



S&DS 265 / 565
Introductory Machine Learning

Unsupervised Learning: PCA

October 11

Yale

Checkpoint

- Assn 2 due Thursday
- Midterm one week from today, in class
- Practice midterms (and solutions) posted on Canvas
- Review sessions scheduled

Unsupervised Learning

Supervised learning is about being able to predict out Y from predictors X_1, X_2, \dots, X_p

Unsupervised learning deals with data that do not have labels Y

We are not trying to predict anything. So what else might we hope to do?

Unsupervised Learning

Supervised learning is about being able to predict out Y from predictors X_1, X_2, \dots, X_p

Unsupervised learning deals with data that do not have labels Y

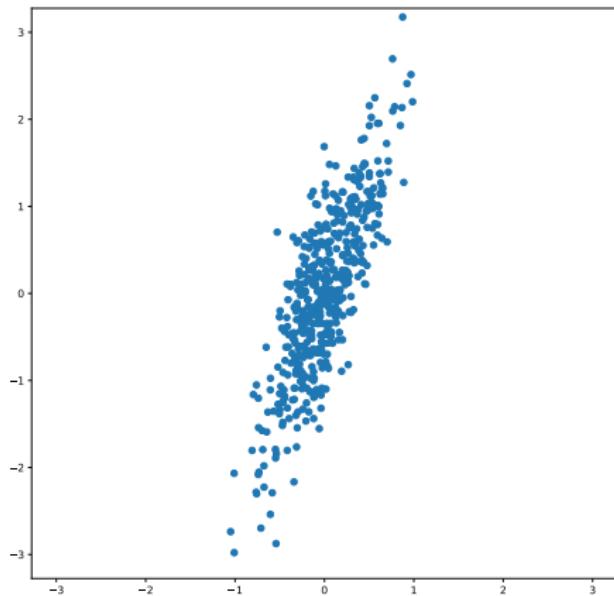
We are not trying to predict anything. So what else might we hope to do?

Consider:

- Are there interesting ways to visualize/summarize the data?
- Are there natural subgroups in the data?
- What are the important types of variation in the data?

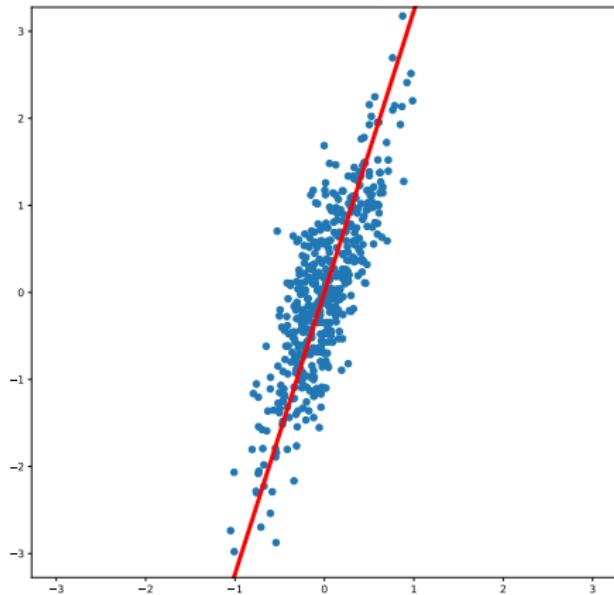
Principal Component Analysis (PCA)

PCA finds the directions of greatest variability in the data.



Principal Component Analysis (PCA)

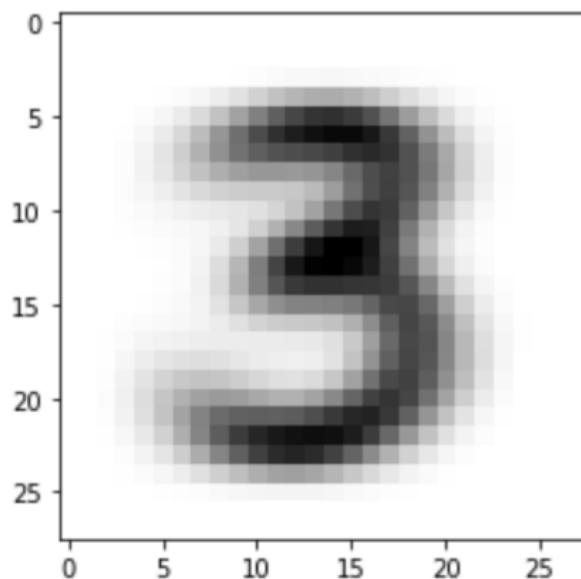
PCA finds the directions of greatest variability in the data.



