In question 2, you solve for $\alpha \in \mathbb{R}^{n}$: $\hat{\mathfrak{f}}(x) = \sum_{i=1}^{n} \alpha_{i} \kappa(x, x_{i}) \in \mathbb{T}$ this is a function Announcements $\alpha_{i} = \mathbb{E}[(z-\alpha)^{2}] = \mathbb{E}[z]$ $\mathbb{E}[(z-1\mathbb{E}[z])^{2}] \ge 0$ on an arbitrarily $\alpha \in \mathbb{E}[(z-\alpha)^{2}] = \mathbb{E}[z]$ $\mathbb{E}[z]$ $\mathbb{E}[(z-1\mathbb{E}[z])^{2}] \ge 0$ fine grid

- Homework 3 due tonight! Milestones graded.
- HW 4 will be posted tonight. Start early. $E[Y|_{X=x}] \stackrel{\text{and}}{=} E[(Y-f(x))^{2}] \qquad \begin{bmatrix} x \\ Y \end{bmatrix} \sim \mathcal{N}(\begin{bmatrix} \mu_{Y} \\ \mu_{Y} \end{bmatrix}, \begin{bmatrix} \Sigma_{xx} \\ \Sigma_{xx} \\ \Sigma_{xx} \end{bmatrix}, \begin{bmatrix} x \\ \Sigma_{xx} \\$
- $\nabla_{w}l(w) = \nabla_{w}E\left[-2wT(x-\mu_{x})(y-\mu_{y}) + wT(x-\mu_{x})(x-\mu_{x})w\right] \leq \frac{1}{2}$
 - = IE[-2(x- μ_x)(Y- μ_y)+ 2(x- μ_x)(x- μ_x)w]
 - $= -2 \Sigma_{YX} + 2 \Sigma_{XX} = 0 \qquad W = \Sigma_{XX} \Sigma_{YX}$

Clustering

Machine Learning – CSE546 Kevin Jamieson University of Washington

November 21, 2016

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Clustering images







Clustering web search results

web news images wikipedia blogs jobs more »	
Clusty race Search advanced preferences	
clusters sources sites All Results (28) Car (28)	Cluster Human contains 8 documents. Search Results 1. Race (classification of human beings) - Wikipedia, the free 한 역, 응 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
Race cars (7) Photos, Races Scheduled (1) Game (4)	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 en.wikipedia.org/wiki/Race_(classification_of_human_beings) - [cache] - Live, Ask 2. Race - Wikipedia, the free encyclopedia to \mathcal{R} .
e Track (2) e Nascar (2) e Equipment And Safety (2) e Other Topics (7)	General. Racing competitions The Race (yachting race), or La course du millénaire, 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 - Sumames - Television - Music - Literature - Video games en.wikipedia.org/wiki/Race - [cache] - Live, Ask
 Photos (22) Game (14) Definition (13) 	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
Team (18) Human (8) Classification Of Human (2)	 Amazon.com: Race: The Reality Of Human Differences: Vincent Sarich や へ あ 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 www.amazon.com/Race-Reality-Differences-Vincent-Sarich/dp/0813340861 - [cache] - Live AMRX Obstanzations Distributional Academic of Paces Distribution (Paces Distribution)
Statement, Evolved (2) Other Topics (4) Weekend (8)	 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
Ethnicity And Race (7) Race for the Cure (8) Race Information (8) more Lal clusters	 race: Definition from Answers.com 원 식 응 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/tace-1 - [cache] - Live Dopefish.com 원 식 응
find in clusters:	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 Apogee Software. www.dopefish.com - [cache] - Open Directory

Hierarchical Clustering

Pick one:

- Bottom up: start with every point as a cluster and merge
- Top down: start with a single cluster containing all points and split

Different rules for splitting/merging, no "right answer"

Gives apparently interpretable tree representation. However, warning: even random data with no structure will produce a tree that "appears" to be structured.



Some Data



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



- Ask user how many clusters they'd like. (e.g. k=5)
- 2. Randomly guess k cluster Center locations



- Ask user how many clusters they'd like. (e.g. k=5)
- 2. Randomly guess k cluster Center locations
- Each datapoint finds out which Center it's closest to. (Thus each Center "owns" a set of datapoints)



- 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

- 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!

