• Fill in the missing plots:

\[ \Sigma = X^T J J X = Z^T J J Z \]

\[ V S V^T = \text{eig}(\Sigma) \quad J = I - \frac{11^T}{n} \]

\[ \mu_X = X^T 1/n \quad \mu_Z = Z^T 1/n \]

\[ X \quad Z \quad \mu_X - \mu_Z \quad V S^{-1/2} V^T (\mu_X - \mu_Z) \]
Matrix Completion

Machine Learning – CSE546
Kevin Jamieson
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November 15, 2016
Singular Value Decomposition (SVD)

Theorem (SVD): Let $A \in \mathbb{R}^{m \times n}$ with rank $r \leq \min\{m, n\}$. Then $A = USV^T$
where $S \in \mathbb{R}^{r \times r}$ is diagonal with positive entries, $U^TU = I$, $V^TV = I$.

$U = [u_1, \ldots, u_r]$  \hspace{1cm} $V = [v_1, \ldots, v_r]$

$A^TAv_i = S_{i,i}v_i$

$AA^Tu_i = S_{i,i}u_i$

$V$ are the first $r$ eigenvectors of $A^TA$ with eigenvalues $\text{diag}(S)$
$U$ are the first $r$ eigenvectors of $AA^T$ with eigenvalues $\text{diag}(S)$
Theorem (SVD): Let $A \in \mathbb{R}^{m \times n}$ with rank $r \leq \min\{m, n\}$. Then $A = USV^T$ where $S \in \mathbb{R}^{r \times r}$ is diagonal with positive entries, $U^TU = I$, $V^TV = I$.

$$U = [u_1, \ldots, u_r] \quad V = [v_1, \ldots, v_r] \quad S = \text{diag}(s_1, \ldots, s_r)$$

$$A = \sum_{k=1}^{r} u_k v_k^T s_k \quad s_1 \geq s_2 \geq \cdots \geq s_r$$

Best rank-1 approximation $\sigma > 0$ and unit vectors $x \in \mathbb{R}^m$, $y \in \mathbb{R}^n$ minimizes:

$$\| \sigma xy^T - A \|_F^2 =$$
Singular Value Decomposition (SVD)

Theorem (SVD): Let $A \in \mathbb{R}^{m \times n}$ with rank $r \leq \min\{m, n\}$. Then $A = USV^T$ where $S \in \mathbb{R}^{r \times r}$ is diagonal with positive entries, $U^TU = I$, $V^TV = I$.

$$U = [u_1, \ldots, u_r] \quad V = [v_1, \ldots, v_r] \quad S = \text{diag}(s_1, \ldots, s_r)$$

$$A = \sum_{k=1}^{r} u_k v_k^T s_k$$

$s_1 \geq s_2 \geq \cdots \geq s_r$

Best rank-1 approximation $\sigma > 0$ and unit vectors $x \in \mathbb{R}^m$, $y \in \mathbb{R}^n$ minimizes:

$$\|\sigma xy^T - A\|_F^2 = \sigma^2 + \text{Tr}(A^TA) - 2\sigma x^TAy$$

$$= \sigma^2 + \left( \sum_{k=1}^{r} s_k^2 \right) - 2\sigma \left( \sum_{k=1}^{r} x^T u_k v_k^T y s_k \right)$$

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Singular Value Decomposition (SVD)

**Theorem (SVD):** Let $A \in \mathbb{R}^{m \times n}$ with rank $r \leq \min\{m, n\}$. Then $A = USV^T$ where $S \in \mathbb{R}^{r \times r}$ is diagonal with positive entries, $U^T U = I$, $V^T V = I$.

$$U = [u_1, \ldots, u_r] \quad V = [v_1, \ldots, v_r] \quad S = \text{diag}(s_1, \ldots, s_r)$$

$$A = \sum_{k=1}^{r} u_k v_k^T s_k$$

$$s_1 \geq s_2 \geq \cdots \geq s_r$$

In general: $\sum_{k=1}^{p} u_i v_i^T s_i = \arg \min_{\text{rank}(Z) = p} \|Z - A\|_F^2$
Matrix completion

Given historical data on how users rated movies in past:

