Carnegie Mellon University
Heinz College

95-865 Australia Lecture 4: Clustering Part II

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HW1 Questionnaire Results

Nearly everyone finds t-SNE really confusing

Many students want more examples/applications

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

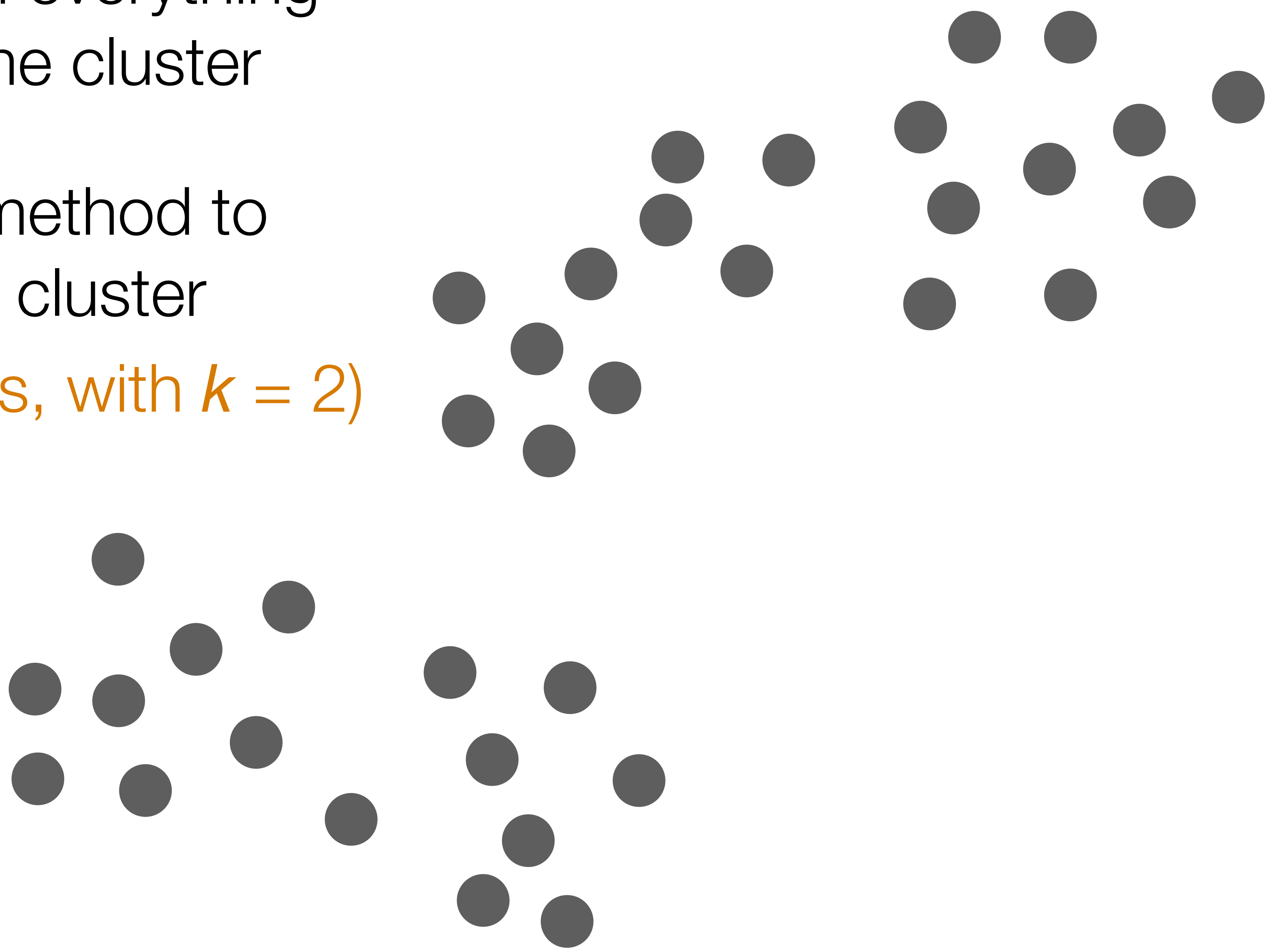
Top-down: Start with everything in 1 cluster and decide on how to recursively split

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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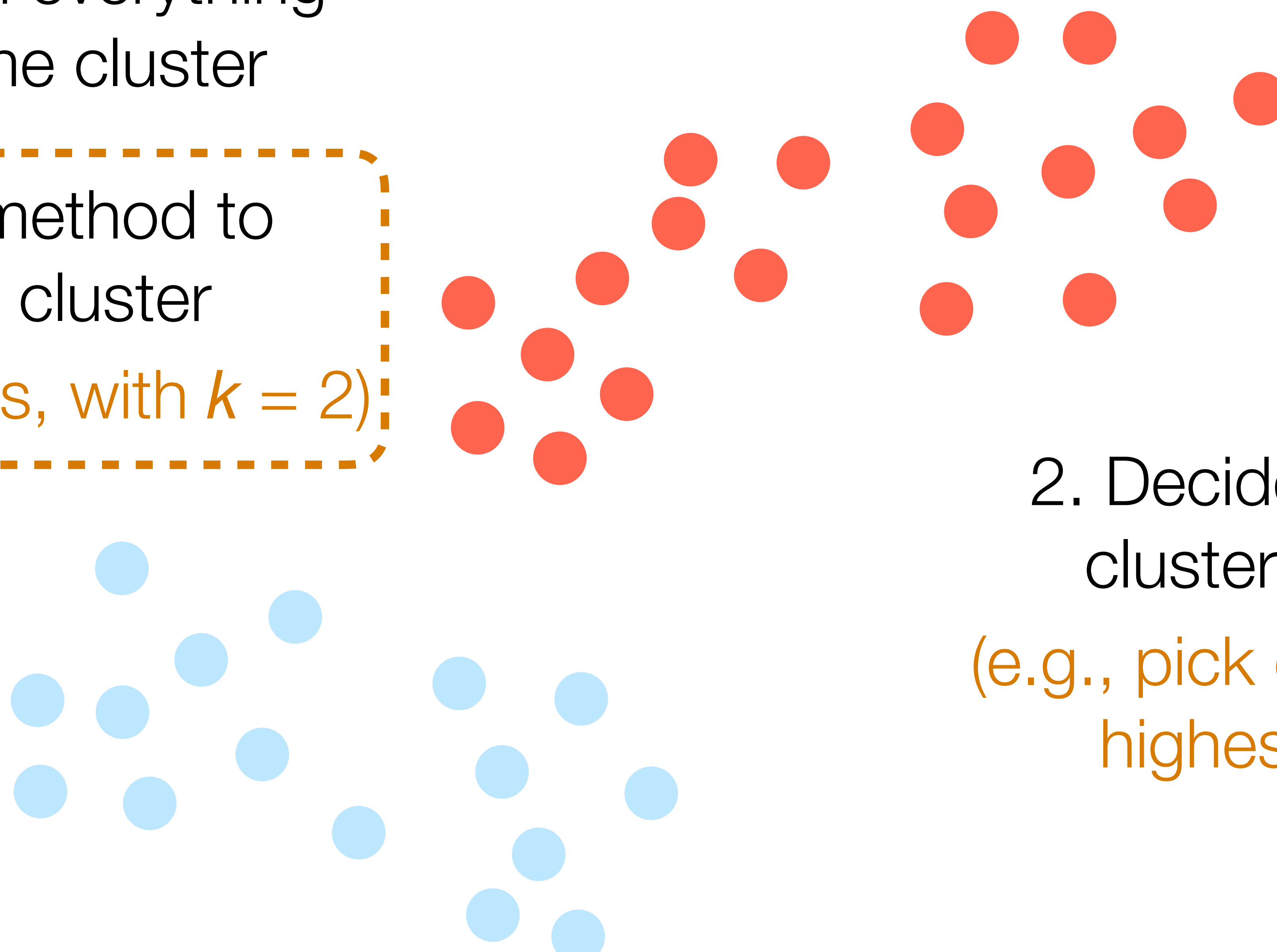

2. Decide on next cluster to split
(e.g., pick cluster with highest RSS)

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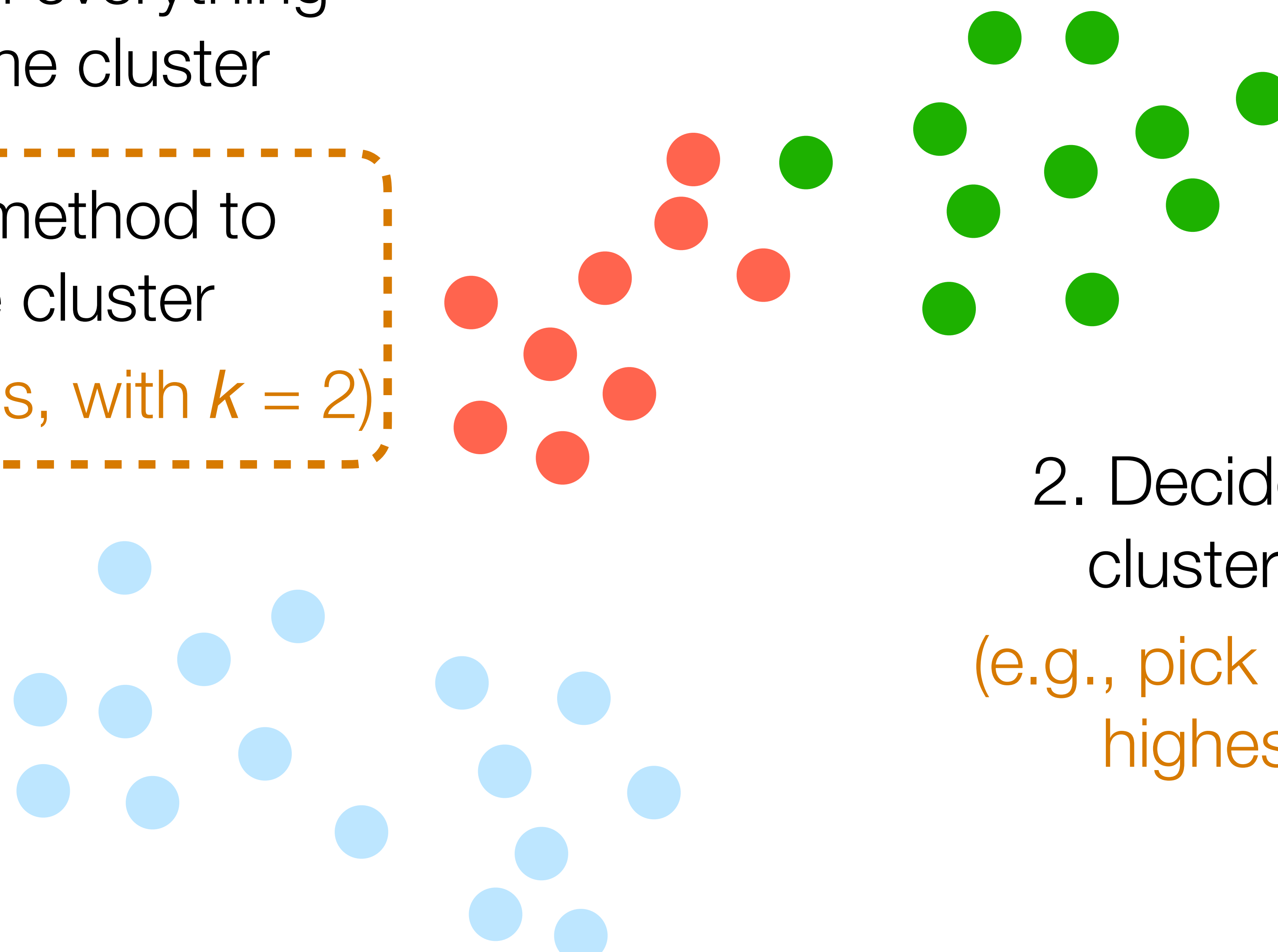

