Lecture Notes for
Machine Learning in Python

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Professor Eric Larson

Dimensionality Reduction

Class Logistics and Agenda

- Logistics:
  - First flipped module in one week!
  - Grading of lab one started…
- Agenda:
  - Dimensionality Reduction
    - PCA (and intro to Randomized PCA)
    - Images Representation with PCA

Class Overview, by topic

Table Data Visualization
Numpy, Pandas, Seaborn
Overviews with some in-depth discussion

Dimension Reduction and Image Processing
Scikit-learn, Scikit Image,
Intuition only, Some mathematics

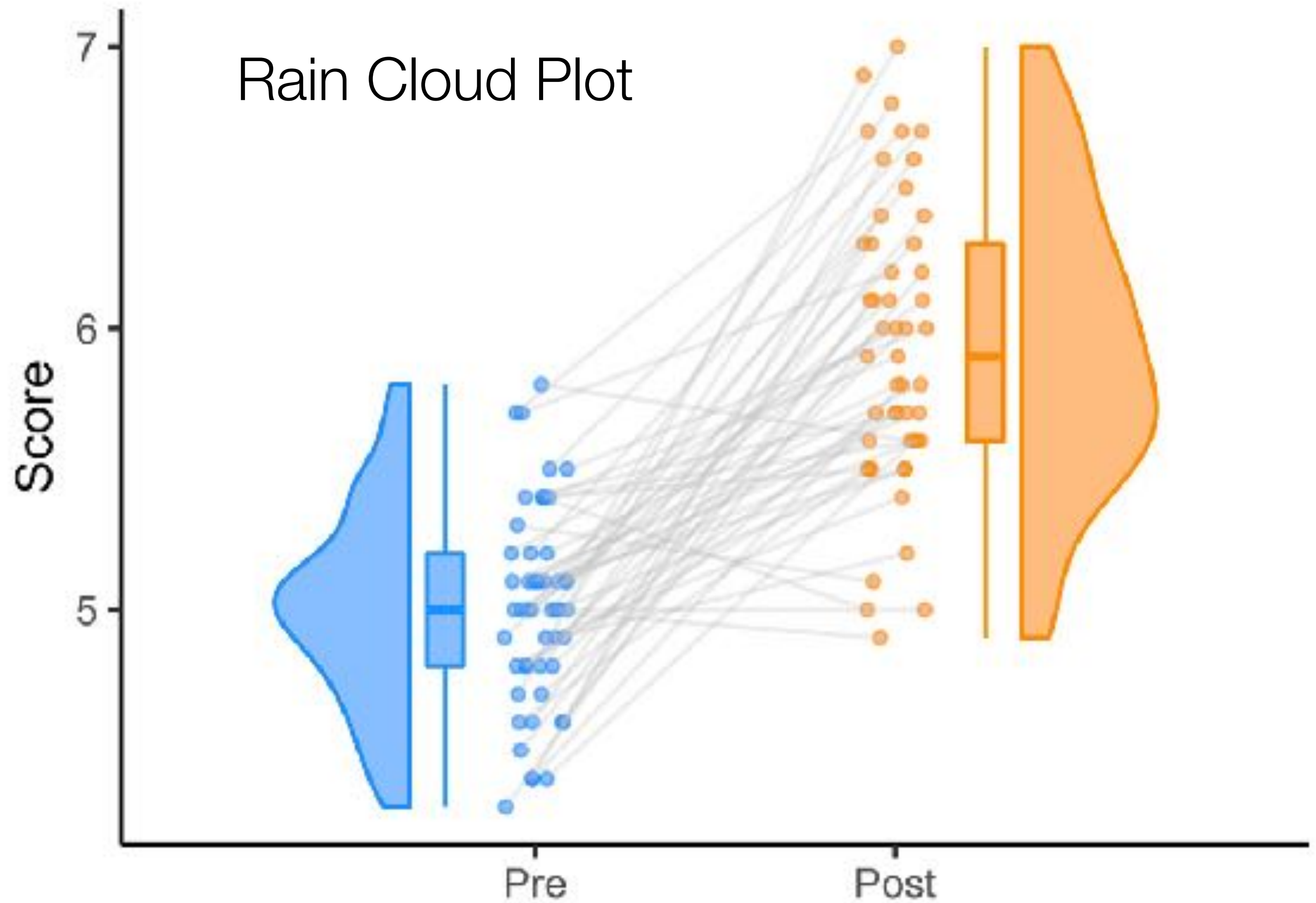
Linear and Logistic Regression
Numpy, Recreate API for Scikit-learn
Detailed mathematics for simple optimization
intuition for advanced optimization

Neural Networks and Back Prop.
Numpy
Detailed mathematics for NN operations

Wide and Deep Networks | **Convolutional Networks** | **Recurrent Networks**
Keras, Tensorflow
Intuition, Detailed implement.