17,700 movies, 480,189 users, 99,072,112 ratings  
(Sparsity: 1.2%)

Predict how the same users will rate movies in the future (for $1 million prize)
Matrix completion

n movies, m users, |S| ratings

\[ \begin{align*}
\text{arg min} & \quad U \in \mathbb{R}^{m \times d}, V \in \mathbb{R}^{n \times d} \\
& \quad \sum_{(i,j,s) \in S} \| (UV^T)_{i,j} - s_{i,j} \|^2_2
\end{align*} \]

How do we solve it? With full information?
Matrix completion

n movies, m users, |S| ratings

\[
\arg \min_{U \in \mathbb{R}^{m \times d}, V \in \mathbb{R}^{n \times d}} \sum_{(i,j,s) \in S} \| (UV^T)_{i,j} - s_{i,j} \|_2^2
\]
Matrix completion

n movies, m users, |S| ratings

\[
\begin{align*}
\arg \min_{U \in \mathbb{R}^{m \times d}, V \in \mathbb{R}^{n \times d}} & \quad \sum_{(i,j,s) \in S} \| (UV^T)_{i,j} - s_{i,j} \|_2^2 \\
\end{align*}
\]

Practical techniques to solve:
- Alternating minimization (Fix U, minimize V. Then fix V and minimize U)
- Stochastic gradient descent on U, V
- Nuclear norm regularization (convex)
Clustering
K-means

Machine Learning – CSE546
Kevin Jamieson
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November 15, 2016
Clustering images

Set of Images

[Goldberger et al.]
Clustering web search results

1. **Race (classification of human beings) - Wikipedia, the free encyclopedia**
   - The term race or racial group usually refers to the concept of dividing humans into populations or groups on the basis of various sets of characteristics. The most widely used human racial categories are based on visible traits (especially skin color, cranial or facial features and hair texture), and self-identification. Conceptions of race, as well as specific ways of grouping races, vary by culture and over time, and are often controversial for scientific as well as social and political reasons.
   - History - Modern debates - Political and...

2. **Race - Wikipedia, the free encyclopedia**
   - General. Racing competitions. The Race (yachting race), or La course du millenaire, a no-rules round-the-world sailing event; Race (biology), classification of flora and fauna; Race (classification of human beings) Race and ethnicity in the United States Census, official definitions of “race” used by the US Census Bureau; Race and genetics, notion of racial classifications based on genetics. Historical definitions of race; Race (bearing), the inner and outer rings of a rolling-element bearing. RACE in molecular biology “Rapid... General - Surnames - Television - Music - Literature - Video games

3. **Publications | Human Rights Watch**
   - The use of torture, unlawful rendition, secret prisons, unfair trials, ... Risks to Migrants, Refugees, and Asylum Seekers in Egypt and Israel... In the run-up to the Beijing Olympics in August 2008, ...
   - www.hrw.org/backgrounder/usa/race - [cache] - Ask

4. **Amazon.com: Race: The Reality Of Human Differences: Vincent Sarich ...**
   - Amazon.com: Race: The Reality Of Human Differences: Vincent Sarich, Frank Miele. Books ... From Publishers Weekly Sarich, a Berkeley emeritus anthropologist, and Miele, an editor ...

5. **AAPA Statement on Biological Aspects of Race**
   - AAPA Statement on Biological Aspects of Race ... Published in the American Journal of Physical Anthropology, vol. 101, pp 569-570, 1996 ... PREAMBLE As scientists who study human evolution and variation, ...
   - www.physanth.org/positions/race.html - [cache] - Ask

6. **race: Definition from Answers.com**
   - race n. A local geographic or global human population distinguished as a more or less distinct group by genetically transmitted physical
   - www.answers.com/topic/race-1 - [cache] - Live

7. **Dopefish.com**
   - Site for newbies as well as experienced Dopefish followers, chronicling the birth of the Dopefish, its numerous appearances in several computer games, and its eventual take-over of the human race. Maintained by Mr. Dopefish himself, Joe Siegler of Aogoee Software.
Some Data
K-means

1. Ask user how many clusters they’d like. *(e.g. k=5)*
K-means

1. Ask user how many clusters they’d like. \((e.g. \, k=5)\)

2. Randomly guess \(k\) cluster Center locations
K-means

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2. Randomly guess \(k\) cluster Center locations