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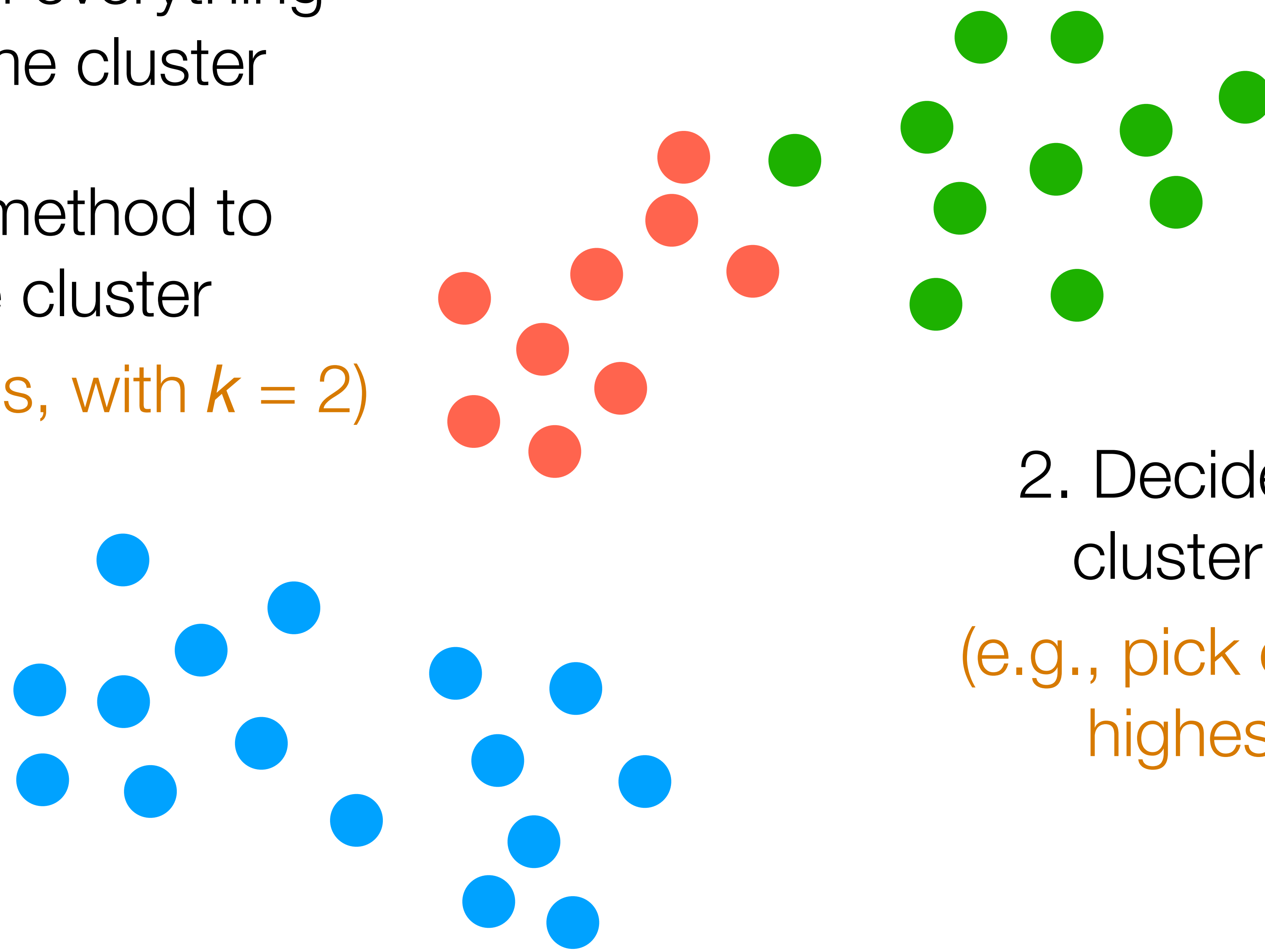

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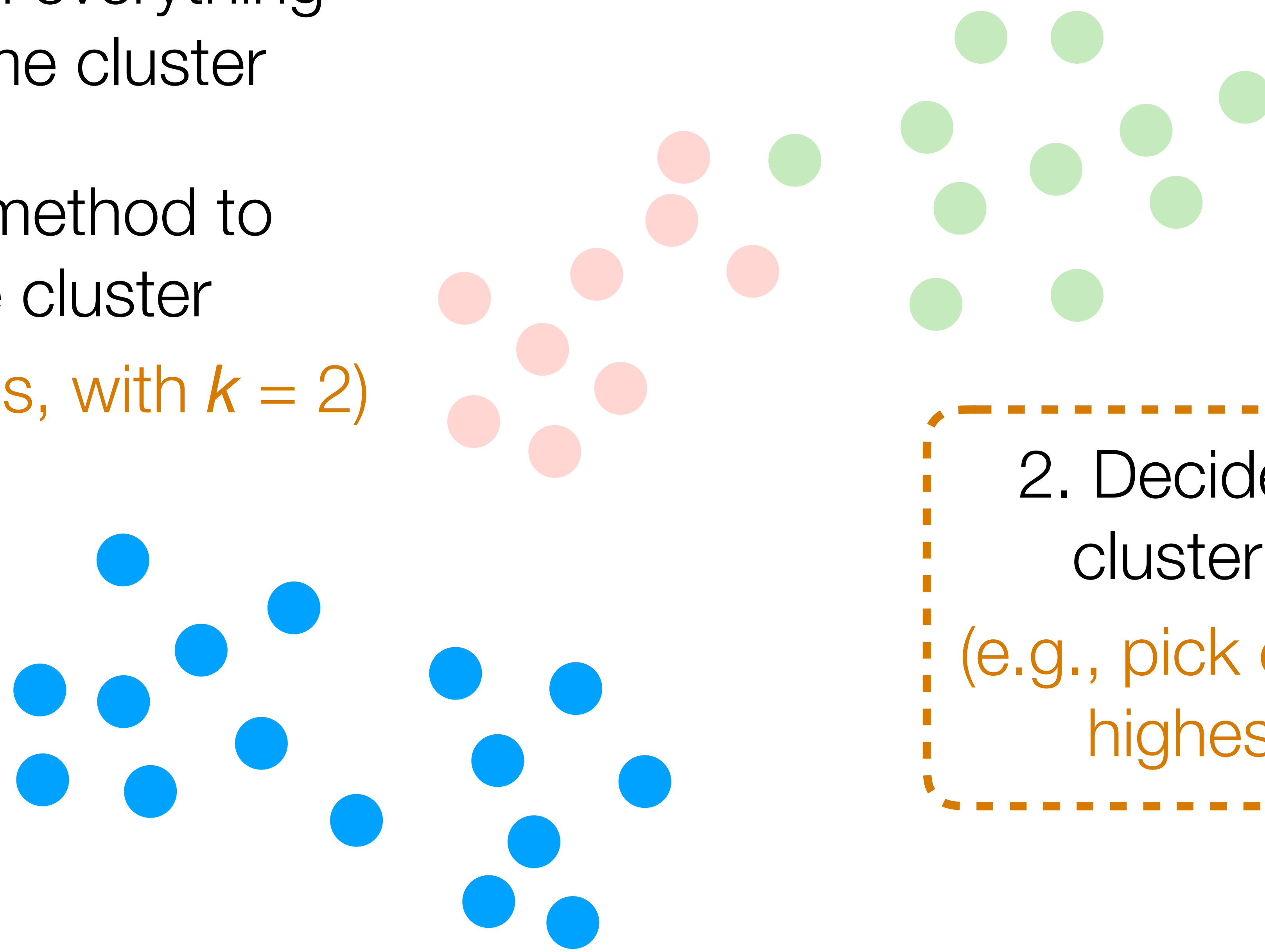

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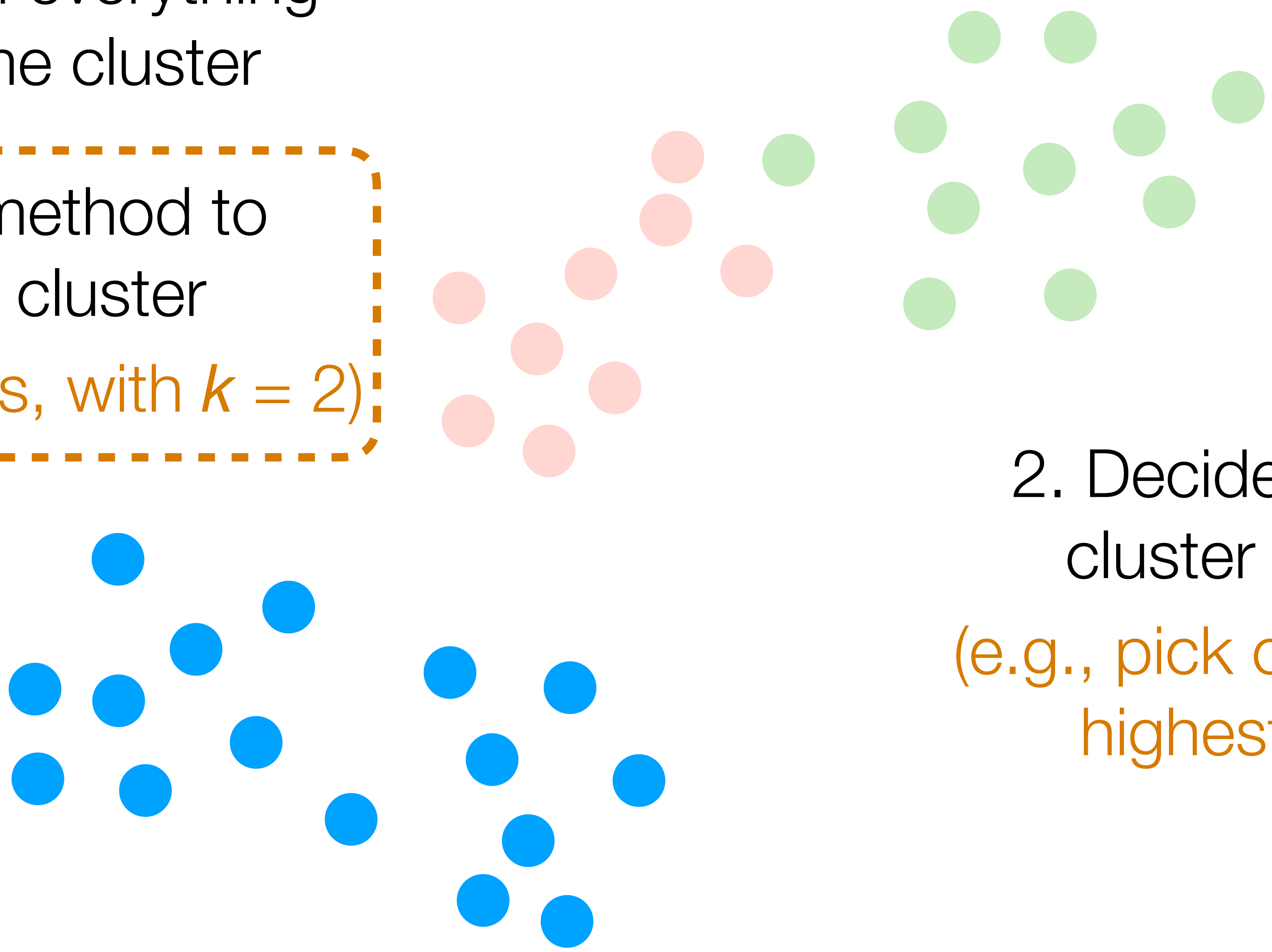

