Clustering and the $k$-means Algorithm

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Clustering

- Goal: Automatically segment data into groups of similar points

- Useful for:
  - Automatically organizing data
  - Understanding hidden structure in some data
  - Representing high-dimensional data in a low-dimensional space

- Examples:
  - Customers according to purchase histories
  - Genes according to expression profile
  - Search results according to topic
  - Facebook users according to interests
  - A museum catalog according to image similarity
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\[ \mathcal{D} = \{x_1, \ldots, x_N\}. \]
Clustering set-up

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- Each data point is \( p \)-dimensional, i.e.,
  \[ x_n = \langle x_{n,1}, \ldots, x_{n,p} \rangle \].
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• Define a distance function between data, \( d(x_n, x_m) \).

• Goal: segment the data into \( k \) groups

\[ \{z_1, \ldots, z_N\} \quad \text{where} \quad z_i \in \{1, \ldots, K\}. \]
Example data

500 2-dimensional data points: $\mathbf{x}_n = \langle x_{n,1}, x_{n,2} \rangle$
• What is a good distance function here?

Squared Euclidean distance is reasonable:

$$d(x_n, x_m) = \sum_{i=1}^{\|x_n - x_m\|^2}$$
Example data

- What is a good distance function here?
- Squared Euclidean distance is reasonable

\[ d(x_n, x_m) = \sum_{i=1}^{p} (x_{n,i} - x_{m,i})^2 = \|x_n - x_m\|^2 \]
Goal: segment this data into \( k \) groups.
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• What should $k$ be?
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• What should \( k \) be?
• Automatically choosing \( k \) is complicated; for now, 4.
Different clustering algorithms use data and distance in different ways
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We discuss \( k \)-means, the simplest clustering algorithm
• Different clustering algorithms use data and distance in different ways
• We discuss $k$-means, the simplest clustering algorithm
• The basic idea is to describe each cluster by its mean value.
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(Note: this works only for distances such that a mean is well-defined.)
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The goal of $k$-means is to assign data to clusters and define these clusters with their means.
\textit{k-means algorithm}

1. Initialization

- Data are $x_1, \ldots, x_N$
- Choose initial cluster means $m_1, \ldots, m_k$ (same dimension as data).

2. Repeat
   - Assign each data point to its closest mean:
     
     $z_n = \text{arg min}_{i \in \{1, \ldots, k\}} d(x_n, m_i)$

   - Compute each cluster mean to be the coordinate-wise average over data points assigned to that cluster:

     $m_k = \frac{1}{N_k} \sum_{n: z_n = k} x_n$

3. Until assignments $z_1, \ldots, z_N$ do not change
**k-means algorithm**

1. **Initialization**
   - Data are $\mathbf{x}_{1:N}$
\textit{k}-means algorithm

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$k$-means example
$k$-means example
\textit{k-means example}
$k$-means example
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OBJ=9.97e+00
$k$-means example

[Plot of $k$-means example]
• How can we measure how well our algorithm is doing?
Objective function

• How can we measure how well our algorithm is doing?
• The $k$-means objective function is the sum of the squared distances of each point to each assigned mean

\[ F(z_1:N, m_1:k) = \frac{1}{2} \sum_{n=1}^{N} ||x_n - m_{z_n}||^2 \]
$k$-means example (look at the objective)
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\[
\text{OBJ} = 9.97 \times 10^0
\]
$k$-means example (look at the objective)
Coordinate descent

\[ F(z_{1:N}, m_{1:k}) = \frac{1}{2} \sum_{n=1}^{N} \| x_n - m_{z_n} \|^2 \]

- Holding the means fixed, assigning each point to its closest mean minimizes \( F \) with respect to \( z_{1:N} \).

- Thus, \( k \)-means is a coordinate descent algorithm.

- It finds a local minimum. (Multiple restarts are often necessary.)
Coordinate descent

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Objective for the example data

Round of k-means

Objective
Compressing images

- Each pixel is associated with a red, green, and blue value.
Compressing images

- Each pixel is associated with a red, green, and blue value
- A $1024 \times 1024$ image is a collection of 1048576 values $\langle x_1, x_2, x_3 \rangle$, which requires 3M of storage
Compressing images

- Each pixel is associated with a red, green, and blue value
- A $1024 \times 1024$ image is a collection of 1048576 values $\langle x_1, x_2, x_3 \rangle$, which requires 3M of storage
- How can we use $k$-means to compress this image?
Vector quantization

- Replace each pixel $x_n$ with its assignment $m_{zn}$ ("paint by numbers").
Vector quantization

- Replace each pixel $x_n$ with its assignment $m_{z_n}$ (“paint by numbers”).
- The $k$ means are called the codebook.
Vector quantization

- Replace each pixel \( x_n \) with its assignment \( m_{z_n} \) ("paint by numbers").
- The \( k \) means are called the \textit{codebook}.
- With \( k = 100 \), we need 7 bits per pixel plus \( 100 \times 3 \) bits \( \approx 897K \).
2 means
4 means
8 means
16 means
32 means
64 means
128 means
256 means
The objective gives a measure of how distorted the compressed picture is relative to the original picture.
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For more clusters, the picture is less distorted.
In many practical settings, Euclidean distance is not appropriate. When?
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- Discrete multivariate data, such as purchase histories
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• For example,
  • Discrete multivariate data, such as purchase histories
  • Positive data, such as time spent on a web-page
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$k$-medoids is an algorithm that only requires knowing distances between data points, $d_{n,m} = d(x_n, x_{m_k})$. 
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$k$-medoids is an algorithm that only requires knowing distances between data points, $d_{n,m} = d(x_n, x_{m_k})$. 

