

GL Applied Data Science Bootcamp

Data Collection and Visualization for Exploratory Data Analysis

August 23, 2021

Introduction



<http://www.carolineuhler.com>

Overview

Overview of this week / module:

- Data collection and visualization for exploratory data analysis
- Network analysis
- Unsupervised learning - clustering

Overview of this lecture:

- Data collection: Mammography case study
- Hypothesis testing
- Visualizing high-dimensional data for exploratory data analysis

Case study: Mammography and breast cancer

- Breast cancer is one of the most common malignancies among women in the United States
 - Mammography: screening women for breast cancer by X-rays
-
- * Does mammography speed up detection by enough to matter?
 - * How would you approach this problem? What is important when setting up a study / experiment?

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 - Mammography: screening women for breast cancer by X-rays
- * Does mammography speed up detection by enough to matter?
- * How would you approach this problem? What is important when setting up a study / experiment?
- ⇒ Perform a **controlled, randomized, double-blind experiment** to minimize the problem of **confounding**

HIP study: First large-scale randomized controlled experiment on mammography performed in 1960s

Table 1. HIP data. Group sizes (rounded), deaths in 5 years of followup, and death rates per 1000 women randomized.

	Group size	<u>Breast cancer</u>		<u>All other</u>	
		No.	Rate	No.	Rate
Treatment					
<u>Screened</u>	20,200	23	1.1	428	21
<u>Refused</u>	10,800	16	1.5	409	38
Total	31,000 ←	39	1.3	837	27
Control	31,000 ←	63	2.0	879	28

Reference: D. A. Freedman. *Statistical Models: Theory and Practice*, 2009.

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- Seems natural to compare those who accepted screening to those who refused or the control group
- But this is an **observational** comparison!
- Becomes clear when comparing the death rates from all other causes
- Instead compare the whole treatment group against the whole control group

* **Intention-to-treat analysis**

Hypothesis testing

- Death rate from breast cancer in control group: 0.0020 ($= \frac{63}{31000}$)
- Death rate from breast cancer in treatment group: 0.0013 ($= \frac{39}{31000}$)

Is the difference in death rates between the treatment and control group sufficient to establish that mammography reduces the risk of death from breast cancer?

⇒ Perform a **hypothesis test**

Hypothesis testing

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$$X_1, \dots, X_{31'000} \sim \text{Bernoulli}(\pi)$$

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Null hypothesis (H_0): $\pi = 0.002$

Alternative (H_A): $\pi < 0.002$ $\pi \neq 0.002$

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$T :=$ Number of deaths under H_0 :

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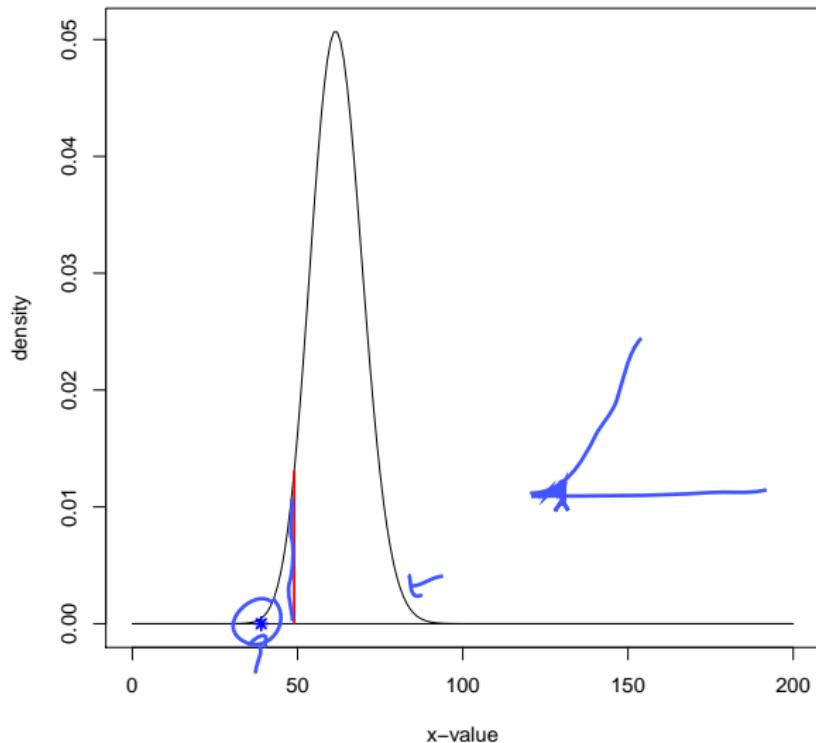
$T :=$ Number of deaths under H_0 :

$$T \sim \text{binomial}(31'000, 0.002)$$

- ④ Determine a **significance level** (α), i.e. the probability of rejecting H_0 when H_0 is true: $\alpha = 0.05$