Handwritten Digits (3s)

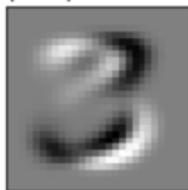
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Handwritten Digits (3s) – Average

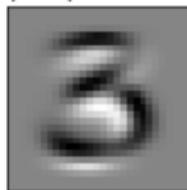


Handwritten Digits (3s) – Principal vectors

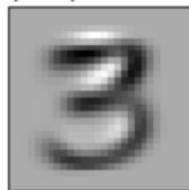
principal vector 1



principal vector 2



principal vector 3



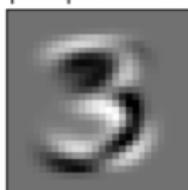
principal vector 4



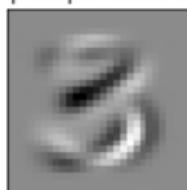
principal vector 5



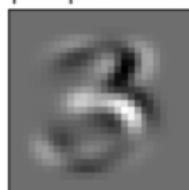
principal vector 6



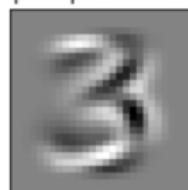
principal vector 7



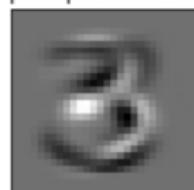
principal vector 8



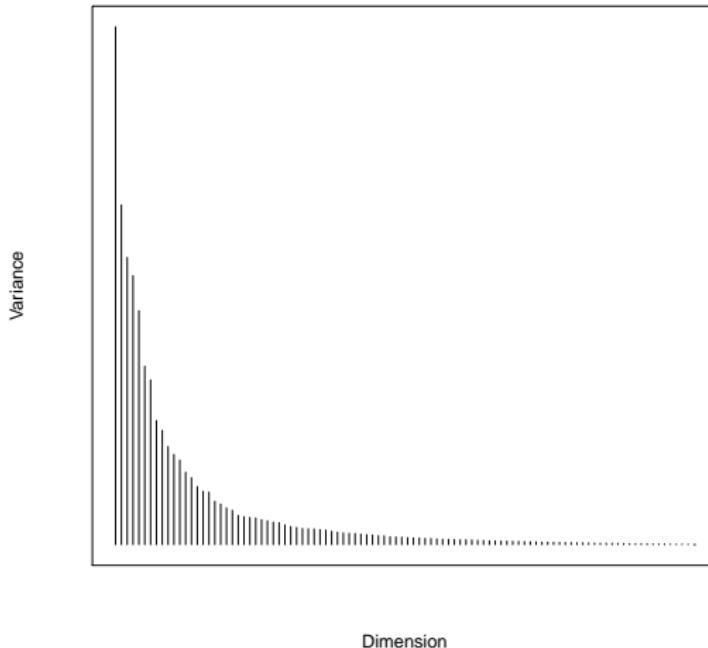
principal vector 9



principal vector 10



Handwritten Digits (3s) – PCA variance

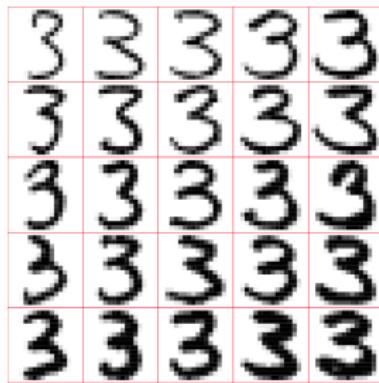
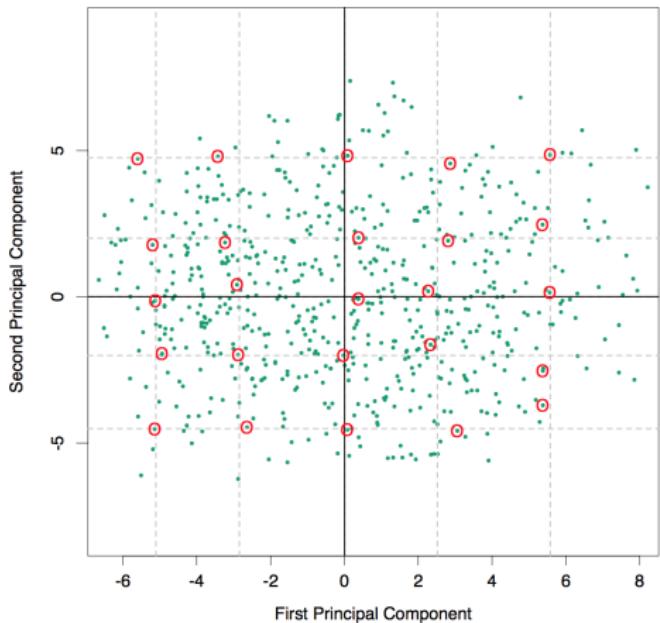


Handwritten Digits (3s)

$$\begin{aligned}\hat{f}(\lambda) &= \bar{x} + \lambda_1 v_1 + \lambda_2 v_2 \\ &= \boxed{3} + \lambda_1 \cdot \boxed{3} + \lambda_2 \cdot \boxed{3}.\end{aligned}$$

Handwritten Digits (3s) – Top 2 components

$$\begin{aligned}\hat{f}(\lambda) &= \bar{x} + \lambda_1 v_1 + \lambda_2 v_2 \\ &= \boxed{\text{3}} + \lambda_1 \cdot \boxed{\text{3}} + \lambda_2 \cdot \boxed{\text{3}}.\end{aligned}$$



Handwritten Digits (3s) – PCA reconstruction



Faces

test face 0



test face 1



test face 2



test face 3



test face 4



test face 5



test face 6



test face 7



test face 8



test face 9



test face 10



test face 11



Eigenfaces (principal vectors)

eigenface 0



eigenface 1



eigenface 2



eigenface 3



eigenface 4



eigenface 5



eigenface 6



eigenface 7



eigenface 8



eigenface 9



eigenface 10