Ethics in Language Models
ConceptNet
Case studies

Last time: visualization



Understanding **Before** Lecture Demo

Understanding **After** Lecture Demo

Dimensionality Reduction: PCA

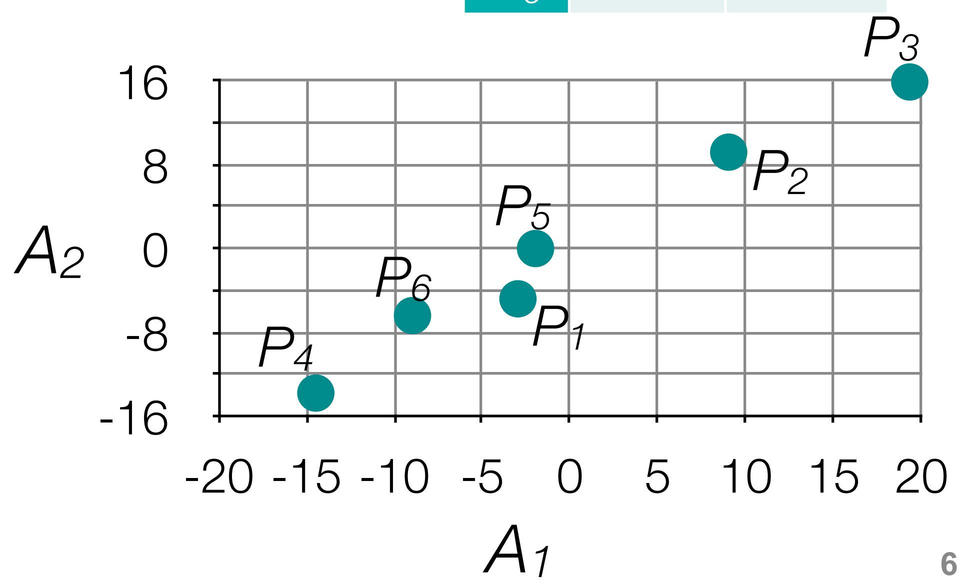
Self Test: Table Data and Dimensions

How many dimensions does this table data have?

A. Two, each point has two features
B. Two, p1 and p2 can be plotted versus one another
C. Six, each column can be plotted in six dimensional space
D. Six, each row is a point in six dimensions

	A_1	A_2
P_1	-2.96	-4.82
P_2	9.03	9.18
P_3	19.33	15.88
P_4	-14.46	-13.82
P_5	-1.96	-0.02
P_6	-8.96	-6.42

$$\mathbb{R}^2$$

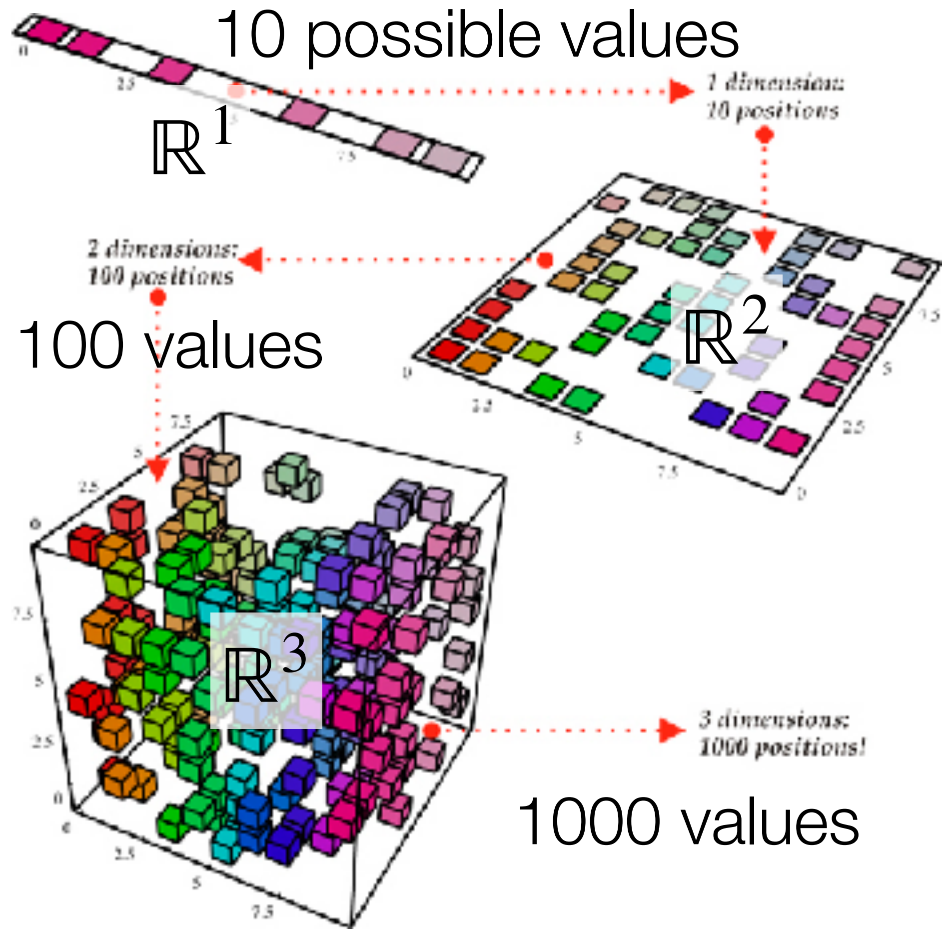


Curse of Dimensionality

Integers from 1-10

- When dimensionality increases, data becomes increasingly sparse in the space that it occupies

- Definitions of density and distance between points, which is critical for clustering and outlier detection, become less meaningful



$$\mathbb{R}^N \leftrightarrow 10^N$$ (or more) values

image source: http://www.iro.umontreal.ca/~bengioy/yoshua_en/research_files/CurseDimensionality.jpg