Binomial distribution

Binomial(31'000, 0.002) with 0.05–quantile and observed # deaths



P-value

- Probability under H_0 to obtain the observed value or a more extreme value of the test statistic
 - ⇒ p-value is always between 0 and 1!
- For mammography study: p-value is 0.0012
- Can be used for hypothesis testing: Reject H_0 if p-value $\leq \underline{\alpha}$
- Quantifies significance of alternative

Hypothesis testing applications outside of healthcare

Hypothesis testing applications outside of healthcare

- Quality management in manufacturing environments: deciding whether new process, technique, method is likely to change number of defective products
- Finance: deciding which investment / instrument is likely to provide satisfactory return
- Business: make informed decisions on which initiatives help grow your business
- Advertising: deciding whether an advertising campaign, marketing technique, etc. is likely to increase sales

Example research findings

Giovannucci et al., Journal of the National Cancer Institute 87 (1995):

Intake of tomato sauce (p -value of 0.001), tomatoes (p -value of 0.03), and pizza (p -value of 0.05) reduce the risk of prostate cancer;

But for example tomato juice (p -value of 0.67), or cooked spinach (p -value of 0.51), and many other vegetables are not significant.

Wonder-pill

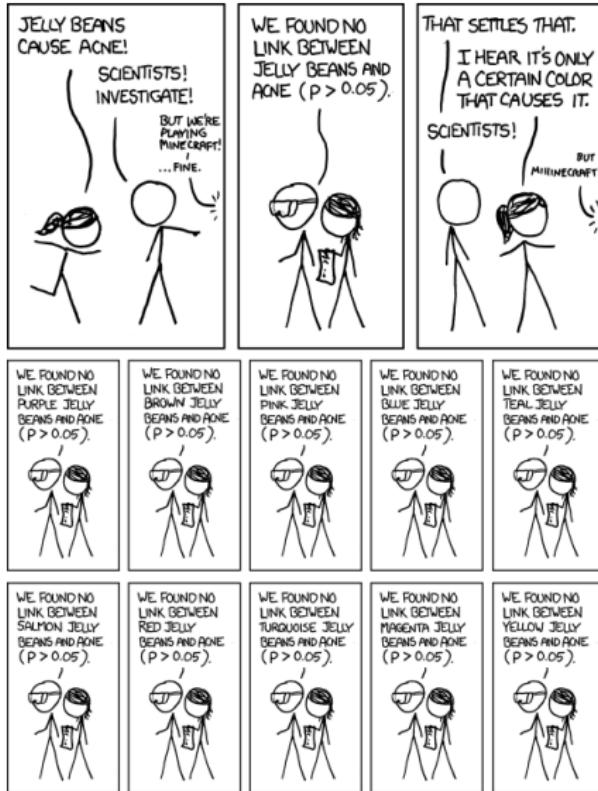
- randomized group of 1000 people
- measure 100 variables before and after taking the pill: weight, blood pressure, etc.
- perform a hypothesis test with a significance level of 5%

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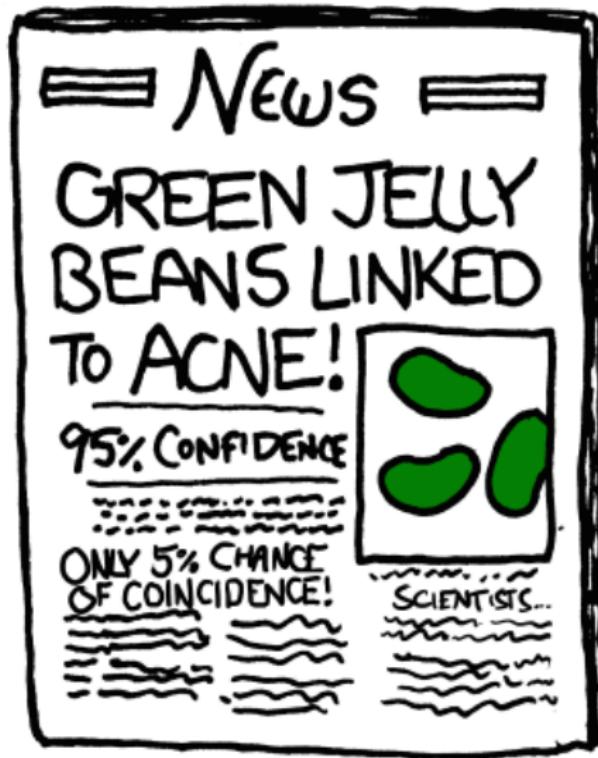
- randomized group of 1000 people
- measure 100 variables before and after taking the pill: weight, blood pressure, etc.
- perform a hypothesis test with a significance level of 5%
- $V := \# \text{ false significant tests}$: $V \sim \text{Binomial}(100, 0.05)$

⇒ in average 5 out of 100 variables show a significant effect!