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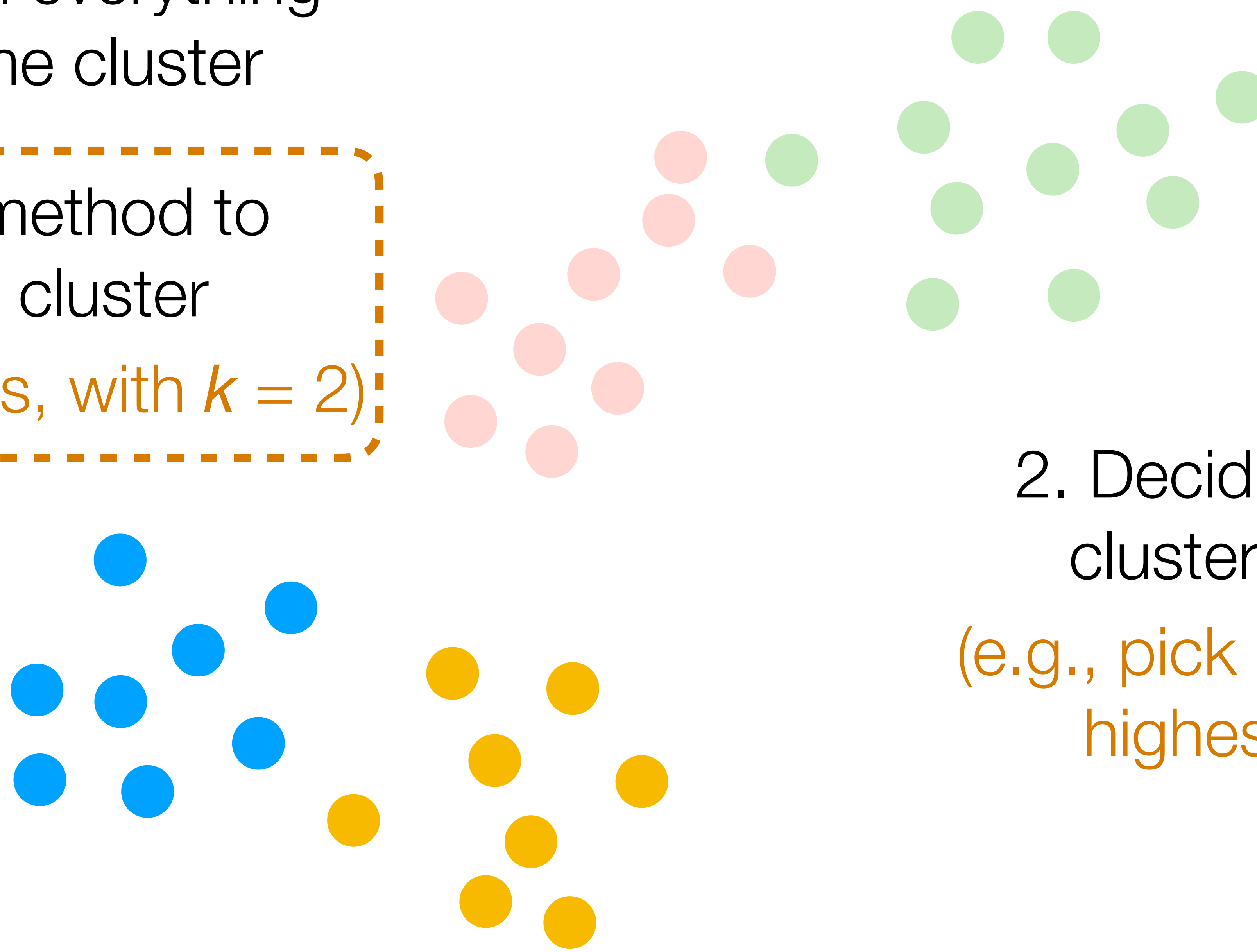

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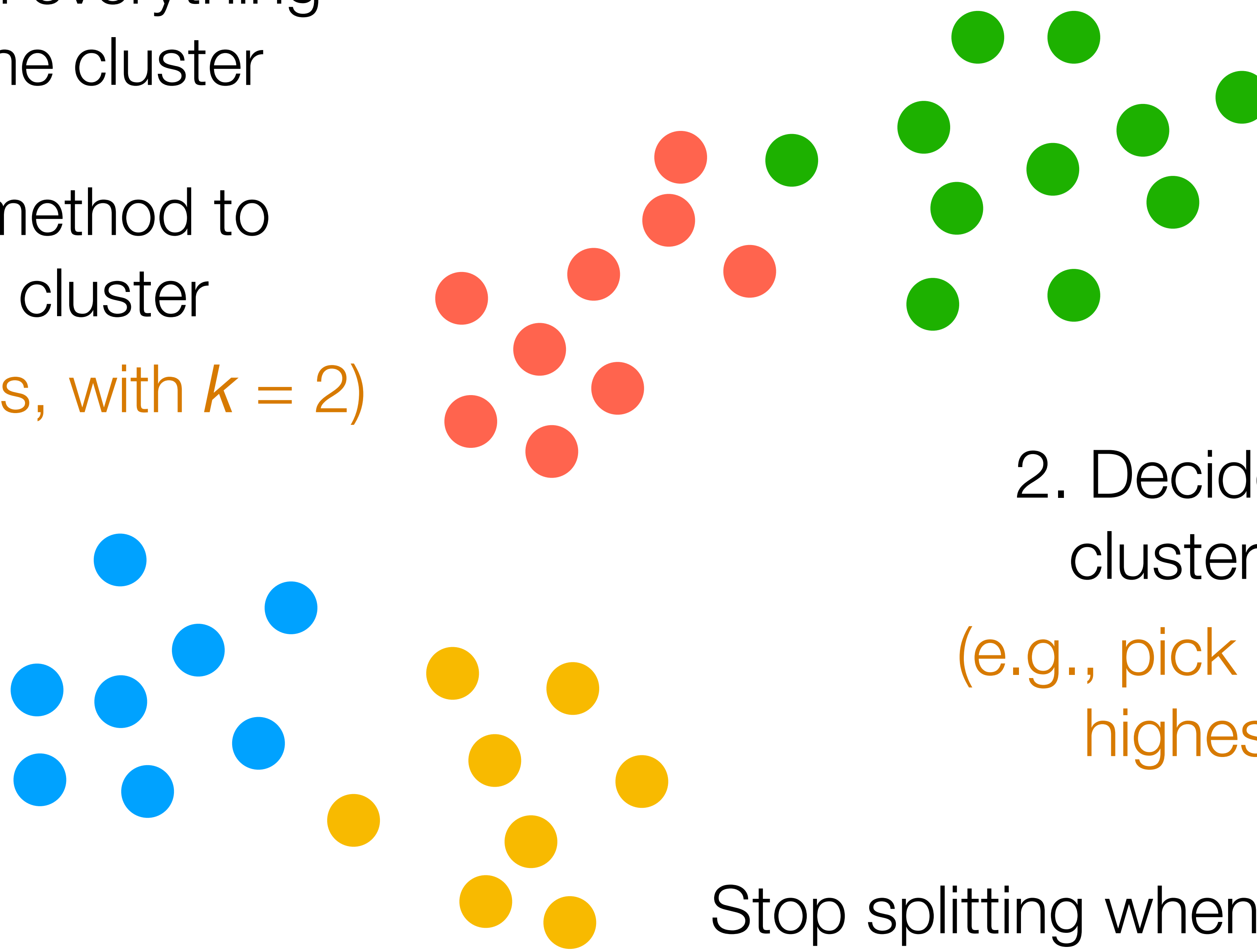


2. Decide on next cluster to split

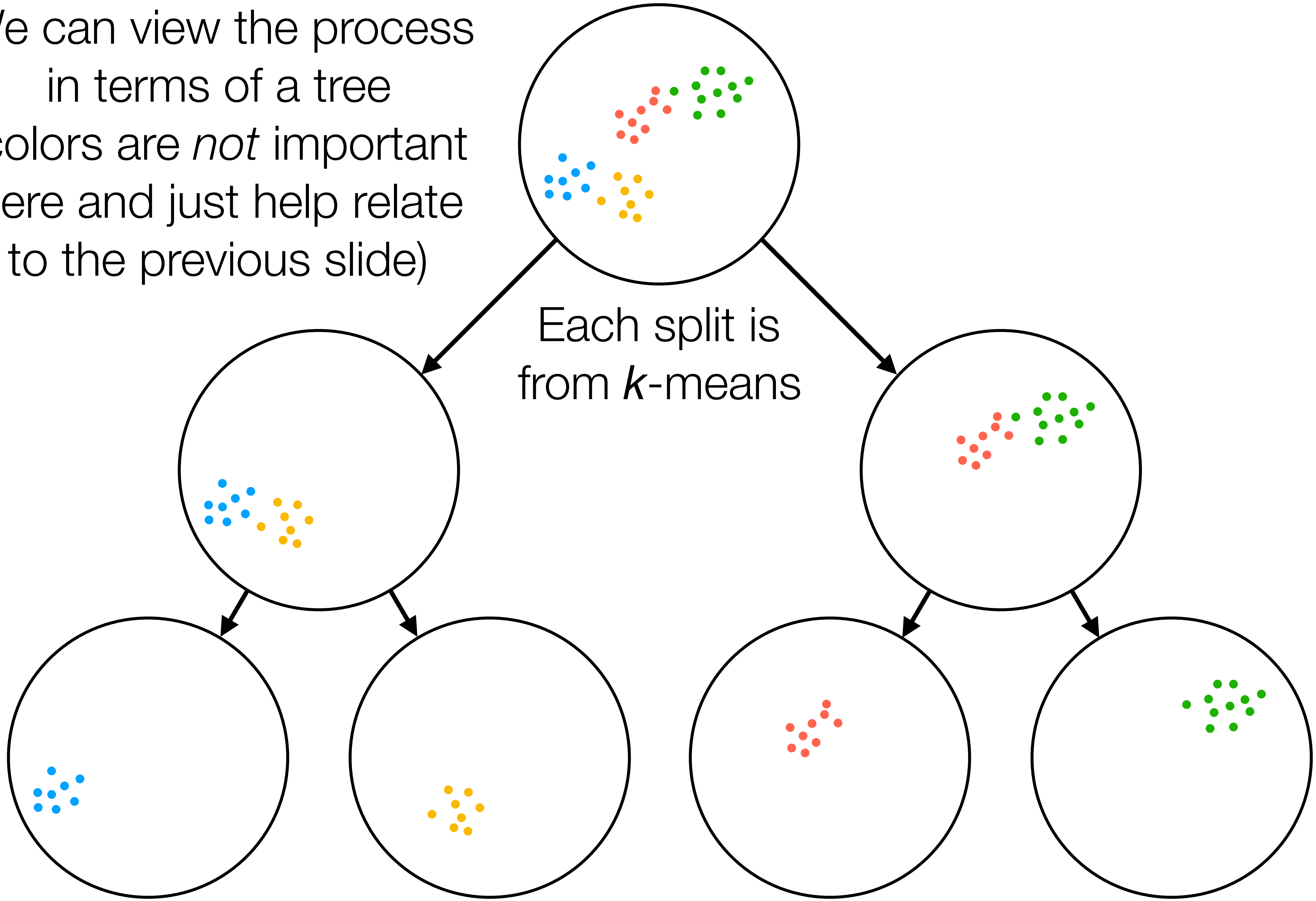
(e.g., pick cluster with highest RSS)

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)



