Clustering: Automatic Selection of $k$, Hierarchical Clustering

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Automatic Selection of $k$

Dirichlet Process Gaussian Mixture Model (DP-GMM):

- Number of clusters is effectively random, and can grow with the amount of data you have!

- While you don't have to choose $k$, you have to choose a different parameter which says basically how likely new points are to form new clusters vs join existing clusters.
### DP-GMM High-Level Idea

<table>
<thead>
<tr>
<th>Cluster 1</th>
<th>Cluster 2</th>
<th>Cluster 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Probability of generating a point from cluster 1 = $\pi_1$</td>
<td></td>
<td>There is a parameter that controls how these $\pi$ values roughly decay $\pi_2$, $\pi_3$, …</td>
</tr>
<tr>
<td>Gaussian mean = $\mu_1$</td>
<td>$\mu_2$</td>
<td>$\mu_3$</td>
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<tr>
<td>Gaussian covariance = $\Sigma_1$</td>
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(Rough idea) How to generate points from this DP-GMM:

1. Flip biased $\infty$-sided coin (the sides have probabilities $\pi_1$, $\pi_2$, $\pi_3$, …)
2. Let $Z$ be the side that we got (it is a positive integer)
3. Sample 1 point from Gaussian mean $\mu_Z$, covariance $\Sigma_Z$

*Remark: For any given dataset, when learning the DP-GMM, there aren't going to be an infinite number of clusters found*
Automatic Selection of $k$

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- Number of clusters is effectively random, and can grow with the amount of data you have!

- While you don't have to choose $k$, you have to choose a different parameter which says basically how likely you are to form new clusters vs try to stick to already existing clusters

- An example of a Bayesian nonparametric model (roughly: a generative model with an infinite number of parameters, where the parameters are random)
Learning a DP-GMM

Two main approaches:

• Finite approximation where you specify some maximum number of possible clusters (the algorithm will find up to that many clusters)

  This is what’s implemented in sklearn

• Algorithm is somewhat similar to $k$-means/EM for GMMs

• Algorithm output: very similar to regular GMM fitting

• Random sampling approach (no finite approximation needed!)

  • Algorithm output: a bunch of samples of different cluster assignments (can pick one with highest probability)

  This is what’s implemented in R (package dpmixsim)
Learning a DP-GMM

Demo
This next algorithm will give you a sense of how we get around specifying the number of clusters directly.

*k*-means approximates
(a special case of) learning GMM's.

What approximates learning DP-GMMs?

This next algorithm will give you a sense of how we get around specifying the number of clusters directly.
DP-means

Step 0. Pick concentration parameter $\lambda > 0$

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radius $\sqrt{\lambda}$
DP-means

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“Step 2b”. Assign closest points to current clusters
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   (a) If it’s not currently covered by gray balls, make it a new cluster center
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Repeat until convergence:

Step 2. For each point:
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Step 3. Recompute cluster centers
As you saw in the DP-GMM demo (and is similar with DP-means), DP-means can produce a few extra small clusters.

In practice: reassign points in small clusters to bigger clusters.
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In practice: reassign points in small clusters to bigger clusters.

Can recompute cluster centers.
Big picture: DP-means & DP-GMM have a “concentration” parameter roughly controlling size of clusters rather than number of clusters

If your problem can more naturally be thought of as having cluster sizes that should not be too large, can use DP-means/DP-GMM instead of k-means/GMM

Real example. Satellite image analysis of rural India to find villages

Each cluster is a village: don’t know how many villages there are total but rough upper bound on radius of village can be specified

→ DP-means provides a decent solution!
Other Ways for Choosing $k$

- Choose a cost function to compute for different $k$
  - In general, not easy! Need some intuition for what “good” clusters are
  - Ideally: cost function should relate to your application of interest
- Pick $k$ achieving lowest cost
Here’s an example of a cost function you don’t want to use

But hey it’s worth a shot
Residual Sum of Squares

Look at one cluster at a time

Cluster 1

Cluster 2
Residual Sum of Squares

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Cluster 2

Residual sum of squares for cluster 1: sum of squared purple lengths
Residual Sum of Squares

Look at one cluster at a time

Measure distance from each point to its cluster center

Residual sum of squares for cluster 1:

$$RSS_1 = \sum_{x \in \text{cluster 1}} \|x - \mu_1\|^2$$
Residual Sum of Squares