Jelly Beans and Acne



Problematic of selective inference



<http://imgs.xkcd.com/comics/significant.png>

Different protection levels

Compute p -values using methods that control:

- family-wise error rate (FWER) $\leq \alpha$, where

$$\text{FWER} = \mathbb{P}(\text{at least one false significant result})$$

- false discovery rate (FDR) $\leq \alpha$, where

FDR = expected fraction of false significant results
among all significant results

Corrections for multiple testing

Bonferroni correction:

- Reject H_0 when: $m \cdot p\text{-value} \leq \alpha$
where m is the total number of hypothesis tests performed
- Bonferroni correction implies $\text{FWER} \leq \alpha$

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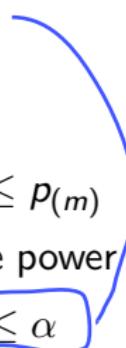
Holm-Bonferroni correction:

- Sort p -values in increasing order: $p_{(1)} \leq \dots \leq p_{(m)}$
- Reject H_0 when: $(m - i + 1)p_{(i)} \leq \alpha$ (more power than Bonferroni)
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→ Bonferroni correction:

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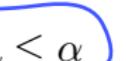
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→ Benjamini-Hochberg correction:

- Sort p -values in increasing order: $p_{(1)} \leq \dots \leq p_{(m)}$
- Reject H_0 when: $mp_{(i)}/i \leq \alpha$
- Benjamini-Hochberg correction implies $\text{FDR} \leq \alpha$

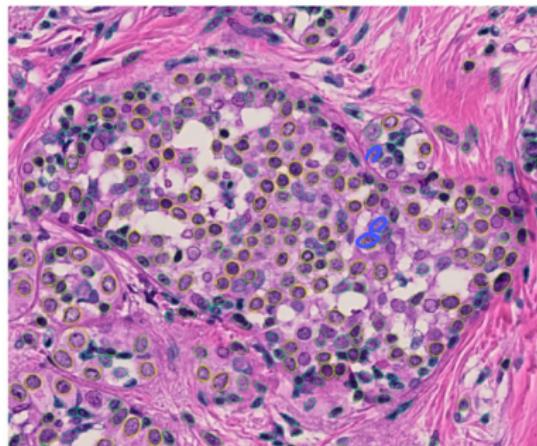


Commonly accepted practice

- No correction for multiple testing when generating hypotheses (but report number of tests performed)
- FDR $\leq 10\%$ in exploratory analysis or screening
 - balance between high power and low # of false significant results
- FWER $\leq 5\%$ in confirmatory analysis
 - food and drug administration (FDA)

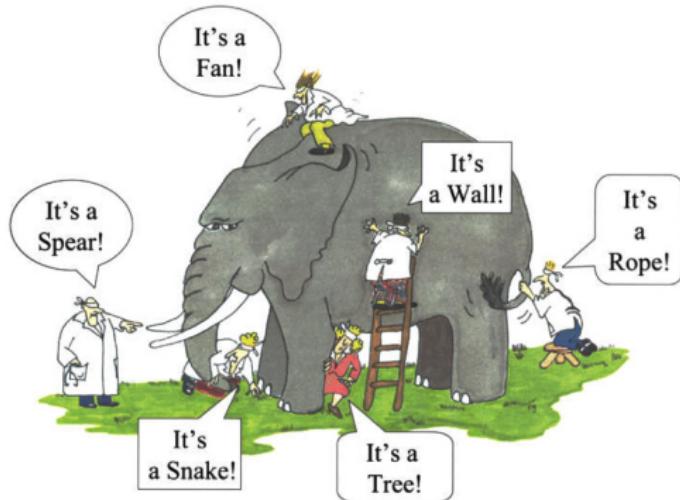
Application: Microscopy Images

- Microscopy images of human tissue slices
- Crop cells (n cells) and summarize each cell by 100 different texture features (i.e., $D = 100$)
- How can we visualize this data set to find clusters or abnormal cells?
- **Input:** $x_1, \dots, x_n \in \mathbb{R}^D$, **Output:** $y_1, \dots, y_n \in \mathbb{R}^d$, where $d \ll D$



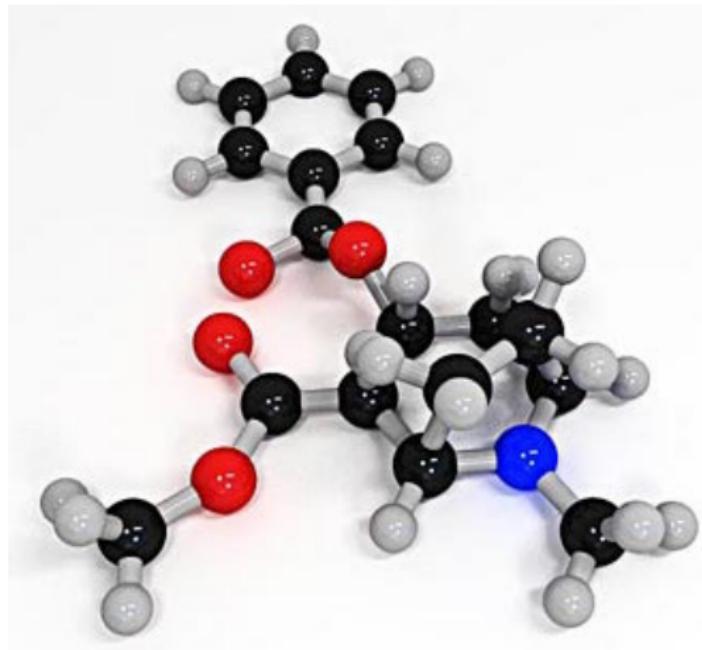
2 different approaches

- Principle component analysis: projection that spreads data as much as possible
- Stochastic neighbor embedding: non-linear embedding that tries to keep close-by points close