No need to define the mean.
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$k$-medoids is an algorithm that only requires knowing distances between data points, \( d_{n,m} = d(x_n, x_{m_k}) \).

No need to define the mean.

Each of the clusters is associated with its most typical example.
**k-medoids algorithm**

1. **Initialization**

   - Data are \( x_1, \ldots, x_N \).
   - Choose initial cluster identities \( m_1, \ldots, m_k \).

2. **Repeat**

   - Assign each data point to its closest center:
     \[
     z_n = \text{arg min}_{i \in \{1, \ldots, k\}} d(x_n, m_i)
     \]

   - For each cluster, find the data point in that cluster that is closest to the other points in that cluster:
     \[
     i_k = \text{arg min}_{n : z_n = k} \sum_{m : z_m = k} d(x_n, x_m)
     \]

3. **Set each cluster center equal to their closest data points**:
   \[
   m_k = x_{i_k}
   \]

4. **Until assignments** \( z_1, \ldots, z_N \) do not change.
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  - Clustering customers for $k$ salespeople in a business

Usually, we seek the "natural" clustering, but what does this mean?
It is not well-defined.
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  - Clustering customers for $k$ salespeople in a business
- Usually, we seek the “natural” clustering, but what does this mean?
- It is not well-defined.
What happens as $k$ increases?
What happens as $k$ increases?

OBJ = 6.60e+01
What happens as $k$ increases?
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Heuristic: A kink in the objective

- Notice the “kink” in the objective between 3 and 5.
Heuristic: A kink in the objective

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- This suggests that 4 is the right number of clusters.
Heuristic: A kink in the objective

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- This suggests that 4 is the right number of clusters.
- Tibshirani (2001) presents a method for finding this kink.
• Spatial and Statistical Inference of Late Bronze Age Polities in the Southern Levant (Savage and Falconer)
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• Cluster the location of archeological sites in Israel
Archeology

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• Cluster the location of archeological sites in Israel
• Make inferences about political history based on the clusters
• Choose \( k \) very carefully, with a complicated computational technique.
• Coping with cold: An integrative, multitissue analysis of the transcriptome of a poikilothermic vertebrate (Gracey et al., 2004)
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• (No mention of how $k = 23$ was chosen.)
• Teachers as Sources of Middle School Students’ Motivational Identity: Variable-Centered and Person-Centered Analytic Approaches (Murdock and Miller, 2003)
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• Used the clusters to identify groups to buttress an analysis of what affects motivation.
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• I.e., the levels of encouragement are corrected for
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• Clustered survey results of 206 students
• Used the clusters to identify groups to buttress an analysis of what affects motivation.
• I.e., the levels of encouragement are corrected for
• Chose the number of clusters to get nice results
<table>
<thead>
<tr>
<th>Table 3. Five-Cluster Solution: Z scores on Each Clustering Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cluster</td>
</tr>
<tr>
<td>---------------------------------------------------------------</td>
</tr>
<tr>
<td>Teacher caring</td>
</tr>
<tr>
<td>Peers' academic support</td>
</tr>
<tr>
<td>Parents' academic support</td>
</tr>
</tbody>
</table>

<table>
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<tr>
<th>Table 4. Means and Standard Deviations for Each Cluster on Grade 8 Motivational Variables</th>
</tr>
</thead>
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<tr>
<td>---------------------------------------------------------------</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>---------------------------------------------------------------</td>
</tr>
<tr>
<td>1. All positive</td>
</tr>
<tr>
<td>2. Peer negative, parents very negative</td>
</tr>
<tr>
<td>3. Peer positive</td>
</tr>
<tr>
<td>4. Negative teacher and peer</td>
</tr>
<tr>
<td>5. Positive teacher and parents</td>
</tr>
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• Implications of Racial and Gender Differences in Patterns of Adolescent Risk Behavior for HIV and other Sexually Transmitted Diseases (Halpert et al., 2004)
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- Clustered survey results of 13,998 students to understand patterns of drug abuse and sexual activity
- K chosen for interpretability and “stability,” which means that they could interpret multiple k-means runs on different data in the same way.
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• Draw the conclusion that patterns exist. What’s wrong with this?
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• Draw the conclusion that patterns exist. What’s wrong with this?