Randomly initialize k centers

$$= \mu^{(0)} = \mu_1^{(0)}, \dots, \, \mu_k^{(0)}$$

Classify: Assign each point j∈{1,...N} to nearest center:

$$\Box \quad C^{(t)}(j) \leftarrow \arg\min_i ||\mu_i - x_j||^2$$

• **Recenter**: μ_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 $\mu_i \leftarrow$ average of its points!

What is K-means optimizing?

 Potential function F(μ,C) of centers μ and point allocations C:

$$F(\mu, C) = \sum_{j=1}^{N_{\perp}} ||\mu_{C(j)} - x_j||^2$$

Optimal K-means:
 min_μmin_c F(μ,C)

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 μ, optimize C

Does K-means converge??? Part 2

• 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 C, optimize μ

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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Typical output of k-means on patches

Similar reduced representation can be used as a feature vector

Coates, Ng, Learning Feature Representations with K-means, 2012

Spectral Clustering

Adjacency matrix: \mathbf{W}

$$\mathbf{W}_{i,j} = \text{weight of edge } (i,j)$$
$$\mathbf{D}_{i,i} = \sum_{j=1}^{n} \mathbf{W}_{i,j} \qquad \mathbf{L} = \mathbf{D} - \mathbf{W}$$

Given feature vectors, could construct:

- k-nearest neighbor graph with weights in {0,1}
- weighted graph with arbitrary similarities $\mathbf{W}_{i,j} = e^{-\gamma ||x_i x_j||^2}$

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

$$\begin{aligned} \mathbf{f}^T \mathbf{L} \mathbf{f} &= \sum_{i=1}^N g_i f_i^2 - \sum_{i=1}^N \sum_{i'=1}^N f_i f_{i'} w_{ii'} \\ &= \frac{1}{2} \sum_{i=1}^N \sum_{i'=1}^N w_{ii'} (f_i - f_{i'})^2. \end{aligned}$$

Spectral Clustering

Adjacency matrix: ${\bf W}$

$$\mathbf{W}_{i,j} = \text{weight of edge } (i,j)$$
$$\mathbf{D}_{i,i} = \sum_{j=1}^{n} \mathbf{W}_{i,j} \qquad \mathbf{L} = \mathbf{D} - \mathbf{W}$$

Given feature vectors, could construct:

 (k=10)-nearest neighbor graph with weights in {0,1}

Popular to use the Laplacian \mathbf{L} or its normalized form $\widetilde{\mathbf{L}} = I - \mathbf{D}^{-1} \mathbf{W}$ as a regularizer for learning over graphs

Mixtures of Gaussians

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(One) bad case for k-means

(One) bad case for k-means

 Some clusters may be "wider" than others

 $\mathbf{Z} = \{y_i\}_{i=1}^n$ is observed data

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

Mixture models $l(\theta|x_i=i) = \theta$ $l(\theta;x_i) = \theta^{x_i}(\theta)^{x_i}$ $l(\theta|x_i=i) = l - \theta$

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

 $\mathbf{Z} = \{y_i\}_{i=1}^n \text{ is observed data}$ $\mathbf{\Delta} = \{\Delta_i\}_{i=1}^n \text{ is unobserved data}$

$$\ell(\theta; y_i, \underline{\Delta_i} = 0) = \log \left(\mathcal{O}_{\theta_i}(y_i)(1 - \pi) \right)$$
$$\ell(\theta; y_i, \underline{\Delta_i} = 1) = \log \left(\mathcal{O}_{\theta_i}(y_i)(1 - \pi) \right)$$

$$\mathcal{L}(\vartheta; Y_i, \Delta_i) = (\mathbf{I} - \Delta_i) \log((\mathbf{I} - \mathbf{\pi}) \mathscr{O}_{\mathcal{O}_i}(Y_i)) + \Delta_i \log(\mathbf{\pi} \mathscr{O}_{\mathcal{O}_i}(Y_i))$$

$$\begin{array}{rcl} Y_{1} & \sim & N(\mu_{1},\sigma_{1}^{2}), \\ Y_{2} & \sim & N(\mu_{2},\sigma_{2}^{2}), \\ Y & = & (1-\Delta) \cdot Y_{1} + \Delta \cdot Y_{2}, \\ \Delta \in \{0,1\} \text{ with } \Pr(\Delta=1) = \pi \\ \theta = (\pi,\theta_{1},\theta_{2}) = (\pi,\mu_{1},\sigma_{1}^{2},\mu_{2},\sigma_{2}^{2}) \end{array}$$