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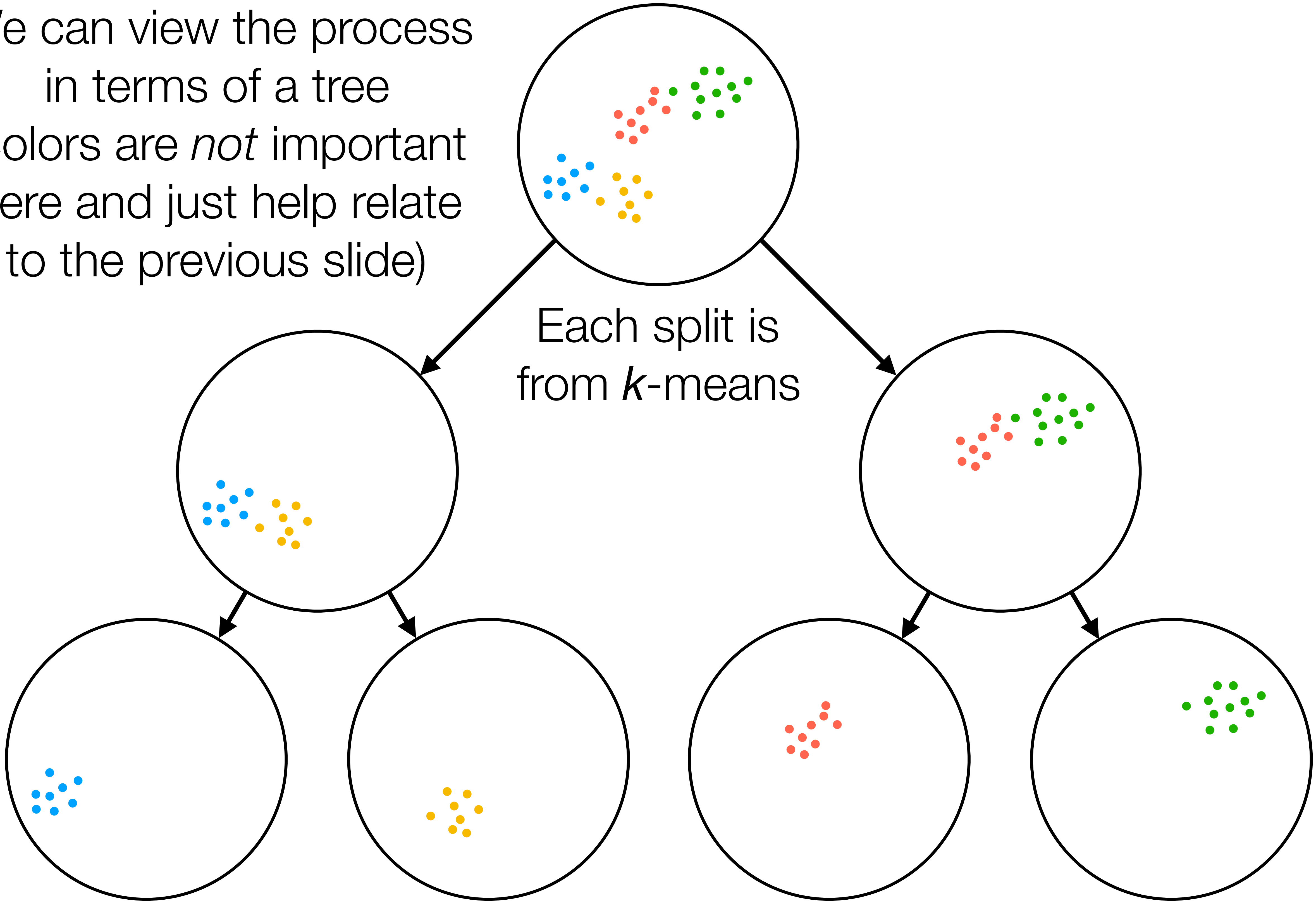
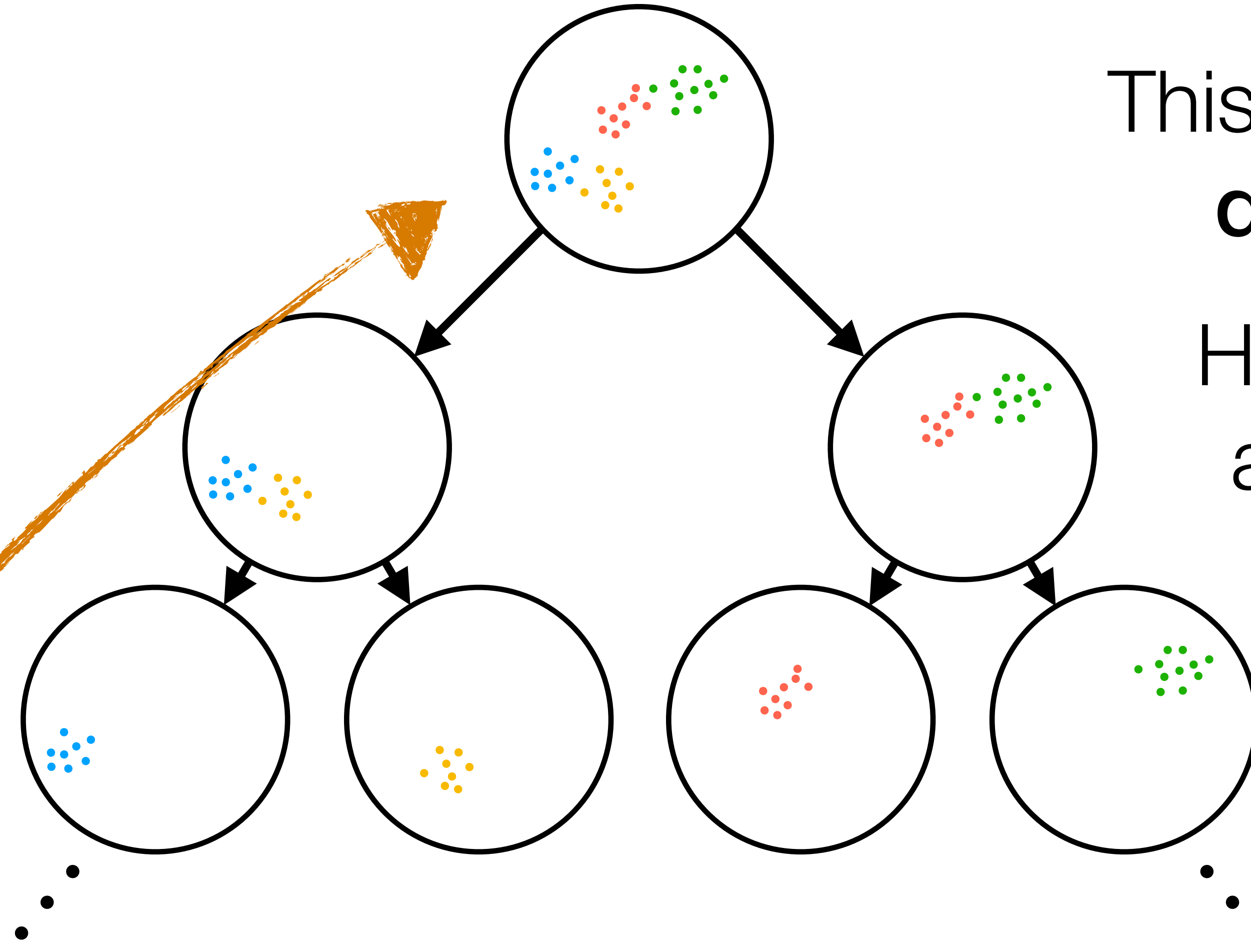


We could keep splitting until the leaves each have 1 point

Divisive Clustering



This tree is called a **dendrogram**

Helpful for visualizing all the intermediate clustering stages

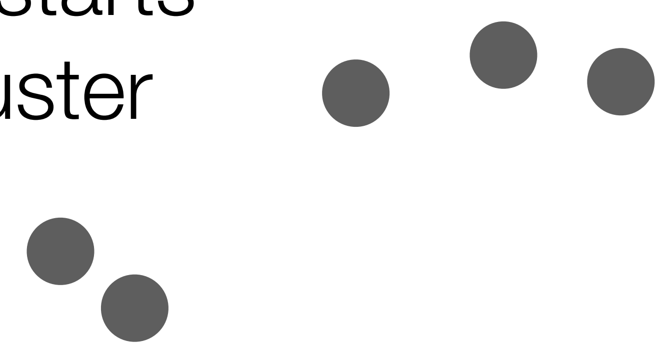
Agglomerative clustering goes the other way

Divisive clustering uses *global* information and keeps splitting

We could keep splitting until the leaves each have 1 point

Agglomerative Clustering

0. Every point starts
as its own cluster



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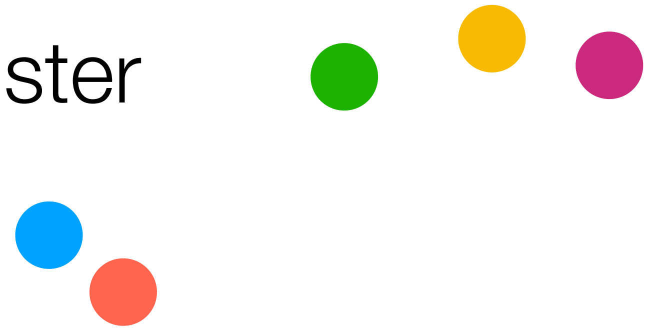

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(e.g., pick pair of clusters with
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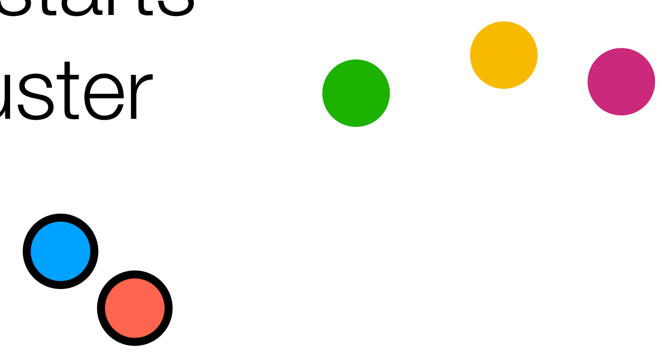

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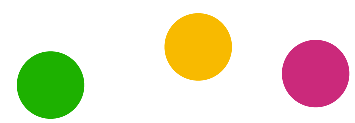

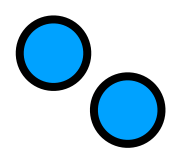

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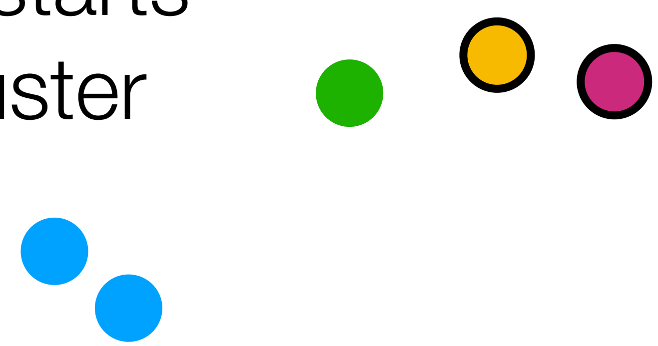

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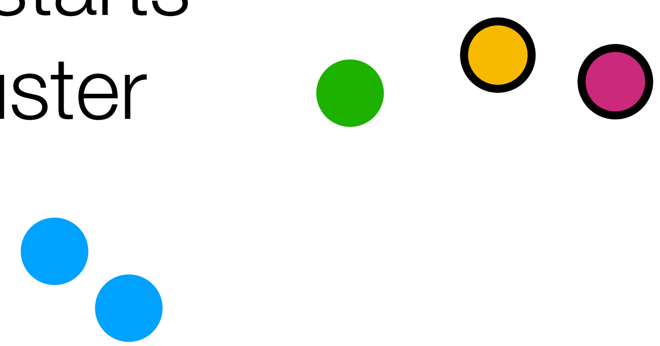

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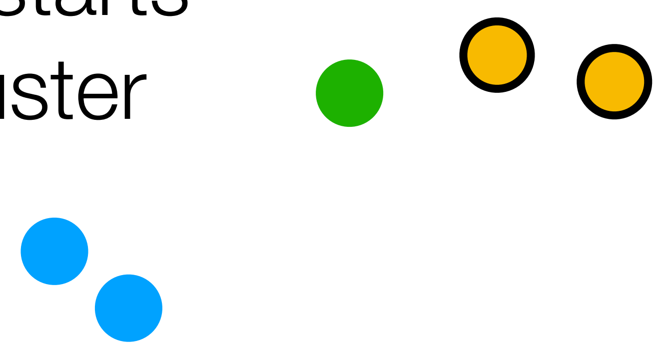

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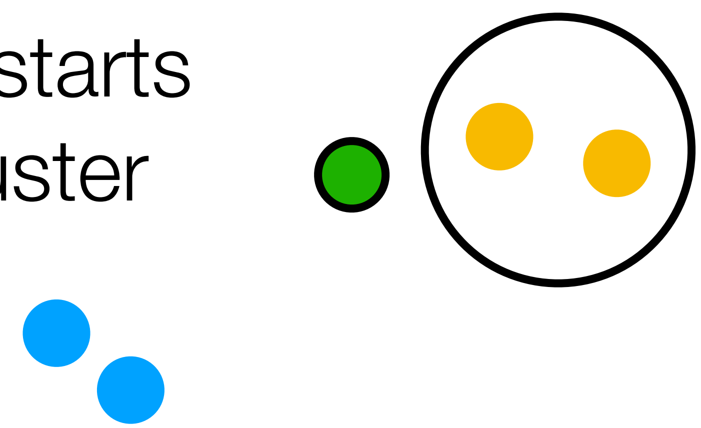

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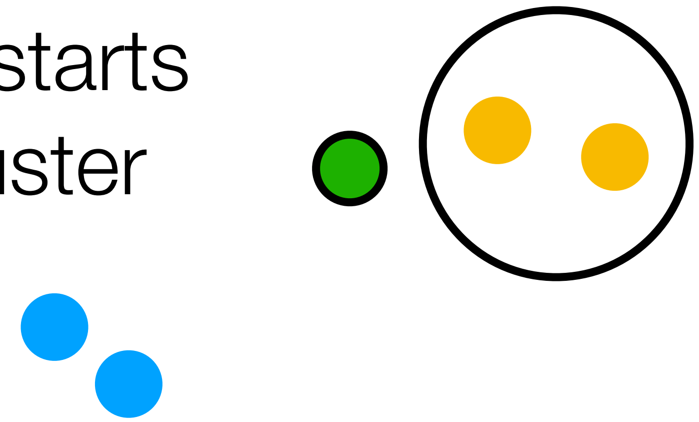

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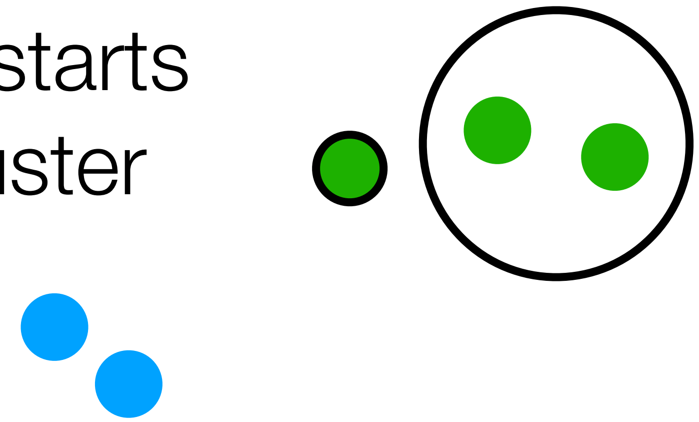