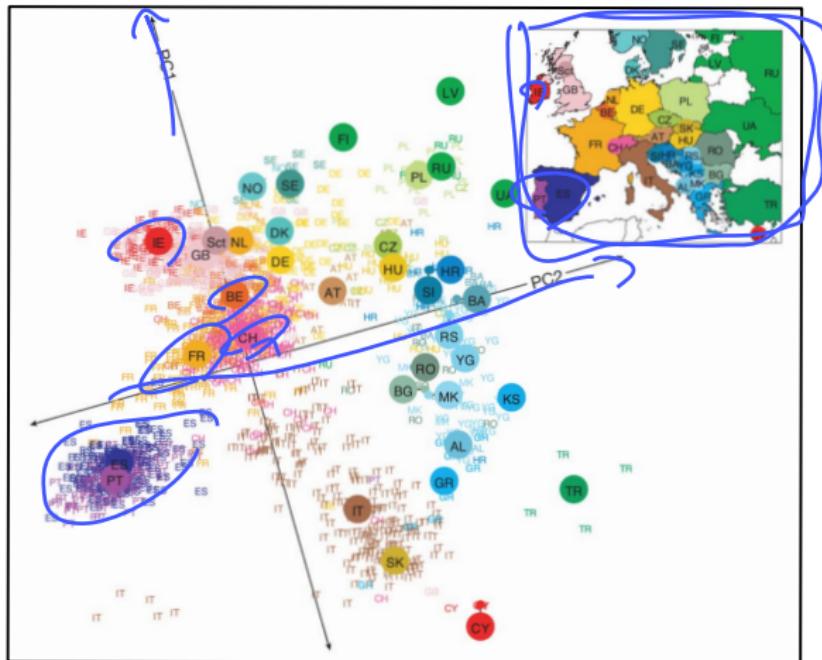


Principle Component Analysis

- **Goal:** Dimension reduction to a few dimensions
- **Intuition:** Find low-dimensional projection with largest spread



PCA application

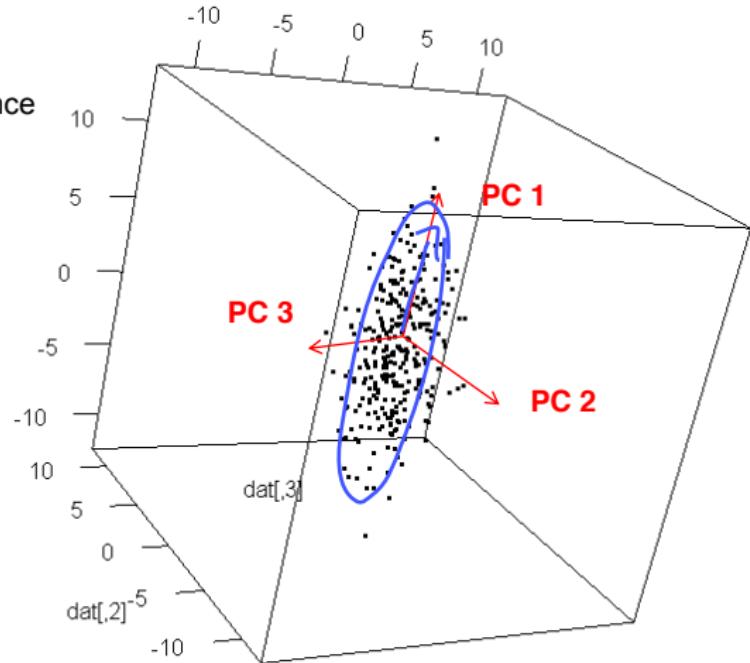


Reference: J. Novembre et al., *Genes mirror geography within Europe*, Nature 456 (2008).

Definition 1: Maximize projection variance

Start with centered data $X \in \mathbb{R}^{n \times p}$

- PC 1 is direction of largest variance
- PC 2 is
 - perpendicular to PC 1
 - again largest variance
- PC 3 is
 - perpendicular to PC 1, PC 2
 - again largest variance
- etc.



Definition 2: Minimize projection residuals

- PC 1: Straight line with smallest orthogonal distance to all points
- PC 1 & PC 2: Plane with smallest orthogonal distance to all points
- etc.