Dimensionality Reduction

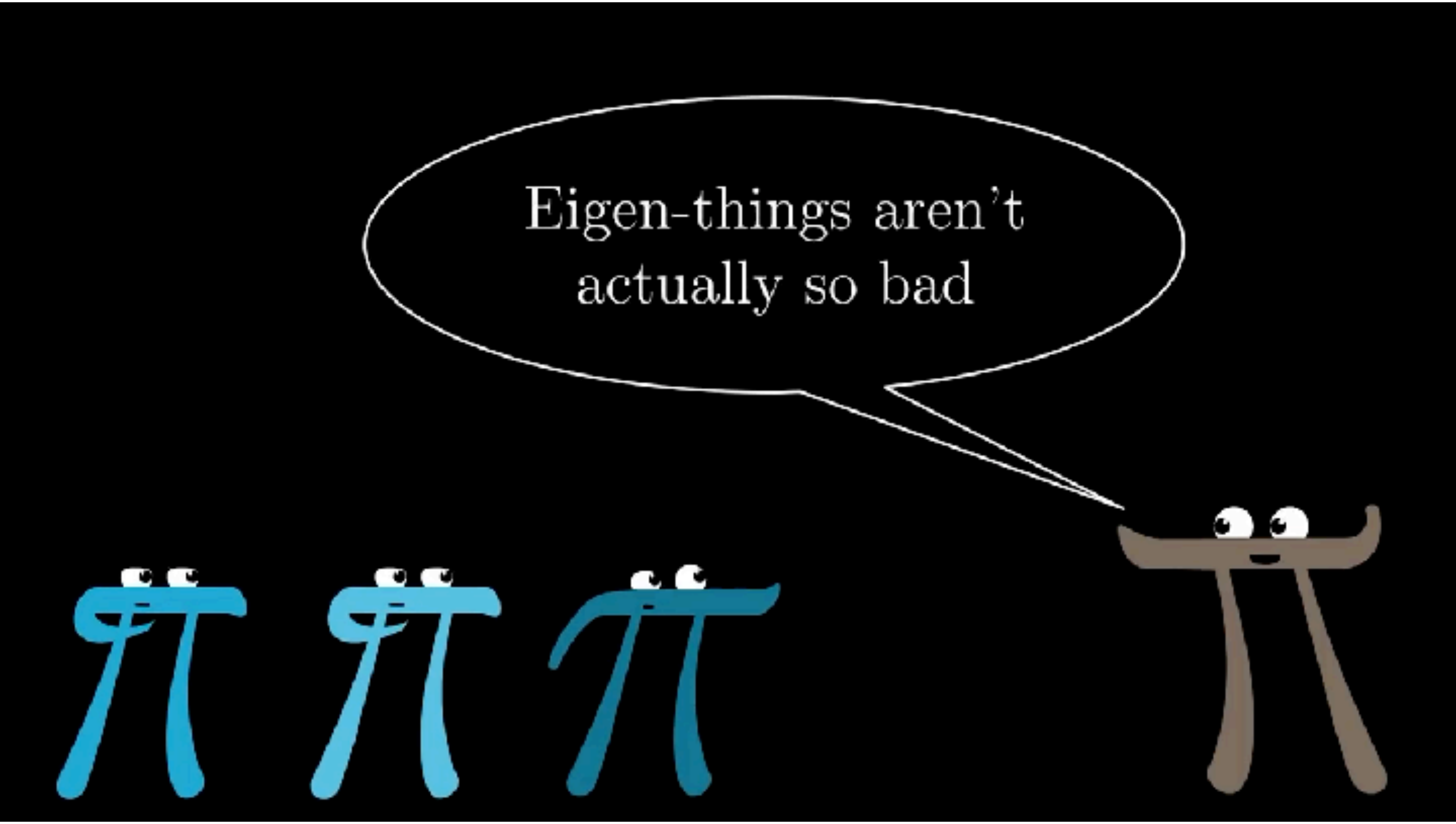
- Purpose:
  - Avoid curse of dimensionality
  - Select subsets of independent features
  - Reduce amount of time and memory required by data mining algorithms
  - Allow data to be more easily visualized
  - May help to eliminate irrelevant features or reduce noise

- Techniques
  - Principle Component Analysis
  - Non-linear PCA
  - Stochastic Neighbor Embedding (tSNE)
  - Uniform Manifold Approximation (UMAP)

I invented PCA…
and *Social Darwinism*

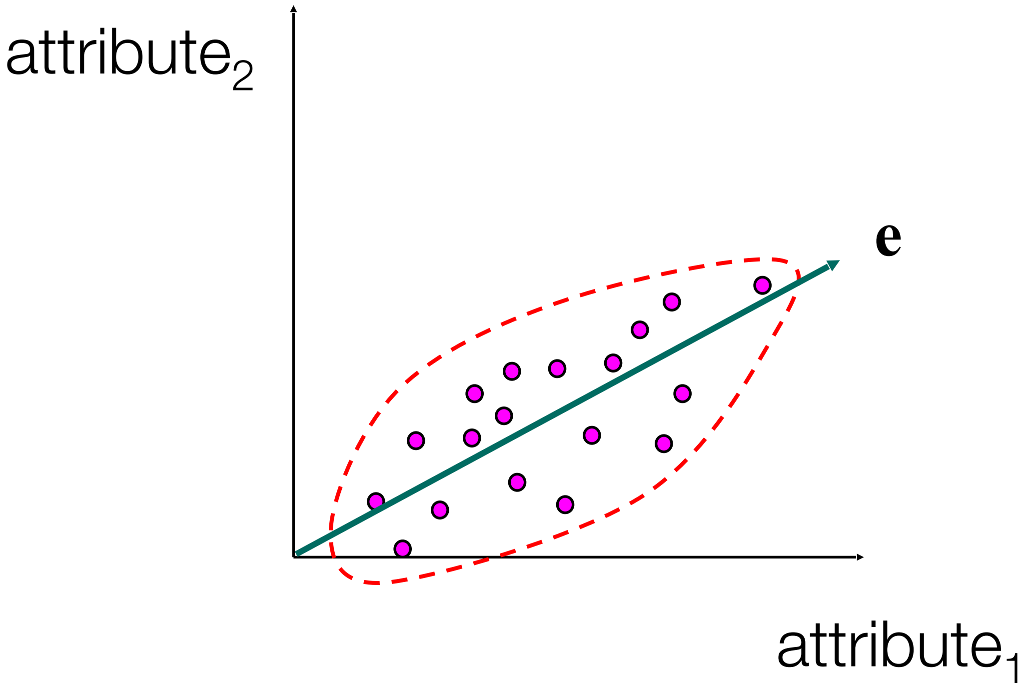
Aside: Eigen Vectors are your friend!