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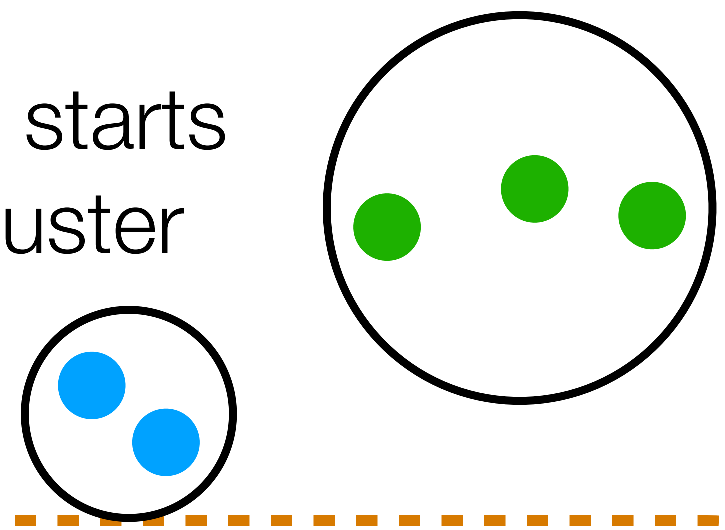

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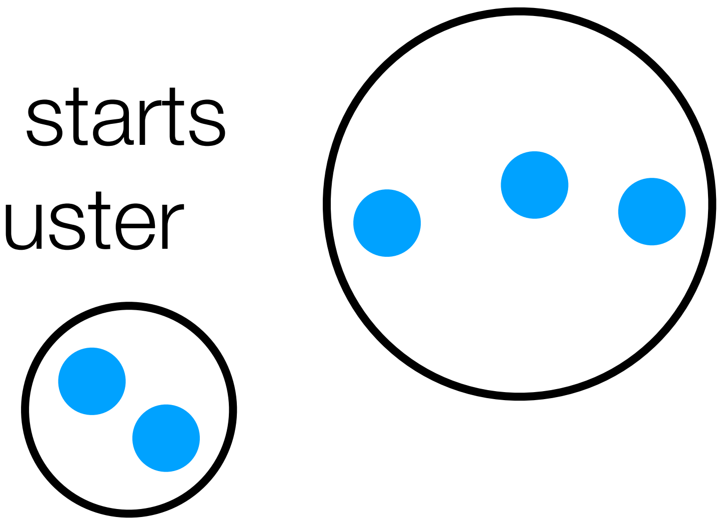

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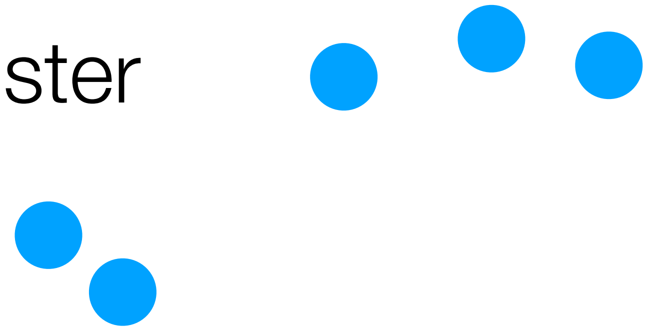

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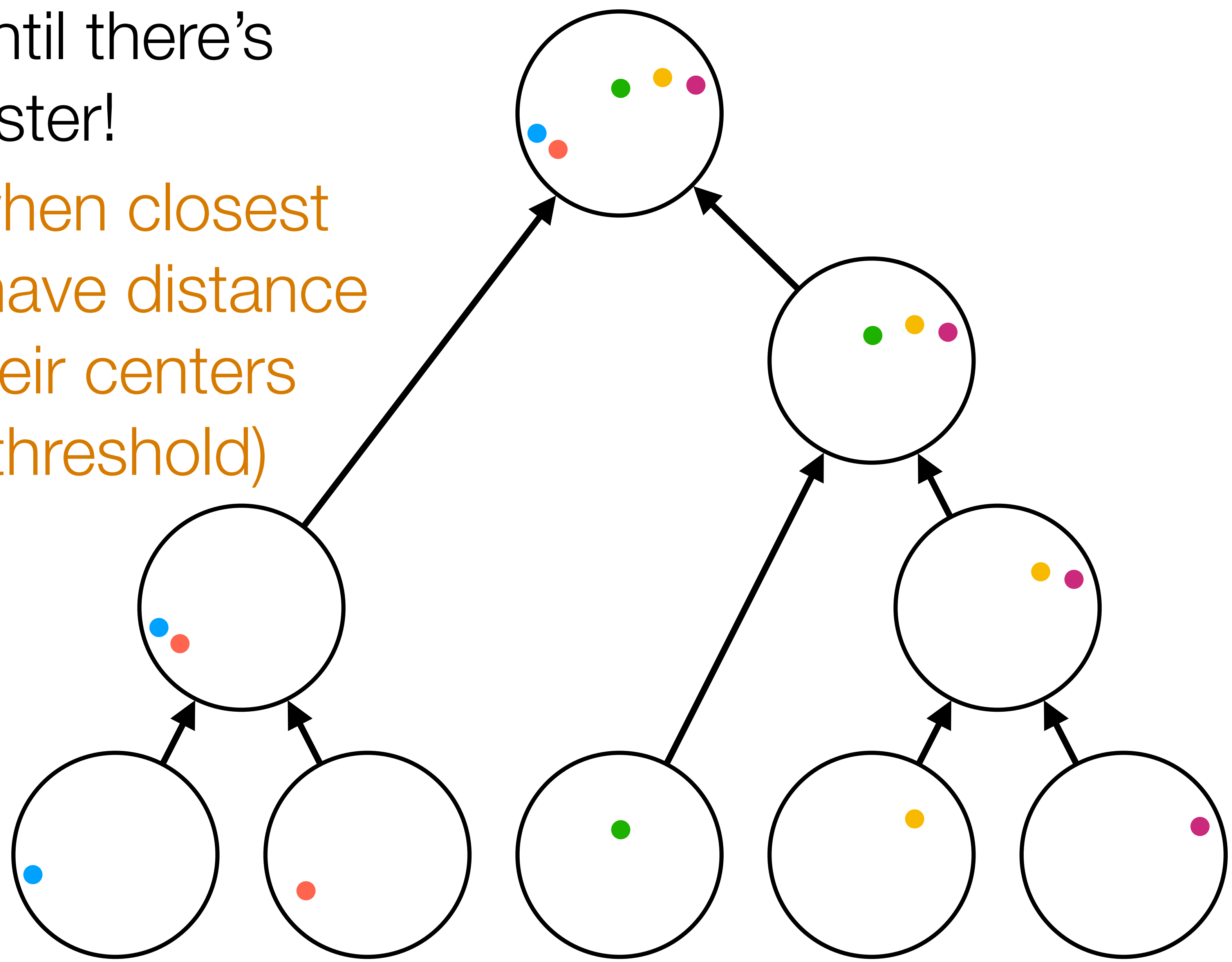
Agglomerative Clustering

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)

Dendrogram

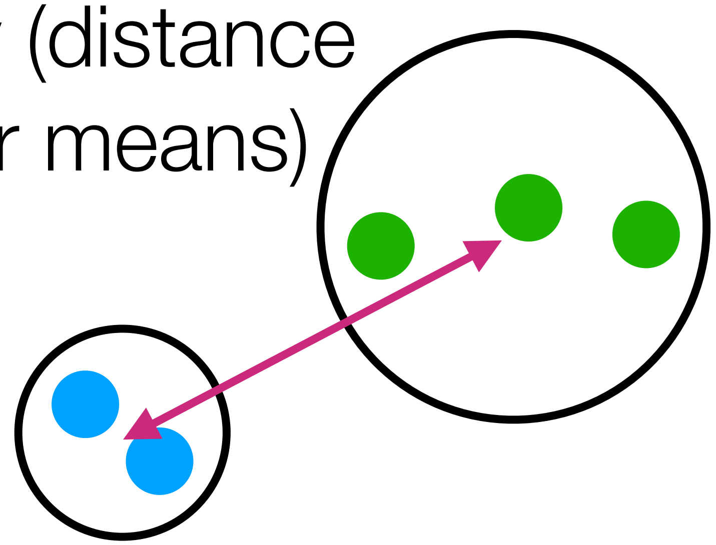


Agglomerative clustering uses *local* information and keeps merging

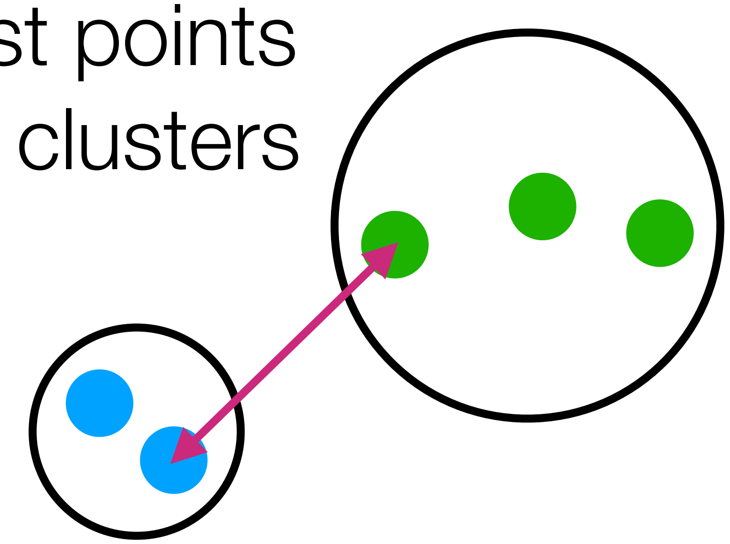
Agglomerative Clustering

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

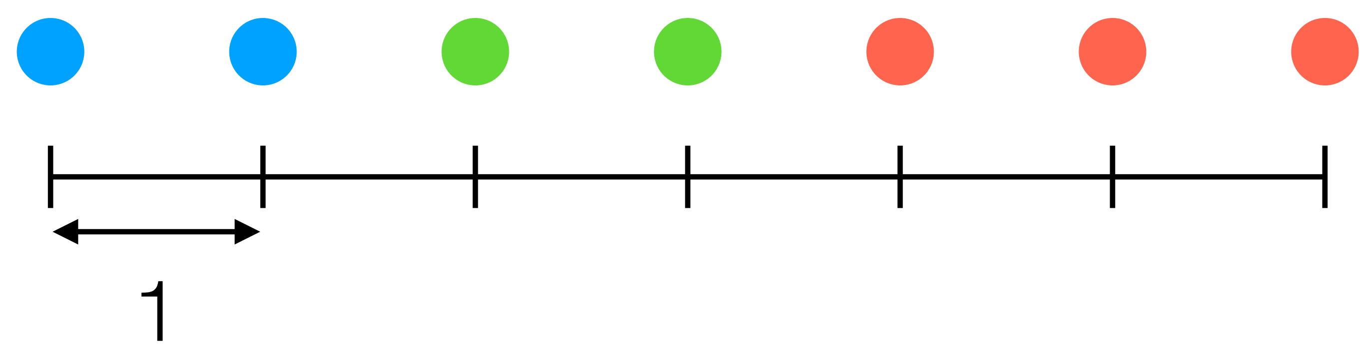
Centroid linkage: what we saw already (distance between cluster means)



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



Example: Single Linkage



What would single linkage merge next?