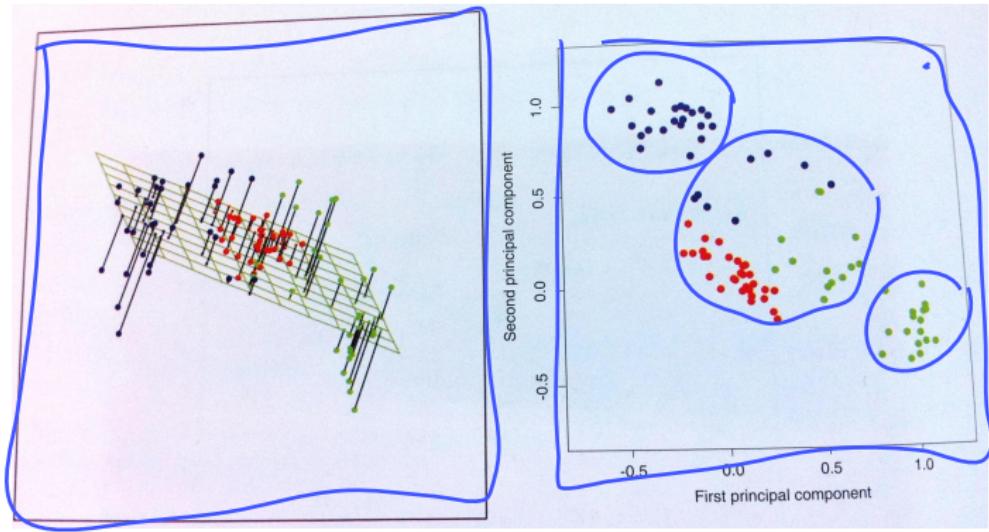


Figure from *Elements of Statistical Learning* by Hastie and Tibshirani

Definition 3: Spectral decomposition

- Covariance matrix (or correlation matrix) $R = \frac{1}{n}X^T X$ is symmetric and positive semidefinite
- Spectral Decomposition Theorem: Every real symmetric matrix R can be decomposed as

$$R = V \Lambda V^T,$$

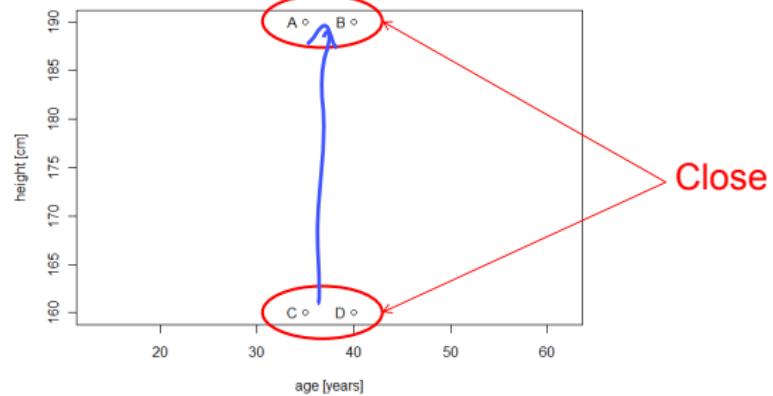
where Λ is diagonal and V is orthogonal

- Columns of V ($=$ eigenvectors of R) are the PCs
- Diagonal entries of Λ ($=$ eigenvalues of R) are variances along PCs

Covariance versus correlation - to scale or not to scale

- Using covariance will find the variable with largest spread as 1. PC
- Use correlation, if different units are compared

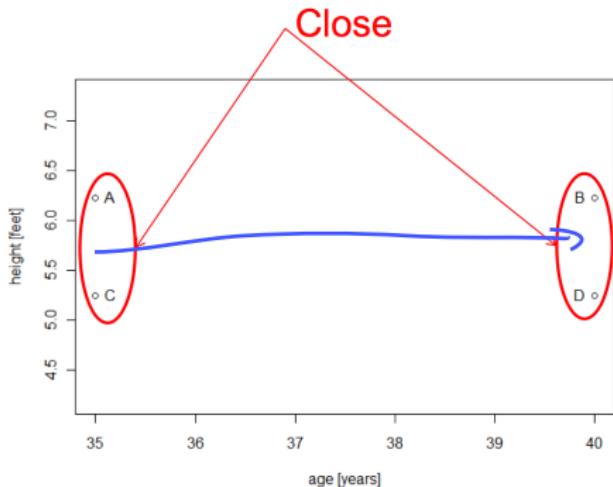
Person	Age (years)	Height (cm)
A	35	190
B	40	190
C	35	160
D	40	160