(Grant Sanderson) **Three Blue One Brown:**
https://www.youtube.com/watch?v=PFDu9oVAE-g



Dimensionality Reduction: PCA

- Goal is to find a projection that captures the largest amount of variation in data

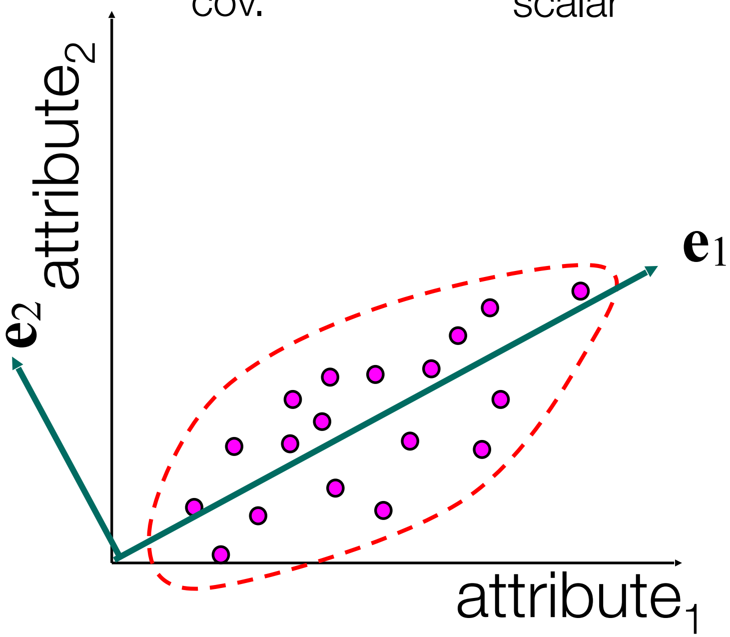


Dimensionality Reduction: PCA

- Find the **eigenvectors** of the **covariance** matrix
- keep the "k" eigenvectors with **largest** eigenvalues

$$\mathbf{C} \cdot \mathbf{e}_i = \lambda_i \mathbf{e}_i$$

cov. scalar



$\mathbf{e}_i$ help define a change of basis from $\mathbf{a}_i$

E_1	E_2
0.749	0.662
0.662	-0.749
λ_1=268.3	λ_2=1.57

Covariance Matrix, $\mathbf{C}$

151.5	132.4
132.4	118.3

	A_1	A_2
1	14	12.6
2	26	26.6
3	36.3	33.3
4	2.5	3.6
5	15	17.4
6	8	11

	$A`_1$	$A`_2$
1	-2.96	-4.82
2	9.03	9.18
3	19.33	15.88
4	-14.46	-13.82
5	-1.96	-0.02
6	-8.96	-6.42

normalize: zero mean
optional: unit std

Dimensionality Reduction: PCA

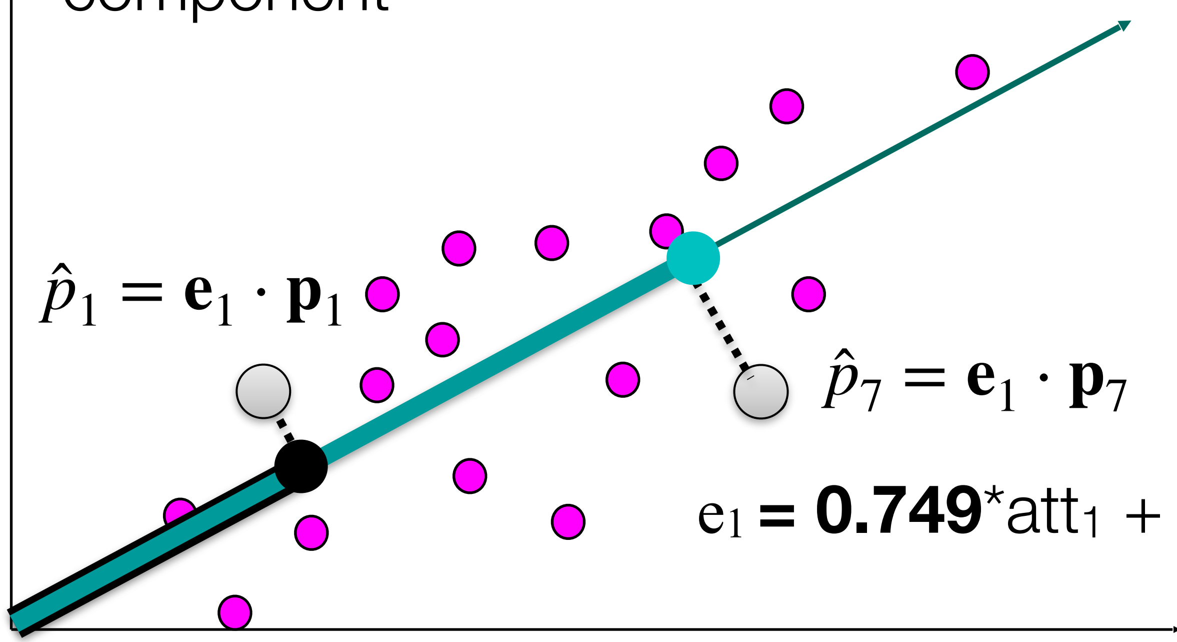
Transform data using dot product between point and principle component (eigenvector)