Distance between blue and green: 1

Distance between blue and red: 3

Distance between green and red: 1

Single linkage would merge either blue with green, or green with red

Agglomerative Clustering

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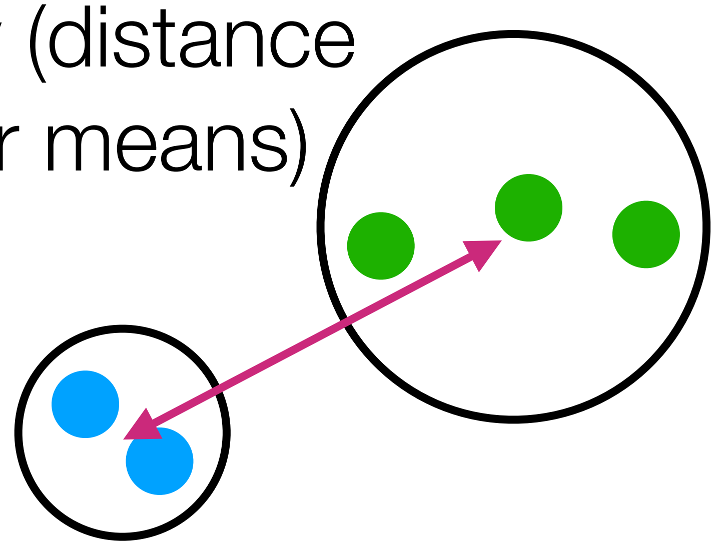

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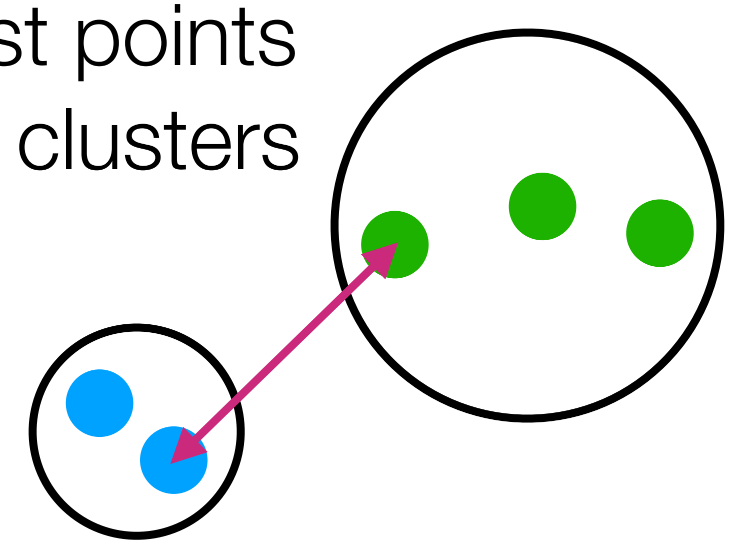
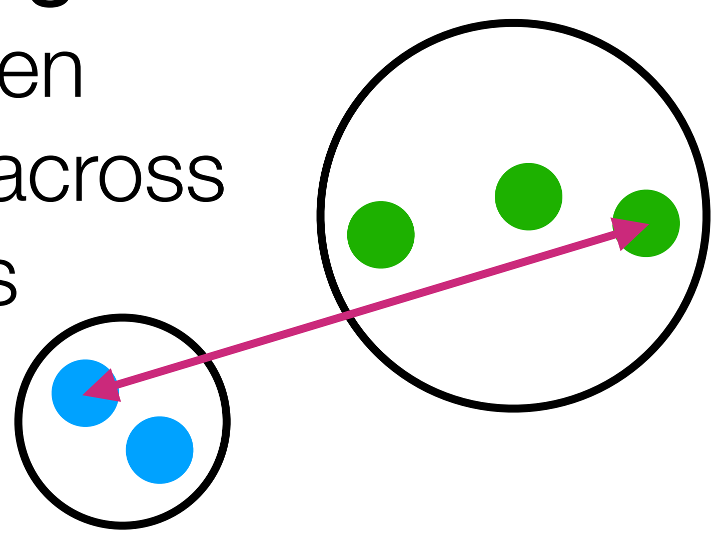
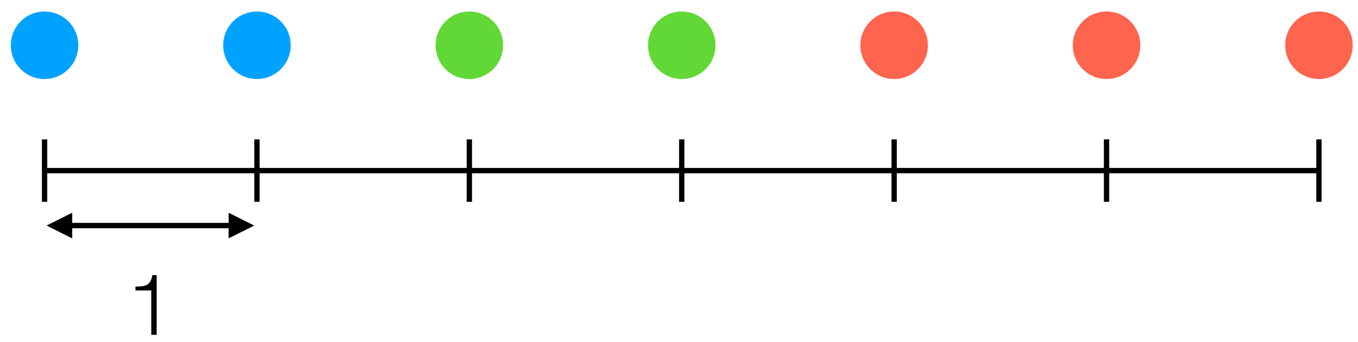


Complete linkage: use distance between farthest points across the two clusters



Example: Complete Linkage



What would complete linkage merge next?

Distance between blue and green: 3

Distance between blue and red: 6

Distance between green and red: 4

Complete linkage would merge blue and green

Agglomerative Clustering

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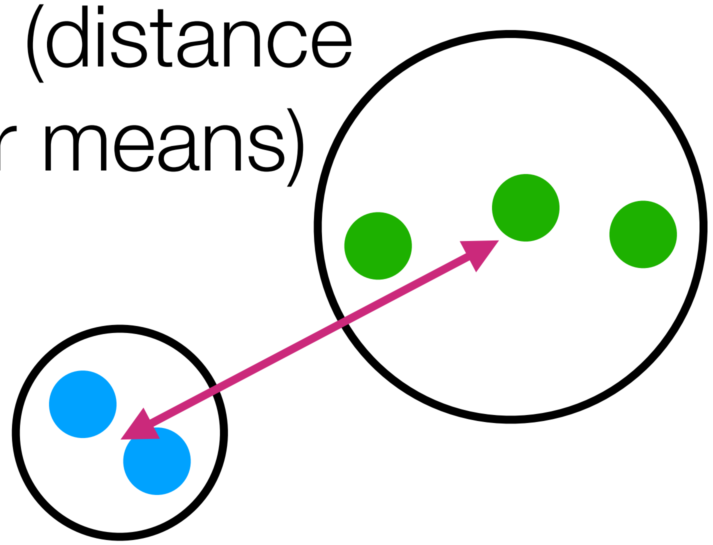

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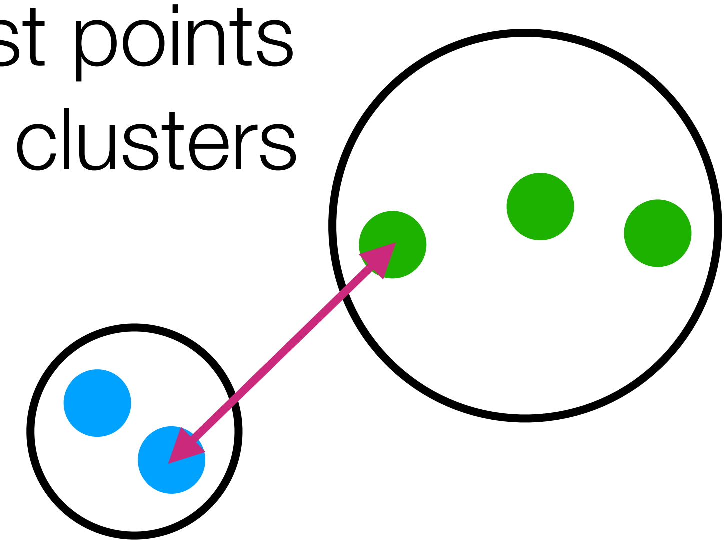

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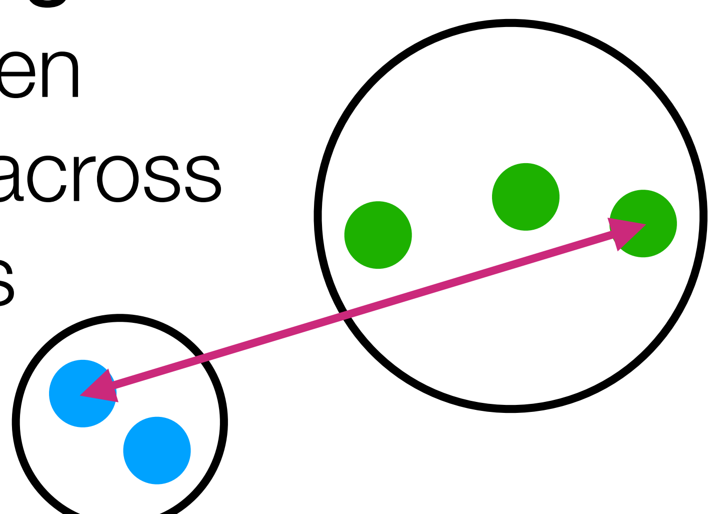


There are other ways as well: none are perfect

Hierarchical Clustering

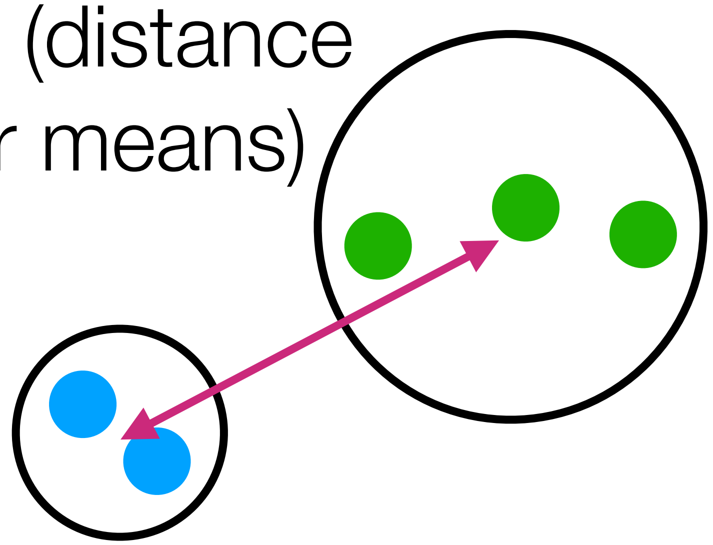
Demo

Agglomerative Clustering

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

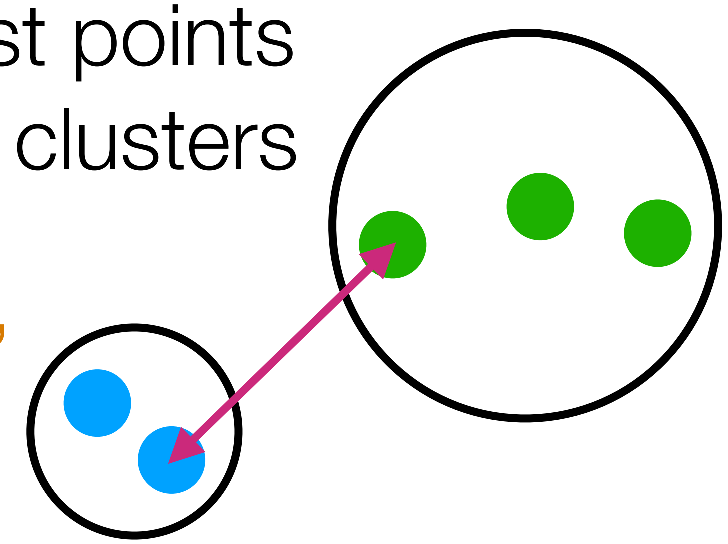
Centroid linkage: what we saw already (distance between cluster means)

Ignores
items in
each cluster



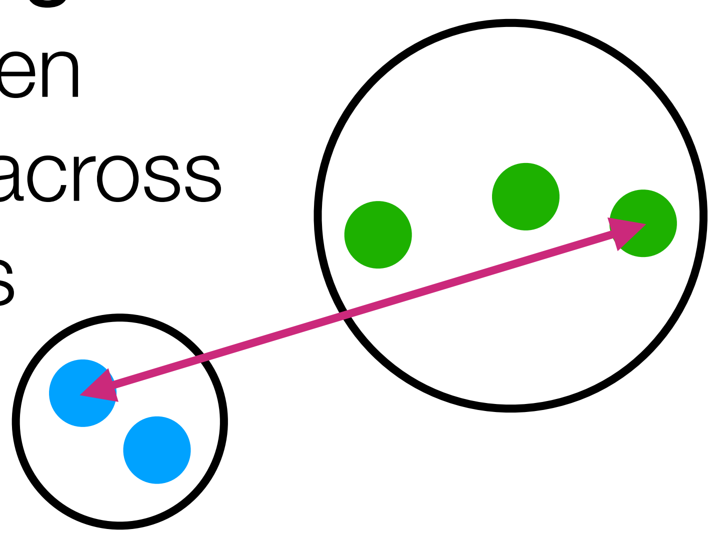
Single linkage: use distance between closest points across the two clusters