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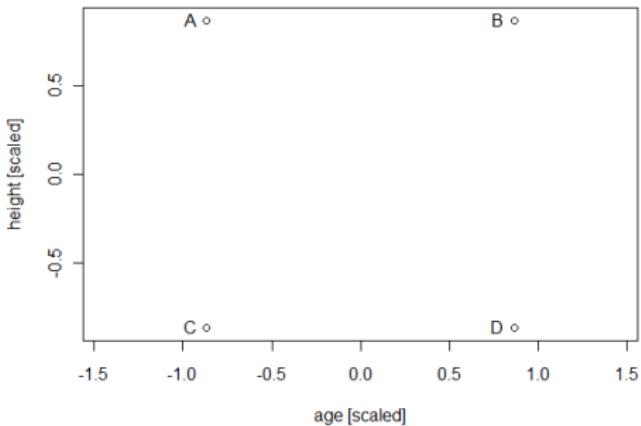
Person	Age (years)	Height (feet)
A	35	6.232
B	40	6.232
C	35	5.248
D	40	5.248



Covariance versus correlation - to scale or not to scale

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Person	Age (years)	Height (feet)
A	-0.87	0.87
B	0.87	0.87
C	-0.87	-0.87
D	0.87	-0.87



Stochastic neighbor embedding (SNE)

- probabilistic approach to place objects from high-dimensional space into low-dimensional space so as to preserve the identity of neighbors
- center a Gaussian on each object in high-dimensional space
- find embedding so that resulting high-dimensional distribution is approximated well by resulting low-dimensional distribution



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- center a Gaussian on each object in high-dimensional space
- find embedding so that resulting high-dimensional distribution is approximated well by resulting low-dimensional distribution
- determine low-dimensional distribution by minimizing **Kullback-Leibler divergence**
- allows ambiguous objects like “bank”, to be close to “river” and “finance” without forcing all outdoor concepts to be located close to corporate concepts

(Symmetric) SNE

- given dissimilarity matrix D , for each object i compute probability of picking j as neighbor:

$$p_{ij} = \frac{\exp(-D_{ij}^2)}{\sum_{k \neq i} \exp(-D_{ik}^2)}$$

- in low-dimensional space, for each point y_i compute probability of picking y_j as neighbor:

$$q_{ij} = \frac{\exp(-\|y_i - y_j\|_2^2)}{\sum_{k \neq i} \exp(-\|y_k - y_i\|_2^2)}$$

- Minimize the KL-divergence

$$\text{KL}(P||Q) = \sum_{i \neq j} p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

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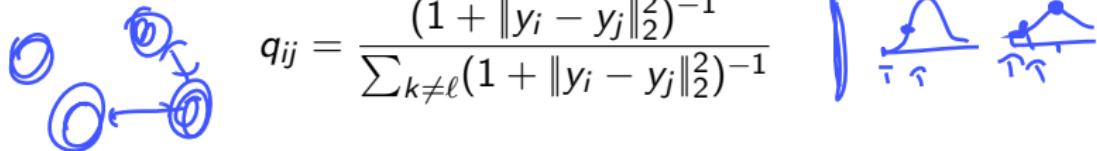
$$\text{KL}(P||Q) = \sum_{i \neq j} p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

- by modeling p_{ij} by $q_{ij} = p_{ij} + x$ you gain less than you lose by choosing $q_{ij} = p_{ij} - x$
- keeps nearby objects nearby and separated objects relatively far

t-SNE

- SNE (non-convex) is optimized using gradient descent from an initial configuration

- SNE (non-convex) is optimized using gradient descent from an initial configuration
- problem with many embedding methods: points often get crowded in the middle
- t-SNE reduces this by using t -distribution with 1 degree of freedom for y 's:



The diagram illustrates the t-SNE optimization process. On the left, four blue circles represent data points in a high-dimensional space. Two points are connected by a double-headed arrow, indicating they are close neighbors. On the right, two bell-shaped curves represent the probability density functions of these points under a t -distribution. The peak of each curve is at the same position as its corresponding point in the high-dimensional space. The width of the curves is determined by the formula for q_{ij} .

$$q_{ij} = \frac{(1 + \|y_i - y_j\|_2^2)^{-1}}{\sum_{k \neq \ell} (1 + \|y_i - y_j\|_2^2)^{-1}}$$

- reduces crowding: moderate distance in high-dim. space can be faithfully modeled by much larger distance in low-dim. space

Case study: Digit recognition

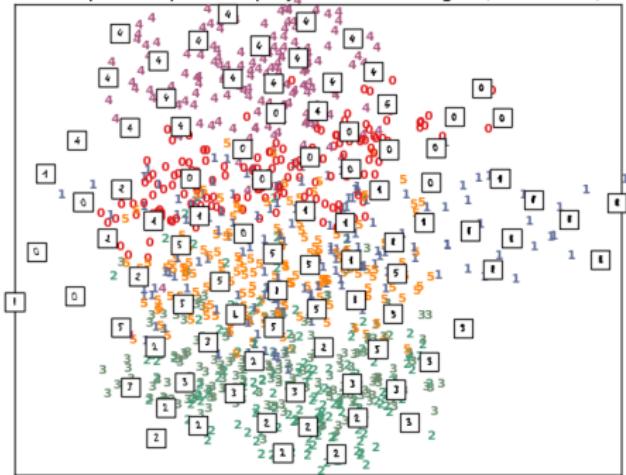
- ~ 1800 hand-written digits (i.e., $n \approx 180$ for each number)
- each (centered) digit was put in a 8×8 -grid (i.e., $D = 64$)
- measure grey value in each part of the grid, i.e. 64 grey values
- **Input:** $x_1, \dots, x_n \in \mathbb{R}^D$, **Output:** $y_1, \dots, y_n \in \mathbb{R}^d$, where $d \ll D$