 $\mathbf{Z} = \{y_i\}_{i=1}^n$ is observed data $\mathbf{\Delta} = \{\Delta_i\}_{i=1}^n$ is unobserved data

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

If we knew Δ , how would we choose θ ? $\mu_i = \frac{1}{\sum_{i=1}^{n} (1 - \Delta_i)} \sum_{i=1}^{n} (1 - \Delta_i) y_i$

$$\begin{array}{rcl} Y_{1} & \sim & N(\mu_{1},\sigma_{1}^{2}), \\ Y_{2} & \sim & N(\mu_{2},\sigma_{2}^{2}), \\ Y & = & (1-\Delta) \cdot Y_{1} + \Delta \cdot Y_{2}, \\ \Delta \in \{0,1\} \text{ with } \Pr(\Delta=1) = \pi \\ \theta = (\pi,\theta_{1},\theta_{2}) = (\pi,\mu_{1},\sigma_{1}^{2},\mu_{2},\sigma_{2}^{2}) \end{array}$$

 $\mathbf{Z} = \{y_i\}_{i=1}^n$ is observed data $\mathbf{\Delta} = \{\Delta_i\}_{i=1}^n$ is unobserved data

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

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

If we knew θ , how would we choose Δ ?

$$\mathbb{E}\left[\Delta_{i} \mid \Theta, \mathcal{Z}\right] = \mathbb{P}\left(A_{i}^{z} = 1 \mid \Theta, \mathcal{Z}\right)$$

$$= \frac{\tau \mathcal{E}\left(\varphi_{2}\left(y_{i}\right)\right)}{(1 - \tau \mathcal{E})\Theta_{1}\left(y_{i}\right) + \tau \mathcal{E}\left(\varphi_{2}\left(y_{i}\right)\right)}$$

$$\begin{array}{rcl} Y_{1} & \sim & N(\mu_{1},\sigma_{1}^{2}), \\ Y_{2} & \sim & N(\mu_{2},\sigma_{2}^{2}), \\ Y & = & (1-\Delta) \cdot Y_{1} + \Delta \cdot Y_{2}, \\ \Delta \in \{0,1\} \text{ with } \Pr(\Delta=1) = \pi \\ \theta = (\pi,\theta_{1},\theta_{2}) = (\pi,\mu_{1},\sigma_{1}^{2},\mu_{2},\sigma_{2}^{2}) \end{array}$$

 $\mathbf{Z} = \{y_i\}_{i=1}^n$ is observed data $\mathbf{\Delta} = \{\Delta_i\}_{i=1}^n$ is unobserved data

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

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

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

$$E[\Delta_i \mid 0, Z] = \hat{\gamma}_i = \frac{\hat{\pi}\phi_{\hat{\theta}_2}(y_i)}{(1-\hat{\pi})\phi_{\hat{\theta}_1}(y_i) + \hat{\pi}\phi_{\hat{\theta}_2}(y_i)}, \ i = 1, 2, \dots, N.$$
(8.42)

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

$$\hat{\mu}_{1} = \frac{\sum_{i=1}^{N} (1 - \hat{\gamma}_{i}) y_{i}}{\sum_{i=1}^{N} (1 - \hat{\gamma}_{i})}, \qquad \hat{\sigma}_{1}^{2} = \frac{\sum_{i=1}^{N} (1 - \hat{\gamma}_{i}) (y_{i} - \hat{\mu}_{1})^{2}}{\sum_{i=1}^{N} (1 - \hat{\gamma}_{i})},$$
$$\hat{\mu}_{2} = \frac{\sum_{i=1}^{N} \hat{\gamma}_{i} y_{i}}{\sum_{i=1}^{N} \hat{\gamma}_{i}}, \qquad \hat{\sigma}_{2}^{2} = \frac{\sum_{i=1}^{N} \hat{\gamma}_{i} (y_{i} - \hat{\mu}_{2})^{2}}{\sum_{i=1}^{N} \hat{\gamma}_{i}},$$

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

Resulting Density Estimator

 $\sum_{i=1}^{n} \pi_{i} \, \theta_{\theta_{i}}(x)$

Expectation Maximization Algorithm

The iterative gaussian mixture model (GMM) fitting algorithm is special case of EM:

Algorithm 8.2 The EM Algorithm.