Dot product is a projection onto component

	E_1
$\mathbf{e}_1$	*0.749*
	0.662

λ=268.3

component



e_1 = **0.749***att$_1$ + **0.662***att$_2$

Reconstruction error:

difference between projection and original point in 2D space

Dimensionality Reduction: PCA

	A_1	A_2
P_1	-2.96	-4.82
P_2	9.03	9.18
P_3	19.33	15.88
P_4	-14.46	-13.82
P_5	-1.96	-0.02
P_6	-8.96	-6.42

zero mean

0.749*att1 + 0.662*att2

$\mathbf{e}_1 \cdot \mathbf{p}_i$

	A_{new}
$\hat{P}_1$	-5.4
$\hat{P}_2$	12.8
$\hat{P}_3$	25.0
$\hat{P}_4$	-19.9
$\hat{P}_5$	-1.4
$\hat{P}_6$	-10.9

Transformed Features

Inverse transform

$\mathbf{e}_1 \cdot \hat{p}_i$

	A_1	A_2
P_1	-2.95	-4.81
P_2	9.0	9.19
P_3	19.2	15.5
P_4	-14.5	-13.2
P_5	-1.96	0.0
P_6	-8.96	-6.3

This projection is called a **Transform**
known as the **Karhunen-Loève Transform (KLT)**

Shown here for two dimensions, but could be anything smaller than original space

$$\mathbb{R}^N \rightarrow \mathbb{R}^M, \quad M < N$$

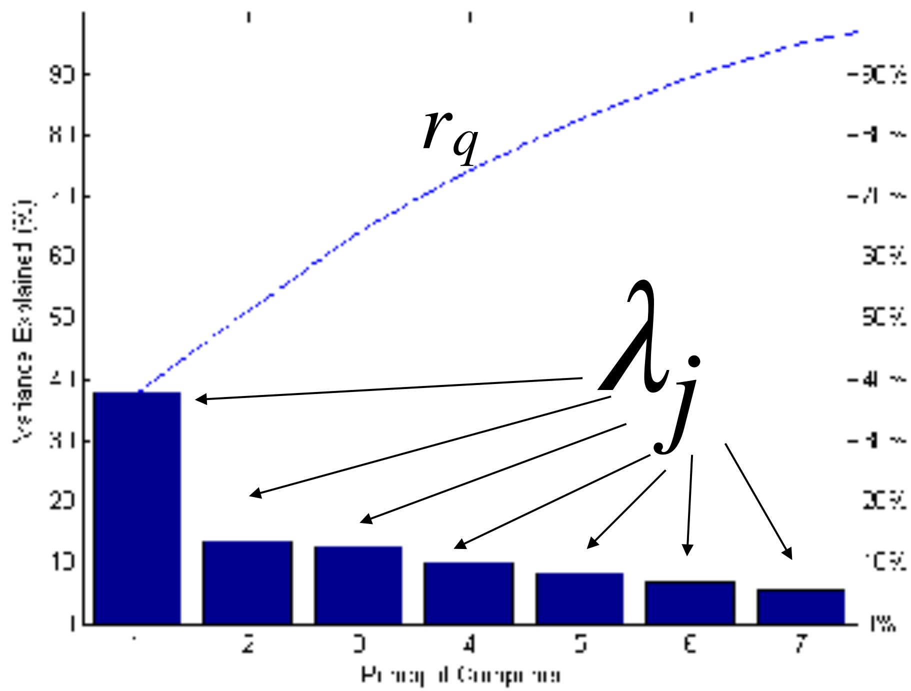
Explained Variance (scree plot)

- Each principle component **explains** a certain **amount of variation** in the data.
- This explained variation is **encoded** in the **eigenvalues** of each **eigenvector**