3. Each datapoint finds out which Center it’s closest to. (Thus each Center “owns” a set of datapoints)
K-means

1. Ask user how many clusters they’d like. (e.g. $k=5$)

2. Randomly guess $k$ cluster Center locations

3. Each datapoint finds out which Center it’s closest to.

4. Each Center finds the centroid of the points it owns
K-means

1. Ask user how many clusters they’d like. (e.g. $k=5$)
2. Randomly guess $k$ cluster Center locations
3. Each datapoint finds out which Center it’s closest to.
4. Each Center finds the centroid of the points it owns…
5. …and jumps there
6. …Repeat until terminated!
K-means

- Randomly initialize $k$ centers
  - $\mu^{(0)} = \mu_1^{(0)}, \ldots, \mu_k^{(0)}$

- **Classify**: Assign each point $j \in \{1, \ldots, N\}$ to nearest center:
  - $C^{(t)}(j) \leftarrow \arg \min_i ||\mu_i - x_j||^2$

- **Recenter**: $\mu_i$ becomes centroid of its point:
  - $\mu_i^{(t+1)} \leftarrow \arg \min_{\mu} \sum_{j:C(j)=i} ||\mu - x_j||^2$
  - Equivalent to $\mu_i \leftarrow \text{average of its points!}$
Does K-means converge?? Part 1

- Optimize potential function:

\[
\min_{\mu} \min_{C} F(\mu, C) = \min_{\mu} \min_{C} \sum_{i=1}^{k} \sum_{j: C(j) = i} ||\mu_i - x_j||^2
\]

- Fix \( \mu \), optimize C
Does K-means converge?? Part 2

- Optimize potential function:

\[
\min_{\mu} \min_{C} F(\mu, C) = \min_{\mu} \min_{C} \sum_{k} \sum_{j : C(j) = i} \|\mu_i - x_j\|^2
\]

- Fix C, optimize \(\mu\)
Vector Quantization, Fisher Vectors

**Vector Quantization** (for compression)

1. Represent image as grid of patches
2. Run k-means on the patches to build code book
3. Represent each patch as a code word.

*FIGURE 14.9. Sir Ronald A. Fisher (1890 – 1962) was one of the founders of modern day statistics, to whom we owe maximum-likelihood, sufficiency, and many other fundamental concepts. The image on the left is a 1024×1024 grayscale image at 8 bits per pixel. The center image is the result of 2×2 block VQ, using 200 code vectors, with a compression rate of 1.9 bits/pixel. The right image uses only four code vectors, with a compression rate of 0.50 bits/pixel.*
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**FIGURE 14.9.** Sir Ronald A. Fisher (1890 – 1962) was one of the founders of modern day statistics, to whom we owe maximum-likelihood, sufficiency, and many other fundamental concepts. The image on the left is a 1024×1024 grayscale image at 8 bits per pixel. The center image is the result of 2×2 block VQ, using 200 code vectors, with a compression rate of 1.9 bits/pixel. The right image uses only four code vectors, with a compression rate of 0.50 bits/pixel.
Vector Quantization (for compression)

1. Represent image as grid of patches
2. Run k-means on the patches to build code book
3. Represent each patch as a code word.

Typical output of k-means on patches

**FIGURE 14.9.** Sir Ronald A. Fisher (1890 – 1962) was one of the founders of modern day statistics, to whom we owe maximum-likelihood, sufficiency, and many other fundamental concepts. The image on the left is a 1024×1024 grayscale image at 8 bits per pixel. The center image is the result of 2×2 block VQ, using 200 code vectors, with a compression rate of 1.9 bits/pixel. The right image uses only four code vectors, with a compression rate of 0.50 bits/pixel

Similar reduced representation can be used as a feature vector

Coates, Ng, *Learning Feature Representations with K-means*, 2012
Spectral Clustering

Adjacency matrix: $W$

$W_{i,j} = \text{weight of edge } (i, j)$

$D_{i,i} = \sum_{j=1}^{n} W_{i,j}$

$L = D - W$

Given feature vectors, could construct:
- $k$-nearest neighbor graph with weights in $\{0,1\}$
- weighted graph with arbitrary similarities $W_{i,j} = e^{-\gamma \|x_i - x_j\|^2}$