A selection from the 64-dimensional digits dataset

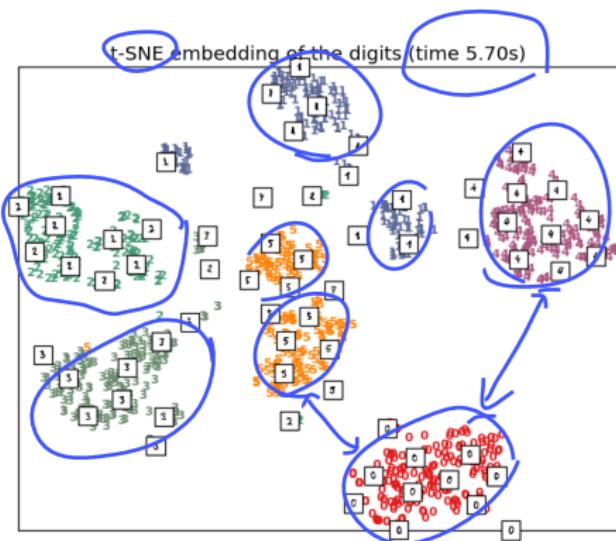
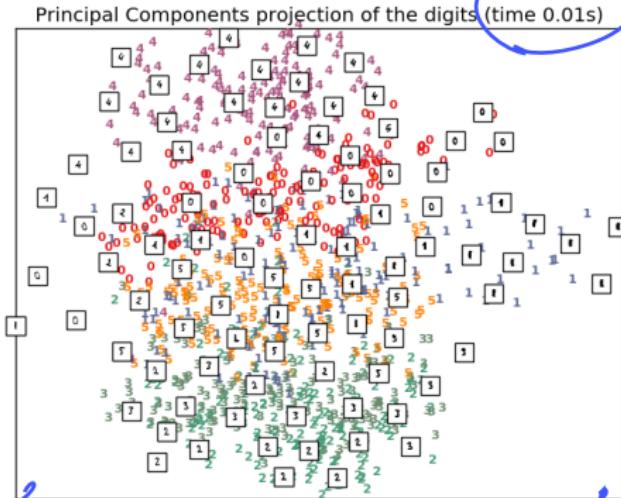
0	1	2	3	4	5	0	1	2	3	4	5	0	5
5	5	0	4	1	3	5	1	0	0	2	2	0	1
4	4	1	5	0	5	2	0	0	1	3	2	1	4
3	4	0	5	3	1	5	4	4	2	2	2	5	5
2	3	4	5	0	1	2	3	4	5	0	1	2	3
0	4	1	3	5	1	0	0	2	2	1	0	1	2
1	5	0	5	2	2	0	0	1	3	2	1	3	4
0	5	7	4	5	4	4	1	2	2	5	5	4	4
5	0	1	2	3	4	5	0	1	2	3	4	5	0
3	5	4	0	0	2	2	2	0	1	2	3	3	4
5	1	0	0	2	2	2	0	1	2	3	3	3	4
5	2	2	0	0	1	3	2	1	3	1	3	4	4
3	1	5	4	2	2	2	5	5	4	4	0	0	1
0	1	2	3	4	5	0	1	2	3	4	5	0	1
5	1	0	0	2	2	2	0	1	2	3	3	3	4
5	2	2	0	0	1	3	2	1	3	1	3	4	5
3	1	5	4	2	2	2	5	5	4	4	0	0	1
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5	1	0	0	2	2	2	0	1	2	3	3	3	4
5	2	2	0	0	1	3	2	1	3	1	3	4	5
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5	1	0	0	2	2	2	0	1	2	3	3	3	4
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0	1	2	3	4	5	0	1	2	3	4	5	0	1
5	1	0	0	2	2	2	0	1	2	3	3	3	4
5	2	2	0	0	1	3	2	1	3	1	3	4	5
3	1	5	4	2	2	2	5	5	4	4	0	0	1
0	1	2	3	4	5	0	1	2	3	4	5	0	1
5	1	0	0	2	2	2	0	1	2	3	3	3	4
5	2	2	0	0	1	3	2	1	3	1	3	4	5
3	1	5	4	2	2	2	5	5	4	4	0	0	1
0	1	2	3	4	5	0	1	2	3	4	5	0	1
5	1	0	0	2	2	2	0	1	2	3	3	3	4
5	2	2	0	0	1	3	2	1	3	1	3	4	5
3	1	5	4	2	2	2	5	5	4	4	0	0	1
0	1	2	3	4	5	0	1	2	3	4	5	0	1
5	1	0	0	2	2	2	0	1	2	3	3	3	4
5	2	2	0	0	1	3	2	1	3	1	3	4	5
3	1	5	4	2	2	2	5	5	4	4	0	0	1
0	1	2	3	4	5	0	1	2	3	4	5	0	1
5	1	0	0	2	2	2	0	1	2	3	3	3	4
5	2	2	0	0	1	3	2	1	3	1	3	4	5
3	1	5	4	2	2	2	5	5	4	4	0	0	1
0	1	2	3	4	5	0	1	2	3	4	5	0	1
5	1	0	0	2	2	2	0	1	2	3	3	3	4
5	2	2	0	0	1	3	2	1	3	1	3	4	5
3	1	5	4	2	2	2	5	5	4	4	0	0	1
0	1	2	3	4	5	0	1	2	3	4	5	0	1
5	1	0	0	2	2	2	0	1	2	3	3	3	4
5	2	2	0	0	1	3	2	1	3	1	3	4	5
3	1	5	4	2	2	2	5	5	4	4	0	0	1
0	1	2	3	4	5	0	1	2	3	4	5	0	1
5	1	0	0	2	2	2	0	1	2	3	3	3	4
5	2	2	0	0	1	3	2	1	3	1	3	4	5
3	1	5	4	2	2	2	5	5	4	4	0	0	1
0	1	2	3	4	5	0	1	2	3	4	5	0	1
5	1	0	0	2	2	2	0	1	2	3	3	3	4
5	2	2	0	0	1	3	2	1	3	1	3	4	5
3	1	5	4	2	2	2	5	5	4	4	0	0	1
0	1	2	3	4	5	0	1	2	3	4	5	0	1
5	1	0	0	2	2	2	0	1	2	3	3	3	4
5	2	2	0	0	1	3	2	1	3	1	3	4	5
3	1	5	4	2	2	2	5	5	4	4	0	0	1
0	1	2	3	4	5	0	1	2	3	4	5	0	1
5	1	0	0	2	2	2	0	1	2	3	3	3	4
5	2	2	0	0	1	3	2	1	3	1	3	4	5
3	1	5	4	2	2	2	5	5	4	4	0	0	1
0	1	2	3	4	5	0	1	2	3	4	5	0	1
5	1	0	0	2	2	2	0	1	2	3	3	3	4
5	2	2	0	0	1	3	2	1	3	1	3	4	5
3	1	5	4	2	2	2	5	5	4	4	0	0	1
0	1	2	3	4	5	0	1	2	3	4	5	0	1
5	1	0	0	2	2	2	0	1	2	3	3	3	4
5	2	2	0	0	1	3	2	1	3	1	3	4	5
3	1	5	4	2	2	2	5	5	4	4	0	0	1
0	1	2	3	4	5	0	1	2	3	4	5	0	1
5	1	0	0	2	2	2	0	1	2	3	3	3	4
5	2	2	0	0	1	3	2	1	3	1	3	4	5
3	1	5	4	2	2	2	5	5	4	4	0	0	1
0	1	2	3	4	5	0	1	2	3	4	5	0	1
5	1	0	0	2	2	2	0	1	2	3	3	3	4
5	2	2	0	0	1	3	2	1	3	1	3	4	5
3	1	5	4	2	2	2	5	5	4	4	0	0	1
0	1	2	3	4	5	0	1	2	3	4	5		