eigenface 11



Racial bias in image databases

Original Research | [Open Access](#) | [Published: 27 October 2021](#)

Bias, awareness, and ignorance in deep-learning-based face recognition

[Samuel Wehrli](#) , [Corinna Hertweck](#), [Mohammadreza Amirian](#), [Stefan Glüge](#) & [Thilo Stadelmann](#)

[AI and Ethics](#) **2**, 509–522 (2022) | [Cite this article](#)

2187 Accesses | **3** Altmetric | [Metrics](#)

Abstract

Face Recognition (FR) is increasingly influencing our lives: we use it to unlock our phones; police uses it to identify suspects. Two main concerns are associated with this increase in facial recognition: (1) the fact that these systems are typically less accurate for marginalized groups, which can be described as “bias”, and (2) the increased surveillance through these systems. Our paper is concerned with the first issue. Specifically, we explore an intuitive technique for reducing this bias, namely “blinding” models to sensitive features, such as gender or race, and show why this cannot be equated with reducing bias. Even when not designed for this task, facial recognition models can deduce sensitive features, such as gender or race, from pictures

Let's go to the notebook

```
pca = PCA(num_components).fit(cimages)
principal_vectors = pca.components_
principal_vectors = principal_vectors.reshape((num_components, height, width))
pcs = pca.fit_transform(cimages)
capprox = pca.inverse_transform(pcs)
labels = ['principal vector %d' % (i+1) for i in np.arange(num_components)]
plot_images(principal_vectors, labels, height, width, int(num_components/5.), 5)
ratio = pca.explained_variance_ratio_.sum()
print('Variance explained by first %d principal vectors: %.2f%%' % (num_components, ratio*100))
```