sum of q largest eigenvalues

$$r_q = \frac{\sum_{j=1}^{q} \lambda_j}{\sum_{\forall i} \lambda_i}$$

sum of all eigenvalues



Dimensionality Reduction: PCA

Genetic profiles distilled to 2 components

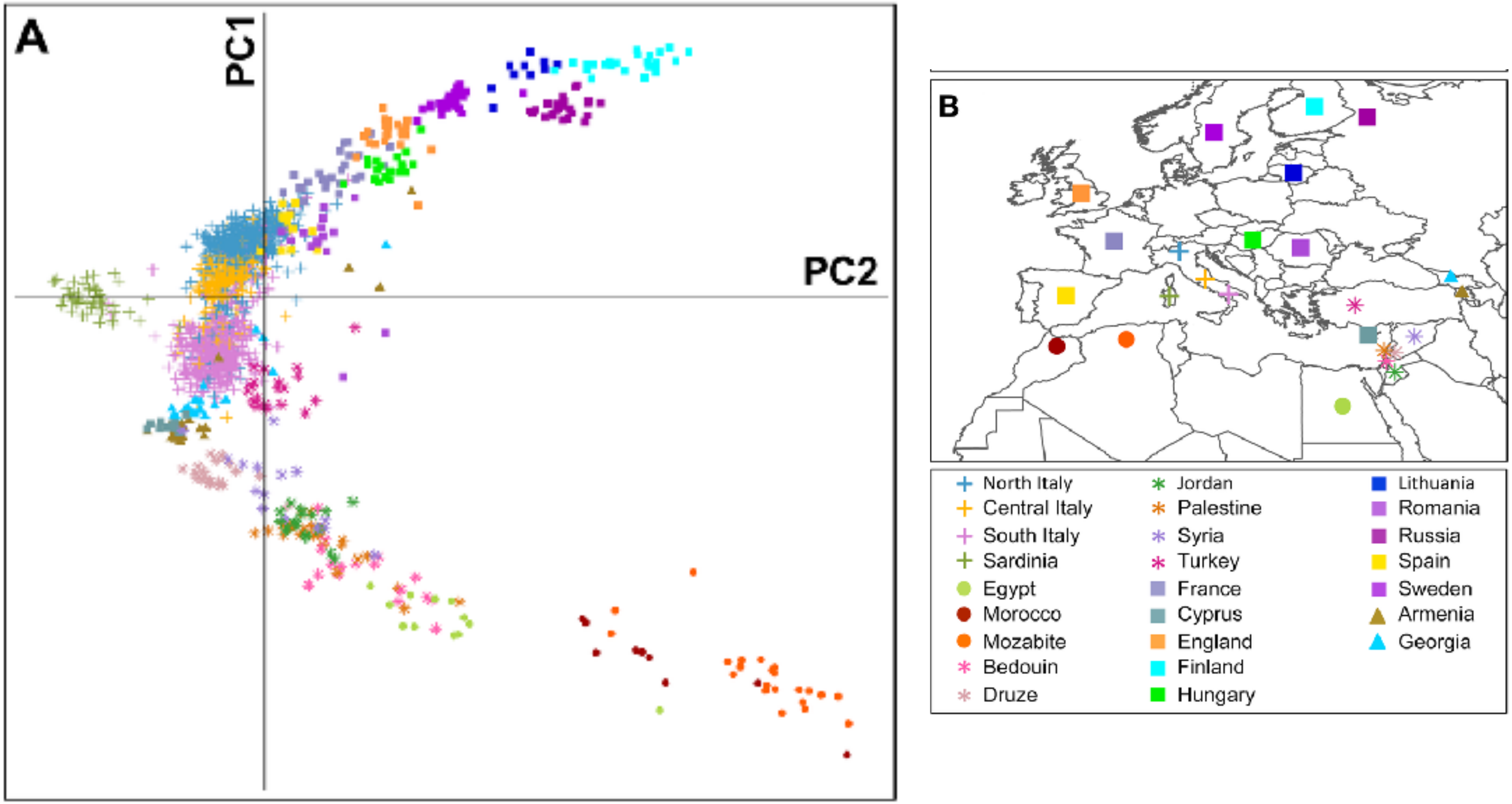


image source: Wikipedia

Dimension Reduction

Demo

```
04.Dimension Reduction and Images.ipynb
```

PCA

biplots

Other Tutorials:

http://scikit-learn.org/stable/auto_examples/decomposition/plot_pca_vs_lda.html#example-decomposition-plot-pca-vs-lda-py

http://nbviewer.ipython.org/github/ogrisel/notebooks/blob/master/Labeled%20Faces%20in%20the%20Wild%20recognition.ipynb

Self Test ML2b.1

Principal Components Analysis works well for categorical data by design.

A. True
B. False
C. It doesn't but people do it anyway

Better option: Mutual Correspondence Analysis

	Eye Color	*Hair Color*
1	*Blue*	*Blon.*
2	*Brown*	*Brown*
3	*Blue*	*Blon.*
4	*Hazel*	*Brown*
5	*Brown*	*Brown*
6	*Brown*	*Blon.*

OHE

	Eye Color			*Hair Color*	
1	*1*	*0*	*0*	*1*	*0*
2	*0*	*1*	*0*	*0*	*1*
3	*1*	*0*	*0*	*1*	*0*
4	*0*	*0*	*1*	*0*	*1*
5	*0*	*1*	*0*	*0*	*1*
6	*0*	*1*	*0*	*1*	*0*

PCA

	A1	*A2*
1	*0.79*	*-0.30*
2	*-0.60*	*-0.13*
3	*0.79*	*-0.30*
4	*0.24*	*0.99*
5	*-0.60*	*-0.13*
6	*-0.1*	*-0.25*

Dimensionality Reduction: Randomized PCA

- **Problem**: PCA on all that data can take a while to compute
  - What if the number of instances is gigantic?
  - What if the number of dimensions is gigantic?
- Can we approximate covariance with a lower rank matrix?
  - By **transforming** our table data, $\boldsymbol{A}$, with another orthogonal matrix, $\boldsymbol{Q}$, we can **approximate** the **covariance matrix**, but with **lower rank**
  - Gives a matrix with typically good enough precision of actual eigenvectors, like using SVD. $\boldsymbol{Q}\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{A}$ is surrogate