Look at one cluster at a time

Measure distance from each point to its cluster center

Repeat similar calculation for other clusters

Residual sum of squares for cluster 2:

\[ \text{RSS}_2 = \sum_{x \in \text{cluster } 2} \|x - \mu_2\|^2 \]
Residual Sum of Squares

\[ \text{RSS} = \text{RSS}_1 + \text{RSS}_2 = \sum_{x \in \text{cluster } 1} \| x - \mu_1 \|^2 + \sum_{x \in \text{cluster } 2} \| x - \mu_2 \|^2 \]

In general if there are \( k \) clusters:

\[ \text{RSS} = \sum_{g=1}^{k} \text{RSS}_g = \sum_{g=1}^{k} \sum_{x \in \text{cluster } g} \| x - \mu_g \|^2 \]

Remark: \( k \)-means tries to minimize RSS
(it does so \textit{approximately}, with no guarantee of optimality)

RSS only really makes sense for clusters that look like circles
Why is RSS not a good way to choose $k$?

What is RSS when $k$ is equal to the number of data points?
A Good Way to Choose $k$

RSS measures *within-cluster variation*

$$W = RSS = \sum_{g=1}^{k} \text{RSS}_g = \sum_{g=1}^{k} \sum_{x \in \text{cluster } g} \|x - \mu_g\|^2$$

Want to also measure *between-cluster variation*

$$B = \sum_{g=1}^{k} (\# \text{ points in cluster } g) \|\mu_g - \mu\|^2$$

Called the **CH index** [Calinski and Harabasz 1974]

A good score function to use for choosing $k$:

$$\text{CH}(k) = \frac{B \cdot (n - k)}{W \cdot (k - 1)}$$

Pick $k$ with highest $\text{CH}(k)$

(Choose $k$ among 2, 3, … up to pre-specified max)

$n =$ total # points
Hierarchical Clustering
Going from Similarities to Clusters

There’s a whole zoo of clustering methods

Two main categories we'll talk about:

**Generative models**

1. Pretend data generated by specific model with parameters
2. Learn the parameters ("fit model to data")
3. Use fitted model to determine cluster assignments

**Hierarchical clustering**

Top-down: Start with everything in 1 cluster and decide on how to recursively split

Bottom-up: Start with everything in its own cluster and decide on how to iteratively merge clusters
Divisive Clustering

0. Start with everything in the same cluster

1. Use a method to split the cluster (e.g., $k$-means, with $k = 2$)
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Stop splitting when some termination condition is reached (e.g., highest cluster RSS is small enough)
Divisive Clustering

We can view the process in terms of a tree (colors are *not* important here and just help relate to the previous slide)

Each split is from \( k \)-means
Divisive Clustering

We can view the process in terms of a tree (colors are *not* important here and just help relate to the previous slide).

Each split is from $k$-means

We could keep splitting until the leaves each have 1 point.
Divisive Clustering

This tree is called a dendrogram. Helpful for visualizing all the intermediate clustering stages.

Agglomerative clustering goes the other way.

Divisive clustering uses *global* information and keeps splitting.

We could keep splitting until the leaves each have 1 point.
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Agglomerative Clustering

Don’t have to keep merging until there’s 1 cluster!
(e.g., stop when closest two clusters have distance between their centers exceed a threshold)

Agglomerative clustering uses *local* information and keeps merging
Agglomerative Clustering

Some ways to define what it means for two clusters to be “close” (needed to find most similar clusters):

**Single linkage:** use distance between closest points across the two clusters

- Can end up chaining together too many things

**Complete linkage:** use distance between farthest points across the two clusters

- Get “crowding” behavior

**Centroid linkage:** what we saw already (distance between cluster means)

- Ignores # items in each cluster

**Average linkage:** use average distance across all possible pairs
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There are other ways as well: none are perfect

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Going from Similarities to Clusters

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The most popular models effectively assume Euclidean distance…
You learn a model ➔ can predict cluster assignments for points not seen in training

Easily works with different distances (not just Euclidean)
Great for problems that don’t need to predict clusters for future points
Different split/merge criteria lead to clusters that look specific ways (e.g., chaining, crowding)
Example: Clustering on U.S. Counties

(using opioid death rate data across 37 years)

No need to predict which cluster new counties should belong to, since we’re already looking at all U.S. counties!

Image source: Amanda Coston
Clustering

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Many more methods we didn’t cover

- sklearn has a whole bunch more (not close to exhaustive)
- Also: remember the recommendation system setup?
- Co-clustering is the problem of clustering both users and items at the same time (sklearn has a few methods)