Variance explained by first 25 principal vectors: 72.46%

principal vector 1 principal vector 2 principal vector 3 principal vector 4 principal vector 5



principal vector 6 principal vector 7 principal vector 8 principal vector 9 principal vector 10



Genes mirror geography within Europe

John Novembre,^{1,2} [Toby Johnson](#),^{4,5,6} [Katarzyna Bryc](#),⁷ [Zoltán Kutalik](#),^{4,6} [Adam R. Boyko](#),⁷ [Adam Auton](#),⁷ Amit Indap,⁷ [Karen S. King](#),⁸ [Sven Bergmann](#),^{4,6} [Matthew R. Nelson](#),⁸ [Matthew Stephens](#),^{2,3} and [Carlos D. Bustamante](#)⁷

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The publisher's final edited version of this article is available at [Nature](#)

This article has been corrected. See the correction in volume 456 on page 274.

See commentary "[Editorial comment should accompany hot papers online](#)." in *Nature*, volume 455 on page 861.

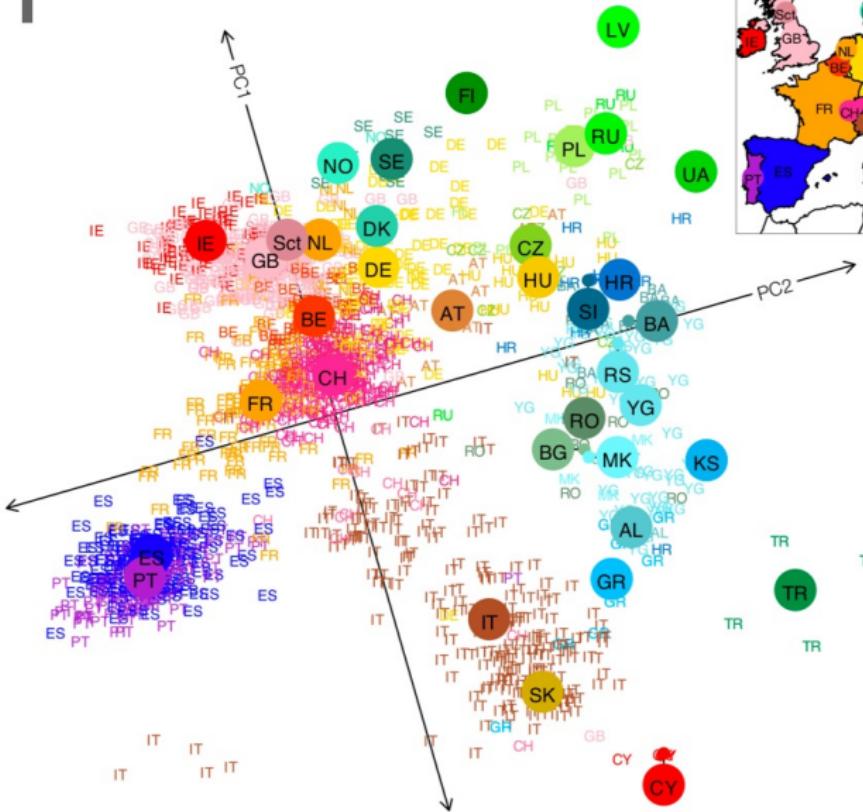
See other articles in PMC that [cite](#) the published article.