Example Objective

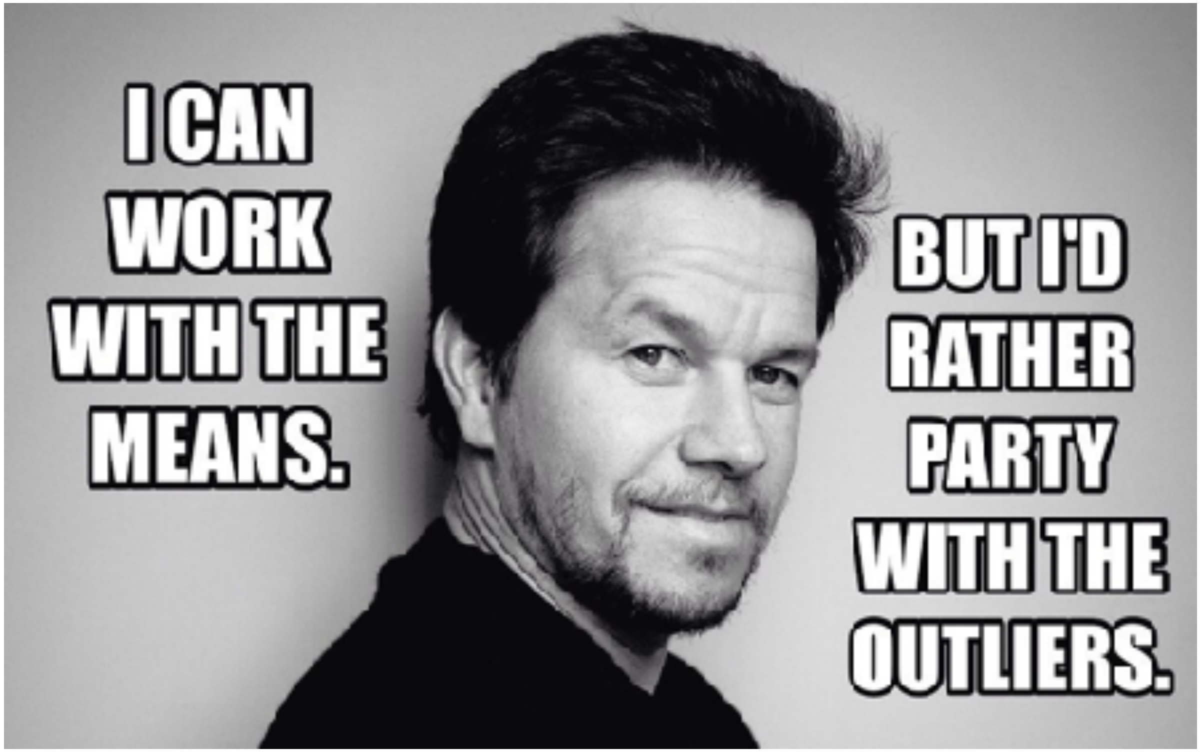
$$\|\mathbf{A} - \underbrace{\mathbf{Q} \cdot \mathbf{Q}^T \mathbf{A}}_{\text{surrogate}} \| < \underbrace{\left(1 + 11\sqrt{k+p} \cdot \min(m, n)\right) \cdot \sigma_{k+1}}_{\text{properties of } \mathbf{A} \text{ and } \mathbf{Q}}$$

Halko, et al., (2009) Finding structure with randomness: Stochastic algorithms for constructing approximate matrix decompositions. https://arxiv.org/pdf/0909.4061.pdf

Just need an intuition about this!!!

