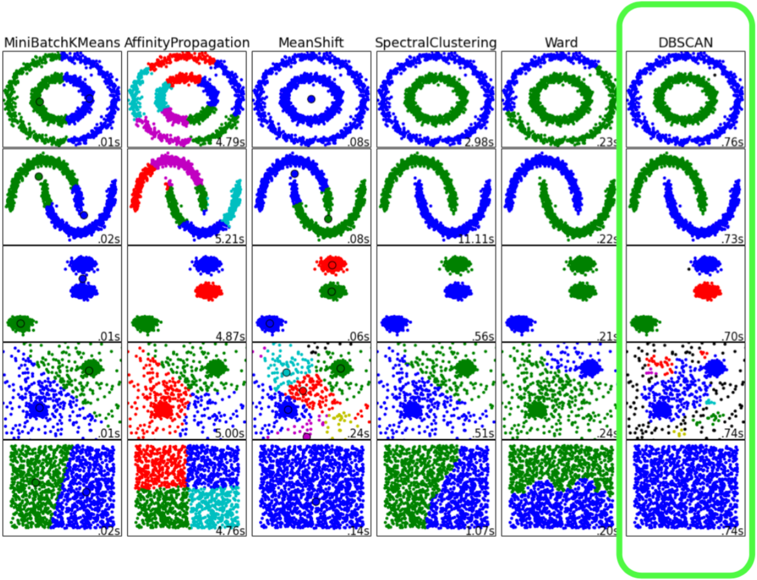
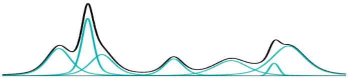

MiniBatchKMeans
AffinityPropagation
MeanShift
SpectralClustering
Ward
DBSCAN
.01s
4.79s
.08s
2.98s
.23s
.76s
.02s
5.21s
.08s
11.11s
.22s
.73s
.01s
4.87s
.06s
.56s
.21s
.70s
.01s
5.00s
.24s
.51s
.24s
.74s
.02s
4.76s
.14s
1.07s
.20s
.74s

Bayesian Mixture Models *(xtra: my grad school jam)*

$$f(X_i | \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi}, \boldsymbol{\pi}) = \sum_{k=1}^{K} \pi_k N(\mu_k, \sigma_k^2)$$



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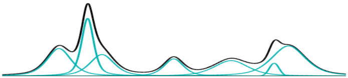
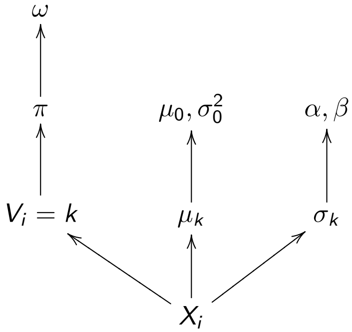


$$\begin{aligned} f(X_i|V_i, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi}) &= N(\mu_k, \sigma_k^2) \\ \Pr(\boldsymbol{V}_i) &= Multinomial(\boldsymbol{\pi}, n = 1) \\ f(\boldsymbol{\pi}) &= Dirichlet(\boldsymbol{\omega}) \\ f(\mu_k) &= N(\mu_0, \sigma_0^2) \\ f(\sigma_k^{-2}) &= Gamma(\alpha, \beta) \end{aligned}$$



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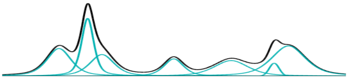

$$\begin{tikzcd}
\omega & & \\
\pi \arrow[u] & \mu_0, \sigma_0^2 & \alpha, \beta \\
V_i = k \arrow[u] & \mu_k \arrow[u] & \sigma_k \arrow[u] \\
& X_i \arrow[ul] \arrow[u] \arrow[ur] &
\end{tikzcd}$$

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\end{aligned}$$

$$\begin{aligned}
&f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi}|\mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega}) = \\
&\prod_{i=1}^{n} \left[\left(\sum_{k=1}^{K} 1_{[V_{ik}=1]} \frac{1}{\sqrt{2\pi}\sigma_k} e^{-\frac{1}{2}\left(\frac{X_i - \mu_k}{\sigma_k}\right)^2} \right) \left(\prod_{k=1}^{K} \pi_k^{V_{ik}} \right) \right] \\
&\quad \times \left(\prod_{k=1}^{K} \frac{1}{\sqrt{2\pi}\sigma_0} e^{-\frac{1}{2}\left(\frac{\mu_k - \mu_0}{\sigma_0}\right)^2} \frac{\beta^\alpha}{\Gamma(\alpha)} \left(\frac{1}{\sigma^2}\right)^{\alpha - 1} e^{-\beta \frac{1}{\sigma^2}} \right) \left(\frac{1}{\mathbf{B}(\omega)} \prod_{k=1}^{K} \pi_k^{\omega_k - 1} \right)
\end{aligned}$$