Let $f \in \mathbb{R}^n$ be a function over the nodes

$$f^T L f = \sum_{i=1}^{N} g_i f_i^2 - \sum_{i=1}^{N} \sum_{i'=1}^{N} f_i f_{i'} w_{ii'}$$

$$= \frac{1}{2} \sum_{i=1}^{N} \sum_{i'=1}^{N} w_{ii'} (f_i - f_{i'})^2.$$
Spectral Clustering

Adjacency matrix: $W$

$W_{i,j} = \text{weight of edge } (i, j)$

$D_{i,i} = \sum_{j=1}^{n} W_{i,j}$ \quad $L = D - W$

Given feature vectors, could construct:
- k-nearest neighbor graph with weights in \{0,1\}
- weighted graph with arbitrary similarities $W_{i,j} = e^{-\gamma \|x_i - x_j\|^2}$

Let $f \in \mathbb{R}^n$ be a function over the nodes

$f^T L f = \sum_{i=1}^{N} g_i f_i^2 - \sum_{i=1}^{N} \sum_{i' = 1}^{N} f_i f_{i'} w_{ii'}$

$= \frac{1}{2} \sum_{i=1}^{N} \sum_{i' = 1}^{N} w_{ii'} (f_i - f_{i'})^2$. 
Spectral Clustering

Adjacency matrix: $W$

$W_{i,j} = \text{weight of edge } (i, j)$

$D_{i,i} = \sum_{j=1}^{n} W_{i,j}$

$L = D - W$

Given feature vectors, could construct:
- (k=10)-nearest neighbor graph with weights in $\{0,1\}$
Mixtures of Gaussians

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November 15, 2016
(One) bad case for k-means

- Clusters may overlap
- Some clusters may be "wider" than others
(One) bad case for k-means

- Clusters may overlap
- Some clusters may be “wider” than others
Mixture models

\[ Y_1 \sim N(\mu_1, \sigma_1^2), \]
\[ Y_2 \sim N(\mu_2, \sigma_2^2), \]
\[ Y = (1 - \Delta) \cdot Y_1 + \Delta \cdot Y_2, \]
\[ \Delta \in \{0, 1\} \text{ with } \Pr(\Delta = 1) = \pi \]

If \( \phi_\theta(x) \) is Gaussian density with parameters \( \theta = (\mu, \sigma^2) \) then

\[
\ell(\theta; Z) = \sum_{i=1}^{n} \log[(1 - \pi)\phi_{\theta_1}(y_i) + \pi\phi_{\theta_2}(y_i)]
\]
Mixture models

\[ Y_1 \sim N(\mu_1, \sigma_1^2), \]
\[ Y_2 \sim N(\mu_2, \sigma_2^2), \]
\[ Y = (1 - \Delta) \cdot Y_1 + \Delta \cdot Y_2, \]
\[ \Delta \in \{0, 1\} \text{ with } \Pr(\Delta = 1) = \pi \]
\[ \theta = (\pi, \theta_1, \theta_2) = (\pi, \mu_1, \sigma_1^2, \mu_2, \sigma_2^2) \]

If \( \phi_\theta(x) \) is Gaussian density with parameters \( \theta = (\mu, \sigma^2) \) then
\[ \ell(\theta; y_i, \Delta_i = 0) = \]
\[ \ell(\theta; y_i, \Delta_i = 1) = \]

\[ Z = \{y_i\}_{i=1}^n \text{ is observed data} \]
\[ \Delta = \{\Delta_i\}_{i=1}^n \text{ is unobserved data} \]
Mixture models

\[ Y_1 \sim N(\mu_1, \sigma_1^2), \]
\[ Y_2 \sim N(\mu_2, \sigma_2^2), \]
\[ Y = (1 - \Delta) \cdot Y_1 + \Delta \cdot Y_2, \]