Case study: Digit recognition

Principal Components projection of the digits (time 0.01s)



Case study: Digit recognition



- tSNE seems to find meaningful clusters
- Note: tSNE embedding is result of non-convex optimization problem: depends on starting configuration; also: axes have NO meaning

For code and figures see

http://scikit-learn.org/stable/auto_examples/manifold/plot_lle_digits.html

References for data collection and hypothesis testing

- For a statistics textbook, including controlled experiments and observational studies (chapters 1 and 2) and hypothesis testing (chapter 26-29):
D. Freedman, R. Pisani, R. Purves. *Statistics*. 2007.
- For how to perform hypothesis testing in R: Chapter 4 in
P. Dalgaard. *Introductory Statistics with R*. 2002.
- For observational studies and experiments, including the HIP study Chapter 1 in
D. Freedman. *Statistical Models: Theory and Practice*. 2009.
- For selective inference and correcting for multiple hypothesis testing:
Lecture by Yoav Benjamini, THE expert for multiple testing issues:
<http://simons.berkeley.edu/talks/yoav-benjamini-2013-12-11a>

References for PCA and tSNE

- For PCA and other projection methods:
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 - T. Hastie, R. Tibshirani & J. Friedman. *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*. Springer, 2009.
- For tSNE:
 - L. van der Maaten & G. E. Hinton. *Visualizing Data using t-SNE*. JMLR, 2008.
 - G. E. Hinton & S. T. Roweis. *Stochastic Neighbor Embedding*. NIPS, 2002.