Markov Chain Monte Carlo (MCMC) *posterior sampling*

A Gibbs sampler for the posterior

$$f(\mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

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Is made by cycling through the *full conditional distributions*

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$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$f(\sigma_k^2 | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Markov Chain Monte Carlo (MCMC) *posterior sampling*

A Gibbs sampler for the posterior

$$f(\mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Is made by cycling through the *full conditional distributions*

$$f(\mu_k | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$f(\sigma_k^2 | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(V_{ik} = 1 | \mathbf{X}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

Markov Chain Monte Carlo (MCMC) *posterior sampling*

A Gibbs sampler for the posterior

$$f(\mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Is made by cycling through the *full conditional distributions*

$$f(\mu_k | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$f(\sigma_k^2 | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(V_{ik} = 1 | \mathbf{X}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Markov Chain Monte Carlo (MCMC) *posterior sampling*

A Gibbs sampler for the posterior

$$f(\mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Is made by cycling through the *full conditional distributions*

$$f(\mu_k | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$f(\sigma_k^2 | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(V_{ik} = 1 | \mathbf{X}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(\boldsymbol{\pi} | \mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

Markov Chain Monte Carlo (MCMC) *posterior sampling*

A Gibbs sampler for the posterior

$$f(\mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Is made by cycling through the *full conditional distributions*

$$f(\mu_k | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$f(\sigma_k^2 | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(V_{ik} = 1 | \mathbf{X}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(\boldsymbol{\pi} | \mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Markov Chain Monte Carlo (MCMC) *posterior sampling*

A Gibbs sampler for the posterior

$$f(\mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Is made by cycling through the *full conditional distributions*

$$f(\mu_k | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$f(\sigma_k^2 | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(V_{ik} = 1 | \mathbf{X}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(\boldsymbol{\pi} | \mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Markov Chain Monte Carlo (MCMC) *posterior sampling*

A Gibbs sampler for the posterior

$$f(\mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Is made by cycling through the *full conditional distributions*

$$f(\mu_k | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$f(\sigma_k^2 | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(V_{ik} = 1 | \mathbf{X}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(\boldsymbol{\pi} | \mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Markov Chain Monte Carlo (MCMC) *posterior sampling*

A Gibbs sampler for the posterior

$$f(\mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Is made by cycling through the *full conditional distributions*

$$f(\mu_k | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$f(\sigma_k^2 | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(V_{ik} = 1 | \mathbf{X}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(\boldsymbol{\pi} | \mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Markov Chain Monte Carlo (MCMC) *posterior sampling*

A Gibbs sampler for the posterior

$$f(\mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Is made by cycling through the *full conditional distributions*

$$f(\mu_k | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$f(\sigma_k^2 | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(V_{ik} = 1 | \mathbf{X}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(\boldsymbol{\pi} | \mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Markov Chain Monte Carlo (MCMC) *posterior sampling*

A Gibbs sampler for the posterior

$$f(\mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Is made by cycling through the *full conditional distributions*

$$f(\mu_k | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$f(\sigma_k^2 | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(V_{ik} = 1 | \mathbf{X}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(\boldsymbol{\pi} | \mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Markov Chain Monte Carlo (MCMC) *posterior sampling*

A Gibbs sampler for the posterior

$$f(\mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Is made by cycling through the *full conditional distributions*

$$f(\mu_k | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$f(\sigma_k^2 | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(V_{ik} = 1 | \mathbf{X}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(\boldsymbol{\pi} | \mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Markov Chain Monte Carlo (MCMC) *posterior sampling*

A Gibbs sampler for the posterior

$$f(\mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Is made by cycling through the *full conditional distributions*

$$f(\mu_k | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$f(\sigma_k^2 | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(V_{ik} = 1 | \mathbf{X}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(\boldsymbol{\pi} | \mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Markov Chain Monte Carlo (MCMC) *posterior sampling*

A Gibbs sampler for the posterior

$$f(\mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Is made by cycling through the *full conditional distributions*

$$f(\mu_k | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$f(\sigma_k^2 | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(V_{ik} = 1 | \mathbf{X}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

$$\Pr(\boldsymbol{\pi} | \mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$

$$\propto f(\mathbf{X}, \mathbf{V}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi} | \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega})$$ (which is proportional to the joint distribution)

Markov Chain Monte Carlo (MCMC) *full conditionals*

$$\Pr(V_{ik} = 1 | \mathbf{X}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2, \boldsymbol{\pi}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega}) \propto \pi_k \frac{1}{\sqrt{2\pi}\sigma_k} e^{-\frac{1}{2}\left(\frac{X_i - \mu_k}{\sigma_k}\right)^2}$$

$$f(\pi | \mathbf{V}, \boldsymbol{mu}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega}) = Dirichlet(\{\omega_k + n_k : k = 1, \cdots K\})$$