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If \( \phi_{\theta}(x) \) is Gaussian density with parameters \( \theta = (\mu, \sigma^2) \) then

\[
\ell(\theta; Z, \Delta) = \sum_{i=1}^{n} (1 - \Delta_i) \log[(1 - \pi) \phi_{\theta_1}(y_i)] + \Delta_i \log(\pi \phi_{\theta_2}(y_i))
\]

If we knew \( \Delta \), how would we choose \( \theta \)?
Mixture models

\[
\begin{align*}
Y_1 & \sim N(\mu_1, \sigma_1^2), \\
Y_2 & \sim N(\mu_2, \sigma_2^2), \\
Y &= (1 - \Delta) \cdot Y_1 + \Delta \cdot Y_2,
\end{align*}
\]

\[\Delta \in \{0, 1\} \text{ with } \Pr(\Delta = 1) = \pi\]

\[\theta = (\pi, \theta_1, \theta_2) = (\pi, \mu_1, \sigma_1^2, \mu_2, \sigma_2^2)\]

If \(\phi_\theta(x)\) is Gaussian density with parameters \(\theta = (\mu, \sigma^2)\) then

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\]

If we knew \(\theta\), how would we choose \(\Delta\)?
Mixture models

\[ Y_1 \sim N(\mu_1, \sigma^2_1), \]
\[ Y_2 \sim N(\mu_2, \sigma^2_2), \]
\[ Y = (1 - \Delta) \cdot Y_1 + \Delta \cdot Y_2, \]
\[ \Delta \in \{0, 1\} \text{ with } \Pr(\Delta = 1) = \pi \]
\[ \theta = (\pi, \theta_1, \theta_2) = (\pi, \mu_1, \sigma^2_1, \mu_2, \sigma^2_2) \]

If \( \phi_\theta(x) \) is Gaussian density with parameters \( \theta = (\mu, \sigma^2) \) then

\[
\ell(\theta; Z, \Delta) = \sum_{i=1}^{n} (1 - \Delta_i) \log[(1 - \pi)\phi_{\theta_1}(y_i)] + \Delta_i \log(\pi\phi_{\theta_2}(y_i))
\]

\[
\gamma_i(\theta) = \mathbb{E}[\Delta_i | \theta, Z] =
\]
Mixture models

Algorithm 8.1 EM Algorithm for Two-component Gaussian Mixture.

1. Take initial guesses for the parameters $\hat{\mu}_1, \hat{\sigma}_1^2, \hat{\mu}_2, \hat{\sigma}_2^2, \hat{\pi}$ (see text).

2. Expectation Step: compute the responsibilities

$$\hat{\gamma}_i = \frac{\hat{\pi} \phi_{\hat{\theta}_2}(y_i)}{(1 - \hat{\pi}) \phi_{\hat{\theta}_1}(y_i) + \hat{\pi} \phi_{\hat{\theta}_2}(y_i)}, \quad i = 1, 2, \ldots, N. \quad (8.42)$$

3. Maximization Step: compute the weighted means and variances:

$$\hat{\mu}_1 = \frac{\sum_{i=1}^{N} (1 - \hat{\gamma}_i) y_i}{\sum_{i=1}^{N} (1 - \hat{\gamma}_i)}, \quad \hat{\sigma}_1^2 = \frac{\sum_{i=1}^{N} (1 - \hat{\gamma}_i) (y_i - \hat{\mu}_1)^2}{\sum_{i=1}^{N} (1 - \hat{\gamma}_i)},$$

$$\hat{\mu}_2 = \frac{\sum_{i=1}^{N} \hat{\gamma}_i y_i}{\sum_{i=1}^{N} \hat{\gamma}_i}, \quad \hat{\sigma}_2^2 = \frac{\sum_{i=1}^{N} \hat{\gamma}_i (y_i - \hat{\mu}_2)^2}{\sum_{i=1}^{N} \hat{\gamma}_i},$$

and the mixing probability $\hat{\pi} = \sum_{i=1}^{N} \hat{\gamma}_i / N.$

4. Iterate steps 2 and 3 until convergence.
Gaussian Mixture Example: Start
After first iteration
After 2nd iteration
After 3rd iteration
After 4th iteration
After 5th iteration
After 6th iteration
After 20th iteration
Some Bio Assay data
GMM clustering of the assay data
Resulting Density Estimator