• $k$-means will find patterns everywhere!
### TABLE 2. Percentage distribution of participants, by cluster, and behavioral patterns defining each cluster

<table>
<thead>
<tr>
<th>Cluster type and behavioral patterns</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Light substance dabblers</strong>—infrequent or no current use of substances†</td>
<td>24.4</td>
</tr>
<tr>
<td>None have had sex</td>
<td></td>
</tr>
<tr>
<td><strong>Abstainers</strong>—none have ever used substances† or had sex</td>
<td>22.7</td>
</tr>
<tr>
<td><strong>Sex dabblers</strong>—all have had sex</td>
<td>14.5</td>
</tr>
<tr>
<td>Median no. of partners=1</td>
<td></td>
</tr>
<tr>
<td>60% used a condom at last sex</td>
<td></td>
</tr>
<tr>
<td>Infrequent use of substances†</td>
<td></td>
</tr>
<tr>
<td><strong>Drinkers</strong>—all consumed alcohol in past 12 mos.</td>
<td>7.4</td>
</tr>
<tr>
<td>49% report binge drinking</td>
<td></td>
</tr>
<tr>
<td>Infrequent or no illicit drug use</td>
<td></td>
</tr>
<tr>
<td>None have had sex</td>
<td></td>
</tr>
<tr>
<td><strong>Smokers</strong>—all smoke cigarettes daily</td>
<td>7.3</td>
</tr>
<tr>
<td>Infrequent use of alcohol/illicit drugs</td>
<td></td>
</tr>
<tr>
<td>62% have had sex</td>
<td></td>
</tr>
<tr>
<td><strong>Alcohol-and-sex dabblers</strong>—all drink occasionally; all have had sex</td>
<td>5.4</td>
</tr>
<tr>
<td>Infrequent tobacco/illicit drug use</td>
<td></td>
</tr>
<tr>
<td><strong>Binge drinkers</strong>—all binge frequently</td>
<td>4.4</td>
</tr>
<tr>
<td>Infrequent cigarette, marijuana and other drug use</td>
<td></td>
</tr>
<tr>
<td>60% binge ≥1 time/wk</td>
<td></td>
</tr>
<tr>
<td>45% have had sex</td>
<td></td>
</tr>
<tr>
<td><strong>Heavy dabblers</strong>—all smoke, drink and binge drink with moderate frequency</td>
<td>3.6</td>
</tr>
<tr>
<td>45% use marijuana; few use other illicit drugs</td>
<td></td>
</tr>
<tr>
<td>91% have had sex</td>
<td></td>
</tr>
<tr>
<td><strong>Combination sex and drug use</strong>—all have had sex; all used alcohol/illicit drug at last sex</td>
<td>3.4</td>
</tr>
<tr>
<td><strong>Marijuana users</strong>—all use marijuana frequently; few have used other illicit drugs</td>
<td>1.7</td>
</tr>
<tr>
<td>94% use alcohol</td>
<td></td>
</tr>
<tr>
<td>79% smoke cigarettes</td>
<td></td>
</tr>
<tr>
<td>74% have had sex</td>
<td></td>
</tr>
<tr>
<td><strong>Multiple partners</strong>—all report ≥14 sexual partners</td>
<td>1.3</td>
</tr>
<tr>
<td>75% report low or moderate use of substances†</td>
<td></td>
</tr>
<tr>
<td><strong>Sex for drugs or money</strong>—all have had sex for drugs or money</td>
<td>1.2</td>
</tr>
<tr>
<td>50% report low or moderate use of substances†</td>
<td></td>
</tr>
<tr>
<td>Median no. of partners=3</td>
<td></td>
</tr>
<tr>
<td><strong>High marijuana use and sex</strong>—all use marijuana frequently; all have had sex</td>
<td>1.1</td>
</tr>
<tr>
<td>All used alcohol/other drug at last sex</td>
<td></td>
</tr>
<tr>
<td>82% have had &gt;1 partner (median=6)</td>
<td></td>
</tr>
<tr>
<td><strong>Marijuana and other drug users</strong>—95% report heavy marijuana use; all use other illicit drugs</td>
<td>0.6</td>
</tr>
<tr>
<td>68% have had sex</td>
<td></td>
</tr>
<tr>
<td>28% used alcohol/other drug at last sex</td>
<td></td>
</tr>
<tr>
<td><strong>Injection-drug users</strong>—all have injected drugs</td>
<td>0.6</td>
</tr>
<tr>
<td>82% have had sex</td>
<td></td>
</tr>
<tr>
<td>Median no. of partners=4</td>
<td></td>
</tr>
<tr>
<td><strong>Males who have sex with males</strong>—all are males who have had sex with another male</td>
<td>0.3</td>
</tr>
<tr>
<td>78% have had multiple partners (median=5)</td>
<td></td>
</tr>
<tr>
<td>49% used marijuana in past 30 days</td>
<td></td>
</tr>
<tr>
<td>50% use alcohol ≥1 time/mo.</td>
<td></td>
</tr>
<tr>
<td>17% have had sex for drugs or money</td>
<td></td>
</tr>
</tbody>
</table>