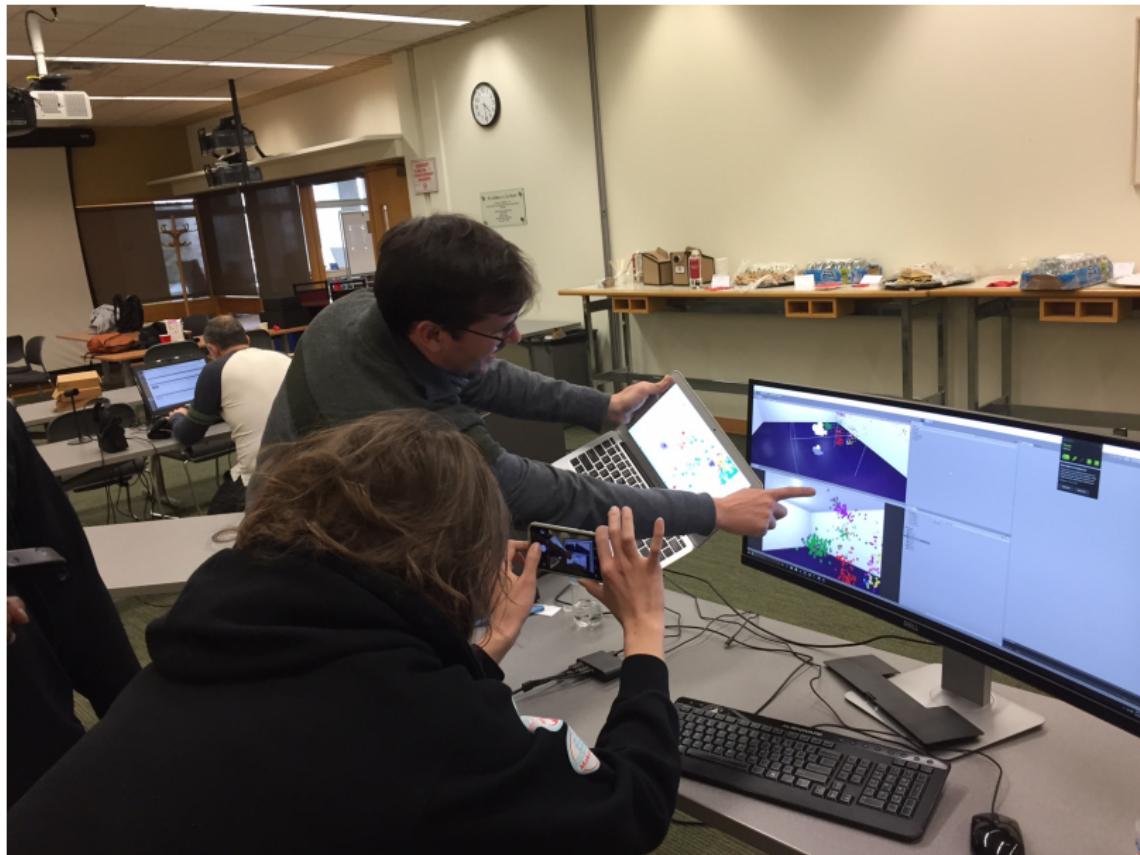
Abstract

Go to:

Understanding the genetic structure of human populations is of fundamental interest to medical, forensic and anthropological sciences. Advances in high-throughput genotyping technology have markedly improved our understanding of global patterns of human genetic variation and suggest the potential to use large samples to uncover variation among closely spaced populations^{1–5}. Here we characterize genetic variation in a sample of 3,000 European individuals genotyped at over half a million variable DNA sites in the human genome. Despite low average levels of genetic differentiation among Europeans, we find a close correspondence between genetic and geographic distances; indeed, a geographical map of Europe arises naturally as an efficient two-dimensional summary of genetic variation in Europeans. The results emphasize that when mapping the genetic basis of a disease phenotype, spurious associations can arise if genetic structure is not properly accounted for. In addition, the results are relevant to the prospects of genetic ancestry testing⁶; an individual's DNA can be used to infer their geographic origin with surprising accuracy—often to within a few hundred kilometres.