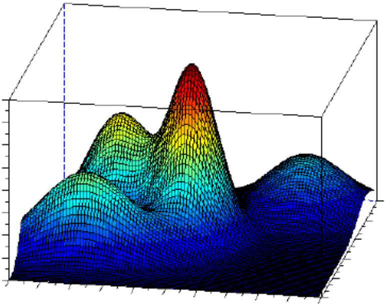
$$n_k = \sum_{V_{ik}=1} 1$$

$$f(\sigma_k^2 | \mathbf{V}, \boldsymbol{\mu}, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega}) = Gamma\left(\frac{n_k}{2} + \alpha, \frac{1}{2} \sum_{V_{ik}=1} (X_i - \mu_k)^2 + \beta\right)$$

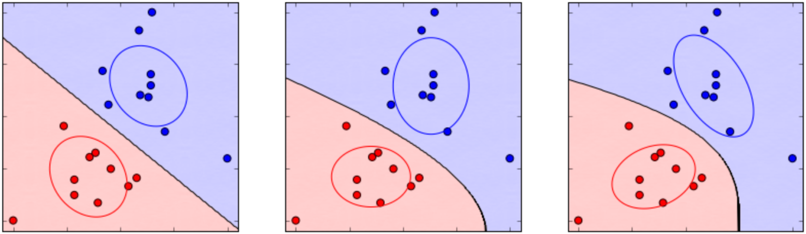
$$f(\mu_k | \mathbf{V}, \boldsymbol{\sigma}^2, \mathbf{X}, \mu_0, \sigma_0^2, \alpha, \beta, \boldsymbol{\omega}) =$$

$$\mathrm{N}\left(\hat{\sigma}_k^2 \left(\frac{\sum_{V_{ik}=1} X_i}{\sigma_k^2} + \frac{\mu_0}{\sigma_0^2}\right), \hat{\sigma}_k^2 = \left(\frac{n_k}{\sigma_k^2} + \frac{1}{\sigma_0^2}\right)^{-1}\right)$$

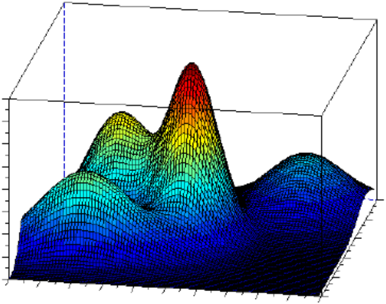
Mixture Models!



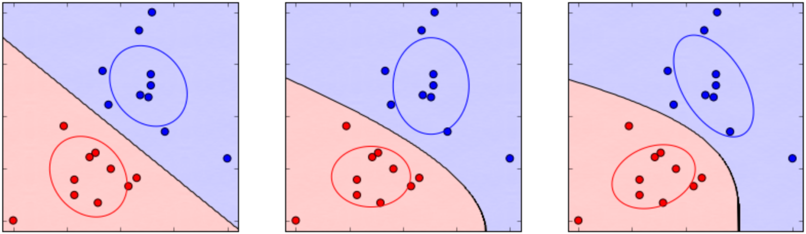
- Used to model "subpopulations"



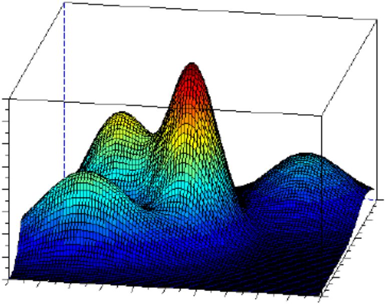
Mixture Models!



- Used to model "subpopulations"
- Or simply complex distributional shapes



Mixture Models!



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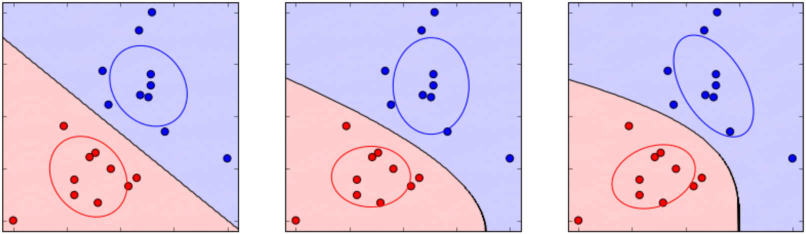

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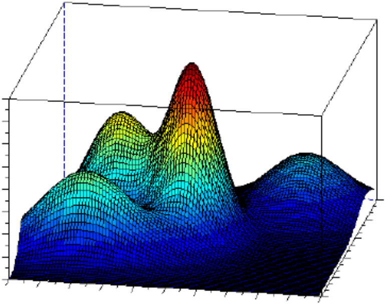

- Used to model "subpopulations"
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- It's *almost nonparametric* like kernel density estimation
- Expectation-Maximization (EM) algorithm is another way to fit mixture models