Has "chaining" behavior



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

Has "crowding" behavior



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Going from Similarities to Clusters

Generative models

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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

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

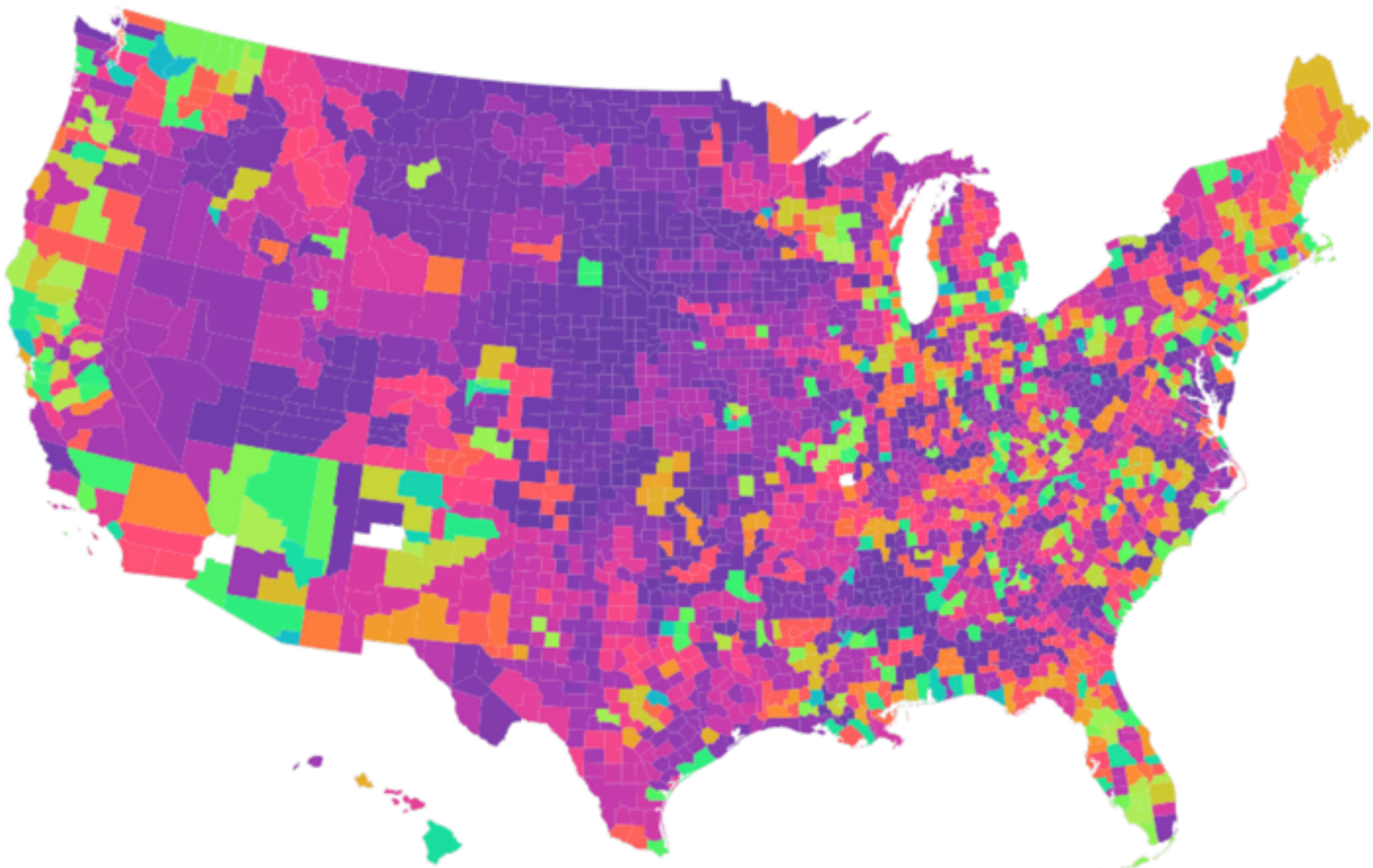
Easily works with different distances (not just Euclidean)

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

Generative models

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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)

How to Choose a Clustering Method?

In general: not easy!

Some questions to think about:

- What features to even cluster on?
- For your application, what distance/similarity makes sense?
- Do you care about cluster assignments for new points?
- After you run a clustering algorithm, make visualizations to interpret the clusters!
- Some times it makes more sense to define your own score function for how good a clustering assignment is

Clustering Last Remarks

- It's possible that several clustering methods give similar results (*which is great!* — it means that there are some reasonably "stable" clusters in your data)
  - Example: *tons* of clustering methods can figure out from senate voting data who Democrats and Republicans are (of course, *without* knowing each senator's political party)
- Ultimately, *you* have to decide on which clustering method and number of clusters make sense for your data
  - Do not just blindly rely on numerical metrics (e.g., CH index)
  - Interpret the clustering results in the context of the application you are looking at

If you can set up a prediction task, then you can use the prediction task to guide the clustering

Is Clustering Structure Enough?

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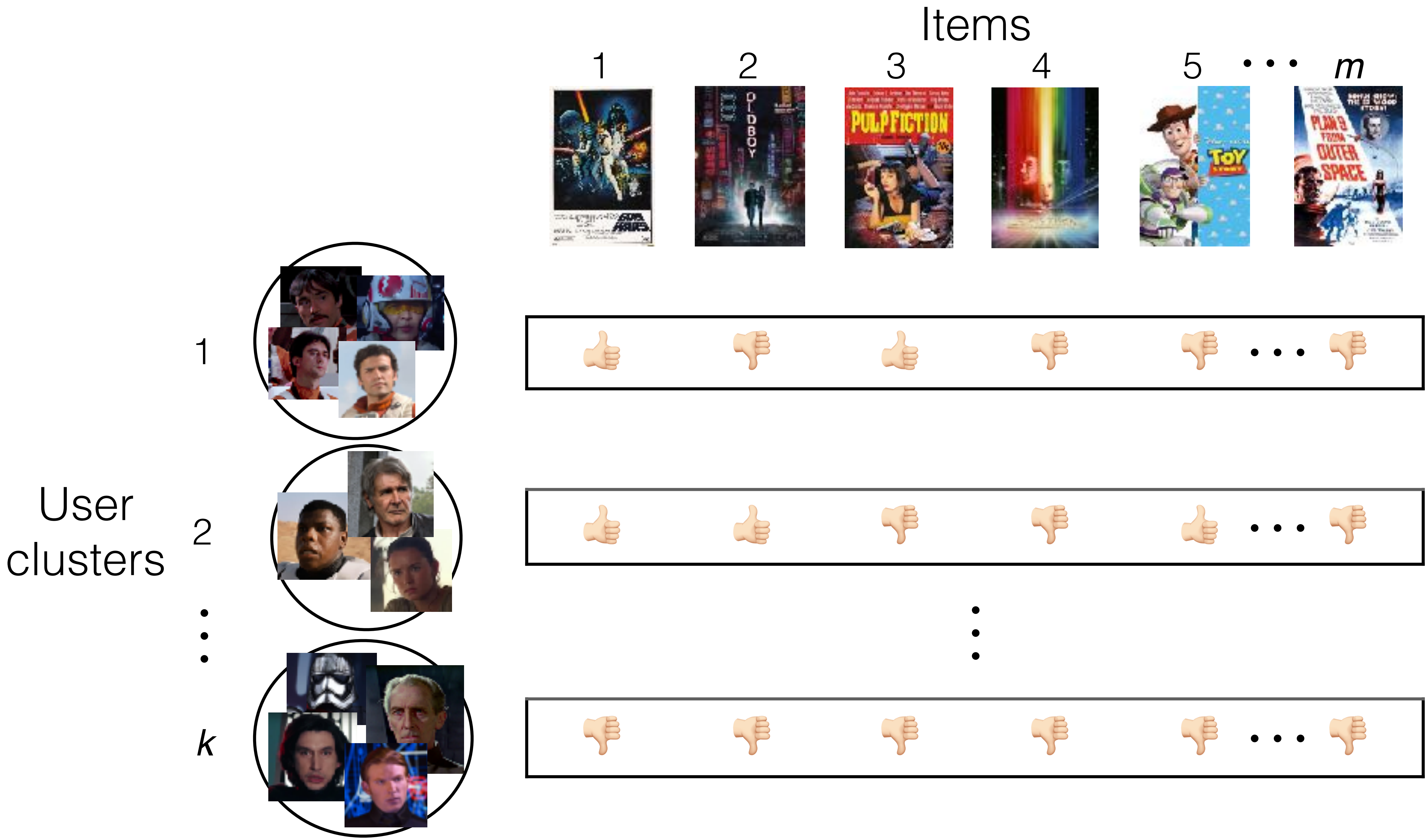