1



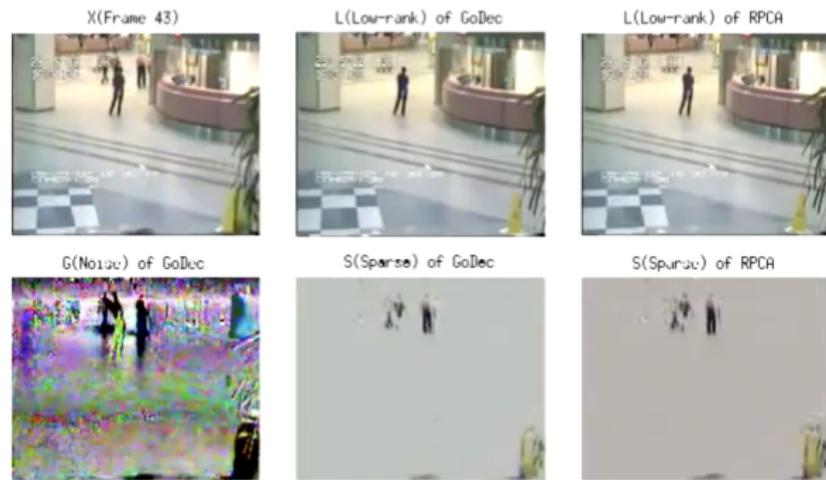


Examples

A couple of other interesting examples of PCA follow (without going into any detail)

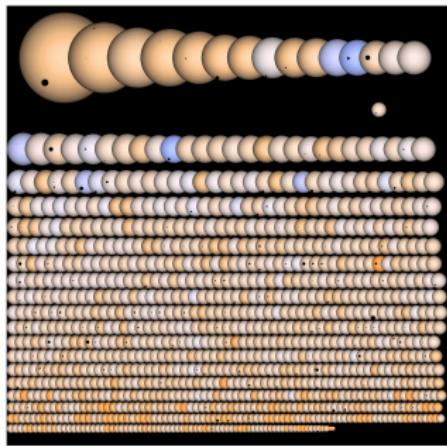
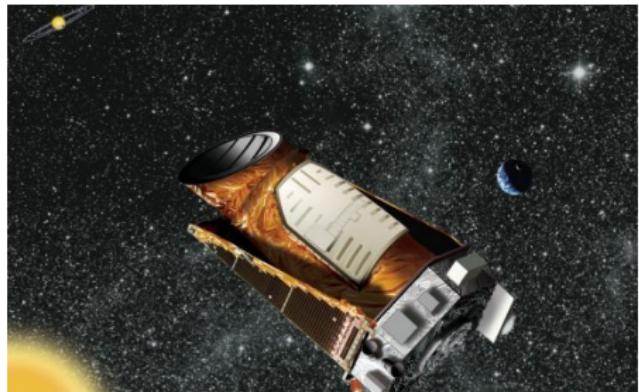
Robust PCA

Robust PCA (low rank plus sparse) can be used for background subtraction in video.



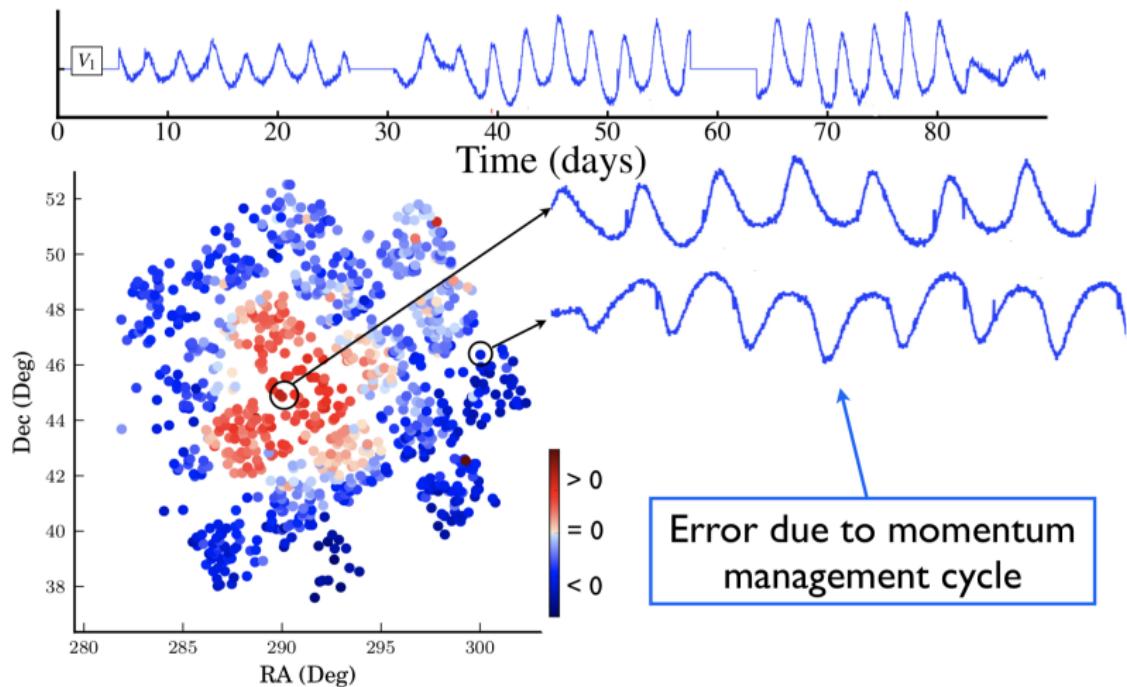
<https://www.youtube.com/watch?v=BTrbow8u4Cw>