- 1. Start with initial guesses for the parameters $\hat{\theta}^{(0)}$.
- 2. Expectation Step: at the jth step, compute

$$Q(\theta', \hat{\theta}^{(j)}) = E(\ell_0(\theta'; \mathbf{T}) | \mathbf{Z}, \hat{\theta}^{(j)})$$
(8.43)

as a function of the dummy argument θ' .

- 3. Maximization Step: determine the new estimate $\hat{\theta}^{(j+1)}$ as the maximizer of $Q(\theta', \hat{\theta}^{(j)})$ over θ' .
- 4. Iterate steps 2 and 3 until convergence.

 $\mathbf{Z} \text{ is observed data } \mathbf{\Delta} \text{ is unobserved data }$

$$\mathbf{T} = (\mathbf{Z}, \boldsymbol{\Delta})$$

f.

Missing data example

$$\begin{split} x_i \sim \mathcal{N}(\mu, \Sigma) & \text{but suppose some entries of } x_i \text{ are missing} \\ \mathbf{\chi}_i = \begin{bmatrix} \mathbf{y}_i \\ \mathbf{\lambda}_i \end{bmatrix} & \mathbf{Z} \text{ is observed data} \\ \ell(\theta | \mathbf{T}, \theta) = -\frac{1}{2} \log(2\pi |\Sigma|) + (x_i - \mu)^T \Sigma^{-1}(x - \mu) & \mathbf{T} = (\mathbf{Z}, \mathbf{\Delta}) \end{split}$$

E Step: $\mathbb{E}[\ell(\theta'; \mathbf{T}) | \mathbf{Z}, \widehat{\theta}^{(j)}]$

Natural choice for $\hat{\theta}^{(0)}$?

Missing data example

 $x_i \sim \mathcal{N}(\mu, \Sigma)$ but suppose some entries of x_i are missing

 \mathbf{Z} is observed data $\boldsymbol{\Delta}$ is unobserved data

 $\mathbf{T} = (\mathbf{Z}, \boldsymbol{\Delta})$

E Step: $\mathbb{E}[\ell(\theta'; \mathbf{T}) | \mathbf{Z}, \widehat{\theta}^{(j)}]$ Natural choice for $\widehat{\theta}^{(0)}$? $\mathbb{E}[Y | X = x] = \mu_Y + \Sigma_{YX} \Sigma_{XX}^{-1} (x - \mu_X)$ M Step: $\widehat{\theta}^{(j+1)} = \arg \max_{\theta'} \mathbb{E}[\ell(\theta'; \mathbf{T}) | \mathbf{Z}, \widehat{\theta}^{(j)}]$

 $\ell(\theta|\mathbf{T},\theta) = -\frac{1}{2}\log(2\pi|\Sigma|) + (x_i - \mu)^T \Sigma^{-1}(x - \mu)$

Missing data example

 $x_i \sim \mathcal{N}(\mu, \Sigma)$ but suppose some entries of x_i are missing

 \mathbf{Z} is observed data $\boldsymbol{\Delta}$ is unobserved data

$$\mathbf{T} = (\mathbf{Z}, \boldsymbol{\Delta})$$

E Step: $\mathbb{E}[\ell(\theta'; \mathbf{T}) | \mathbf{Z}, \widehat{\theta}^{(j)}]$

Natural choice for $\widehat{\theta}^{(0)}$?

 $\mathbb{E}[Y|X = x] = \mu_Y + \Sigma_{YX} \Sigma_{XX}^{-1} (x - \mu_X)$ M Step: $\widehat{\theta}^{(j+1)} = \arg \max_{\theta'} \mathbb{E}[\ell(\theta'; \mathbf{T}) | \mathbf{Z}, \widehat{\theta}^{(j)}]$

 $\ell(\theta|\mathbf{T},\theta) = -\frac{1}{2}\log(2\pi|\Sigma|) + (x_i - \mu)^T \Sigma^{-1}(x - \mu)$

Connection to matrix factorization?

Density Estimation

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Kernel Density Estimation

Kernel Density Estimation

Are

$$f(x) = \sum_{m=1}^{M} \alpha_m \phi(x; \mu_m, \boldsymbol{\Sigma}_m)$$

Ace

Are

Kernel Density Estimation

Generative vs Discriminative