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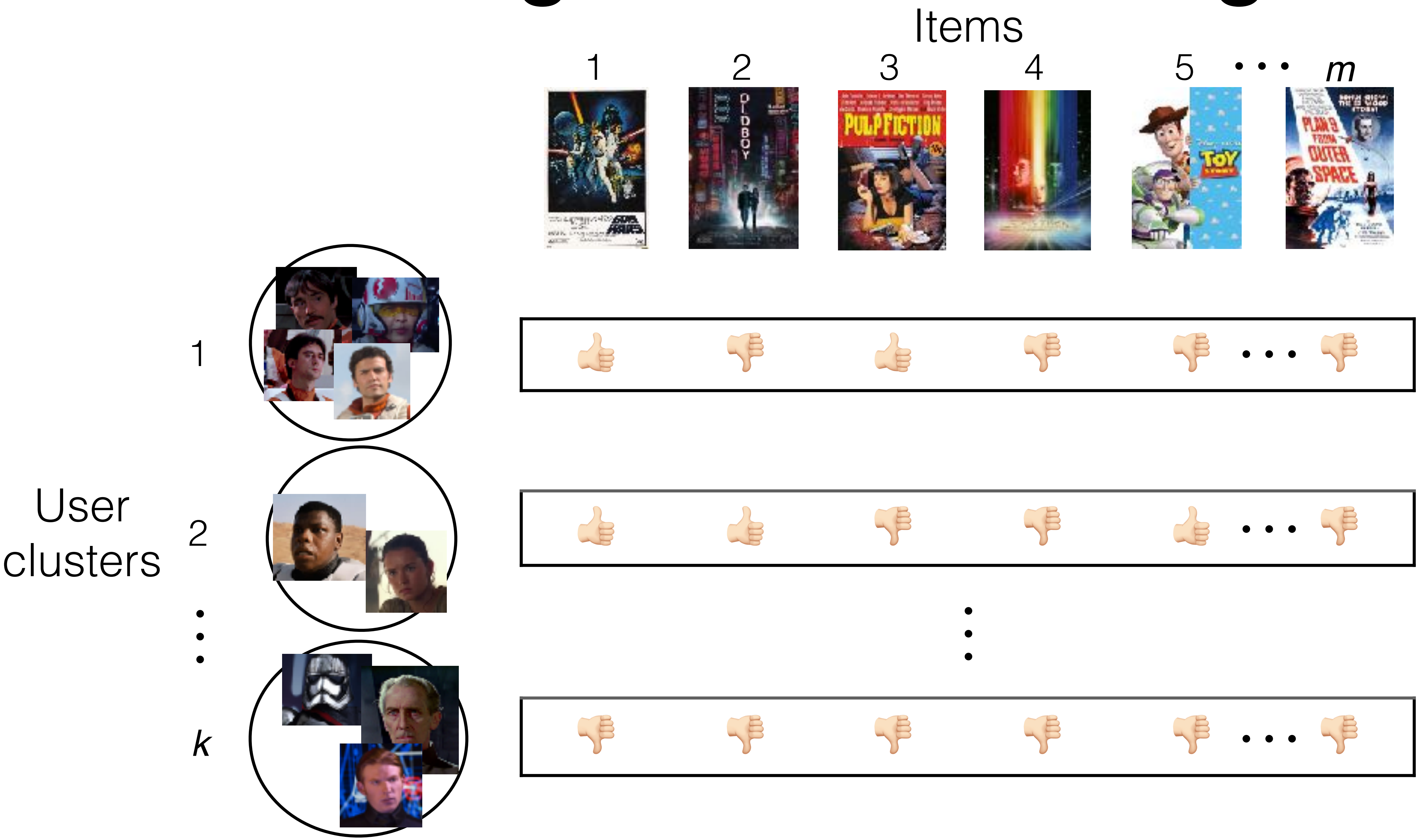
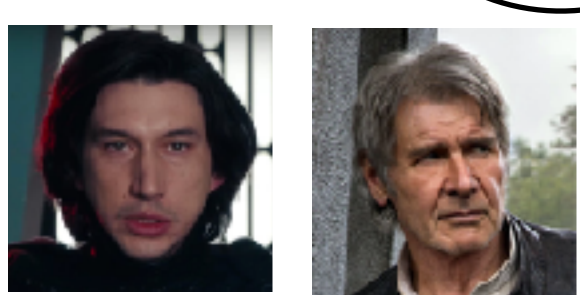
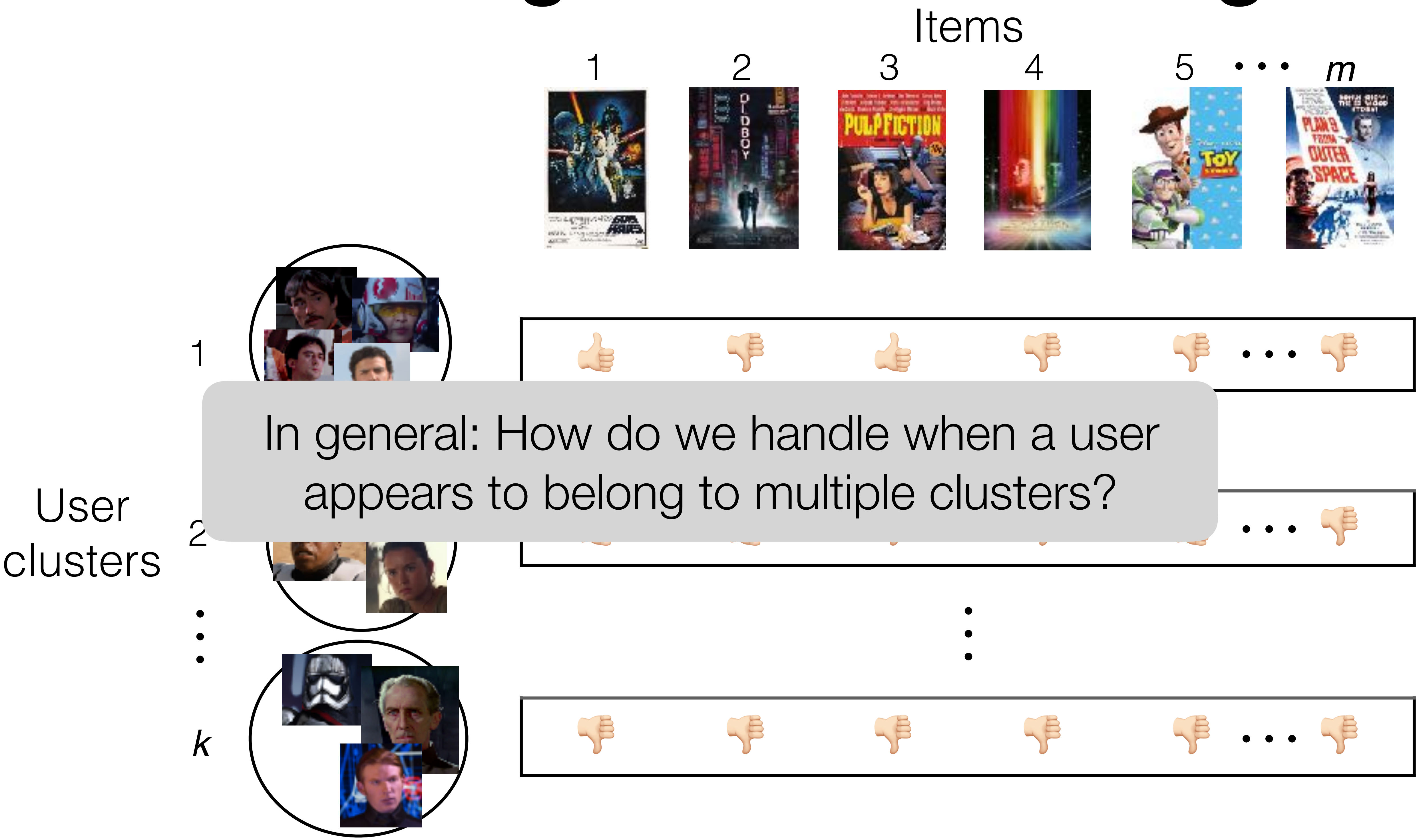


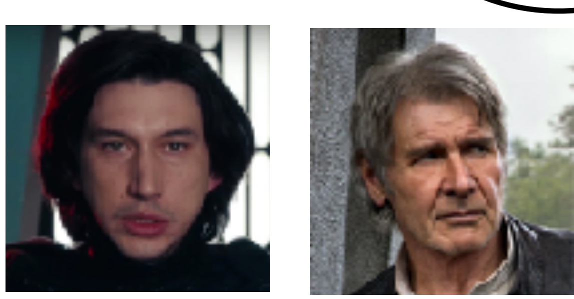


What if these two users shared a Netflix account (and used the same user profile)?

Is Clustering Structure Enough?



In general: How do we handle when a user appears to belong to multiple clusters?



What if these two users shared a Netflix account (and used the same user profile)?

Topic Modeling

Movie recommendation

Each user is part of multiple “clusters”/topics

Each cluster/topic consists of a bunch of movies
(example clusters: “sci-fi epics”, “cheesy rom-coms”)

Text

Each document is part of multiple topics

Each topic consists of a bunch of regularly co-occurring words
(example topics: “sports”, “medicine”, “movies”, “finance”)

Health care

Each patient’s health records explained by multiple “topics”

Each topic consists of co-occurring “events”
(example topics: “heart condition”, “severe pancreatitis”)

Topic Modeling

Movie recommendation

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Each cluster/topic consists of a bunch of movies
(ex s”)

In all of these examples:

- Each data point (a feature vector) is part of multiple topics
- Each topic corresponds to specific feature values in the feature vector likely appearing

Each to words
(exar nce”)

Health care

Each patient’s health records explained by multiple “topics”

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(example topics: “heart condition”, “severe pancreatitis”)

Latent Dirichlet Allocation (LDA)

- Easy to describe in terms of text (but works for not just text)
- Input: “document-word” matrix, and pre-specified # topics *k*

i-th row, *j*-th column: # times word *j* appears in doc *i*

- Output: what the *k* topics are (details on this shortly)

LDA Example

		Document	
		Alice's text	Bob's text
Topic	weather	0.1	0.5
	food	0.9	0.5

		Topic	
		weather	food
Word	cold	0.3	0.1
	hot	0.7	0.3
	apple	0.0	0.5
	pie	0.0	0.1

Each word in Alice's text is generated by:

1. Flip 2-sided coin for Alice
2. If weather: flip 4-sided coin for weather
   If food: flip 4-sided coin for food

LDA Example

		Document	
		Alice's text	Bob's text
Topic	weather	0.1	0.5
	food	0.9	0.5

		Topic	
		weather	food
Word	cold	0.3	0.1
	hot	0.7	0.3
	apple	0.0	0.5
	pie	0.0	0.1

Each word in Bob's text is generated by:

1. Flip 2-sided coin for Bob
2. If weather: flip 4-sided coin for weather
   If food: flip 4-sided coin for food

LDA Example

		Document	
		Alice's text	Bob's text
Topic	weather	0.1	0.5
	food	0.9	0.5

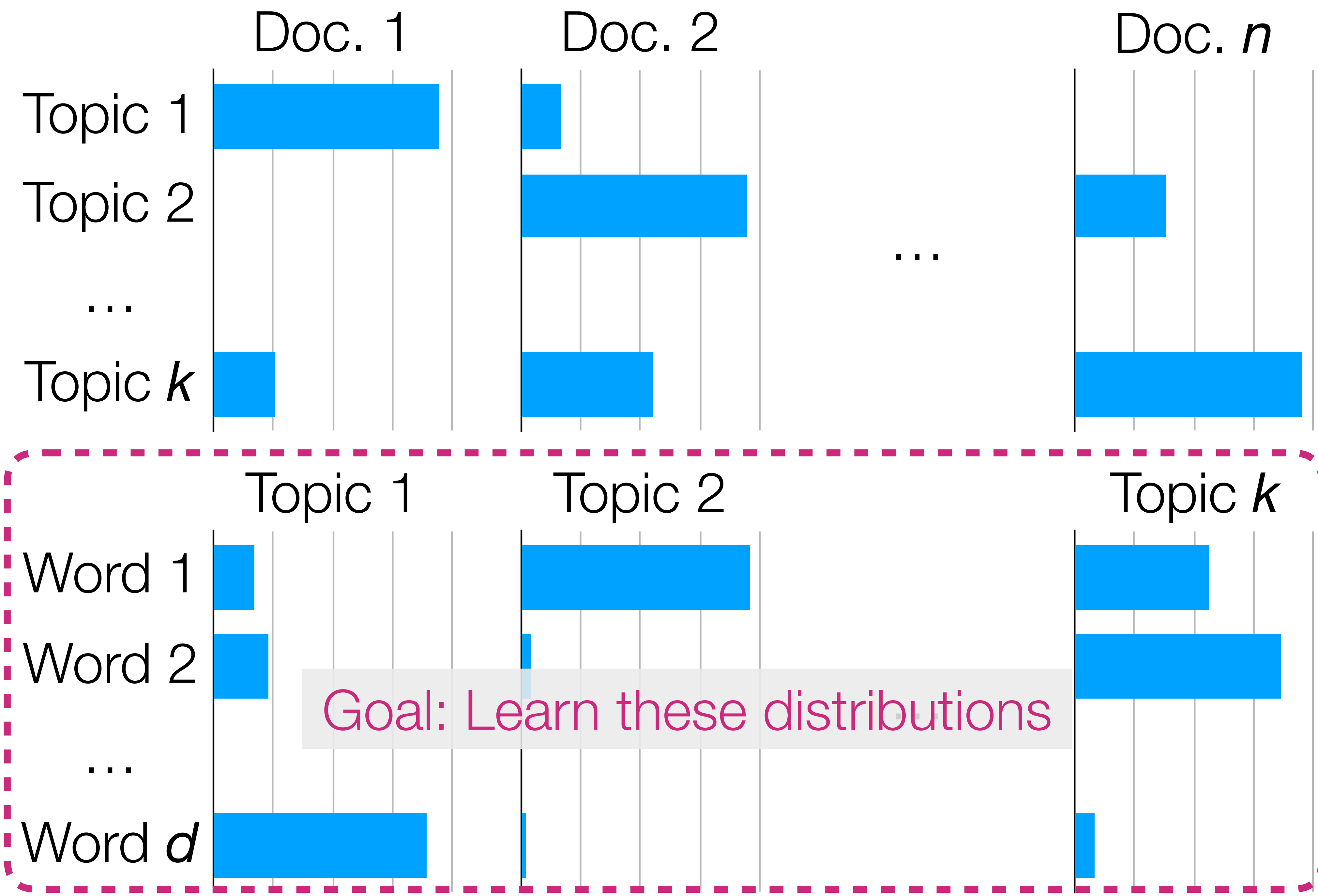
		Topic	
		weather	food
Word	cold	0.3	0.1
	hot	0.7	0.3
	apple	0.0	0.5
	pie	0.0	0.1

Each word in doc. *i* is generated by:

1. Flip 2-sided coin for doc. *i*
2. If weather: flip 4-sided coin for weather
   If food: flip 4-sided coin for food

"Learning the topics" means figuring out these 4-sided coin probabilities

LDA



LDA models each word in document *i* to be generated as:

- Randomly choose a topic *Z* (use topic distribution for doc *i*)
- Randomly choose a word (use word distribution for topic *Z*)

LDA

- Easy to describe in terms of text (but works for not just text)
- Input: “document-word” matrix, and pre-specified # topics *k*

$$
\begin{array}{cc|cccc}
 & & & \textbf{Word} & & \\
 & & 1 & 2 & \dots & d \\
\hline
 & 1 & & & & \\
\textbf{Document} & 2 & & & & \\
 & \vdots & & & & \\
 & n & & & &
\end{array}
$$

i-th row, *j*-th column: # times word *j* appears in doc *i*

- Output: the *k* topics’ distribution of words

How to Choose Number of Topics *k*?

Something like CH index is also possible:

For a specific topic, look at the *m* most probable words ("top words")

Coherence (within cluster/topic variability):

$$\sum_{\substack{\text{top words } v,w \\ \text{that are not the same}}} \log \frac{(\text{\# documents with at least one appearance of } v \text{ and } w) + \varepsilon}{\text{\# documents with at least one appearance of } w}$$

choose something small like 0.01

Inter-topic similarity (between cluster/topic variability):

Can average each of these across the topics

Count # top words that do not appear in any of the other topics' *m* top words

(number of "unique words")

LDA

Demo (to be done by TA Erick)