Kepler telescope

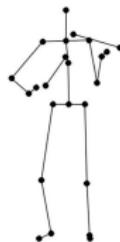


Kepler telescope

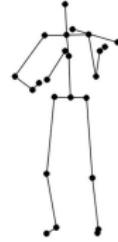
Identification of correlated errors using robust PCA



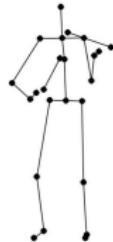
RESULTS: PC VISUALISATION, TECHNICAL VS. NON-TECHNICAL MOTION



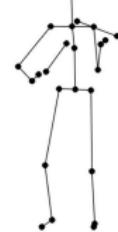
Original



PC1 (45% of variance accounted)
Side-to-side swaying (non-technical)



PC2 (25% of variance accounted)
Right arm string crossing (technical)



PC3 (15% of variance accounted)
Left-right rotation (non-technical)

PCA: Algorithm

- ① Center the data: $x_i \mapsto x_i - \bar{x}$
- ② Compute the $d \times d$ sample covariance $S = \frac{1}{n} \sum_{i=1}^n x_i x_i^T$
- ③ Find the first k eigenvectors of S
- ④ Project the data onto those k vectors

PCA: Algorithm

- ① Center the data: $x_i \mapsto x_i - \frac{1}{n} \sum_{j=1}^n x_j = x_i - \bar{x}$
- ② Compute the $d \times d$ sample covariance $S = \frac{1}{n} \sum_{i=1}^n x_i x_i^T$. Note that

$$\frac{1}{n} \sum_i (x_{ij} - \bar{x})^2$$

is the sample variance of j th coordinate of data.

- ③ Find the first k eigenvectors of S ,

$$\phi_1, \dots, \phi_k \in \mathbb{R}^d, \quad S\phi_j = \lambda_j \phi_j$$

- ④ Project the data onto those k vectors:

$$x_i \mapsto \bar{x} + (\phi_1^T x_i) \phi_1 + \dots + (\phi_k^T x_i) \phi_k$$

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principal vector 6 principal vector 7 principal vector 8 principal vector 9 principal vector 10



Dimension reduction—another demo

- Flower Power: PCA and classification (30 points)



In this problem you will carry out principal components analysis and classification on the iris data. The task will be to reduce the dimension from four to two using PCA, and then to train logistic regression models on the projected data.

+ Code + Text

```
[ ] import pandas as pd
import numpy as np
from sklearn.model_selection import train_test_split
from sklearn.decomposition import PCA
from sklearn.linear_model import LogisticRegression

import matplotlib.pyplot as plt
%matplotlib inline
```

PCA: Summary

- PCA is an unsupervised method
- Finds directions of greatest variation in the data
- The directions are called the *principal vectors*; the weightings on the vectors are called the *principal components*
- The first few vectors may be interpretable
- Orthogonality makes interpretation difficult for the higher components
- Can be used for visualization or dimensionality reduction