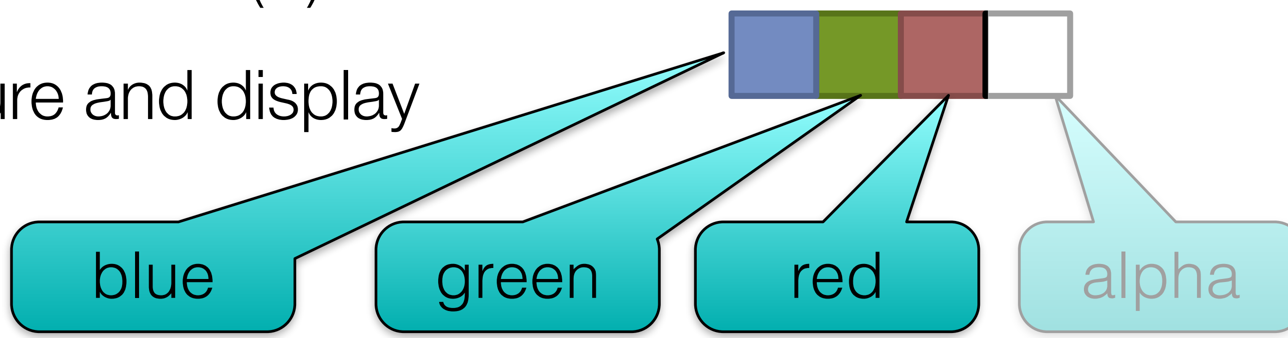
Image Representation

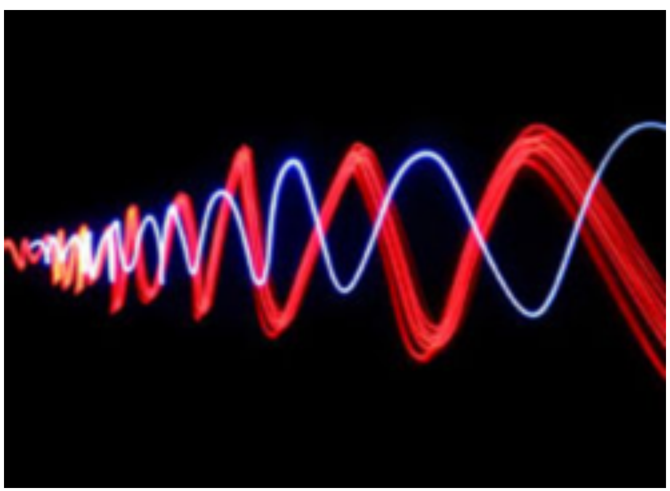
Our first @ResearchMark meme

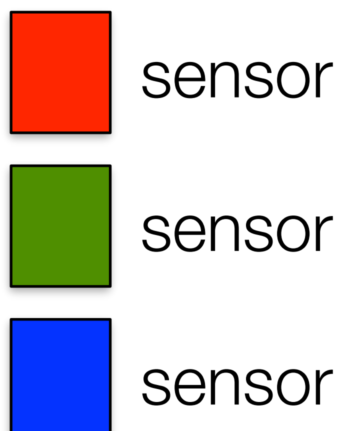


Images as data

- an image can be represented in many ways
- most common format is a matrix of pixels
    - each “pixel” is BGR(A)
- used for capture and display







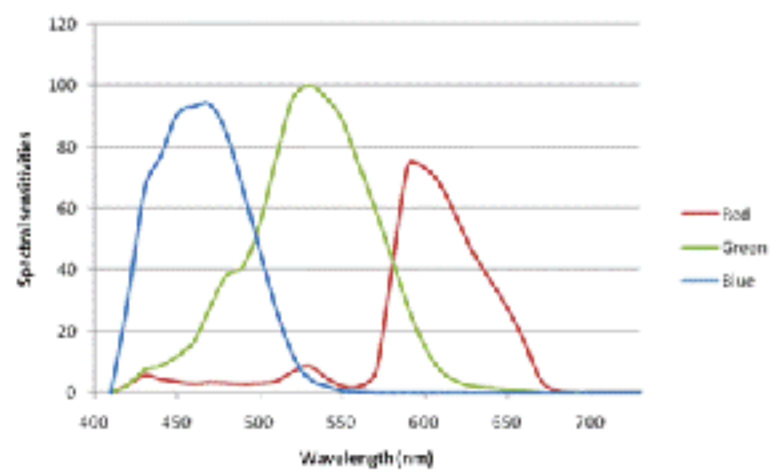


Image Representation

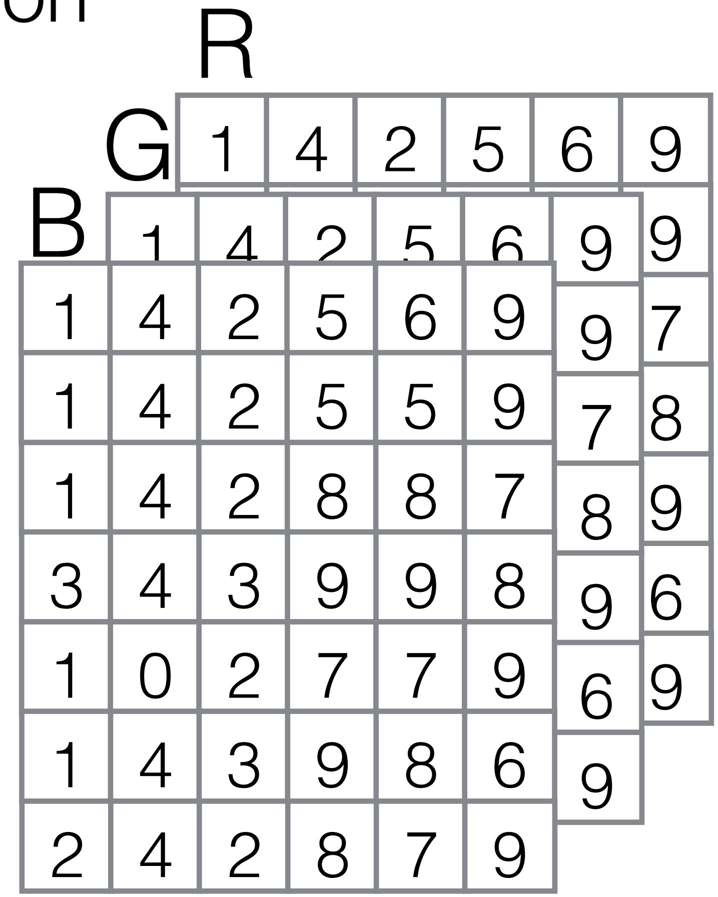
- need a compact representation

- **grayscale**
  0.3*R+0.59*G+0.11*B,
  "luminance"

gray

1	4	2	5	6	9
1	4	2	5	5	9
1	4	2	8	8	7
3	4	3	9	9	8
1	0	2	7	7	9
1	4	3	9	8	6
2	4	2	8	7	9

Numpy Matrix
image[rows, cols]



Numpy Matrix
image[rows, cols, channels]

Image Representation, Features

Problem: need to represent image as table data

- need a compact representation

1	4	2	5	6	9
1	4	2	5	5	9
1	4	2	8	8	7
3	4	3	9	9	8
1	0	2	7	7	9
1	4	3	9	8	6
2	4	2	8	7	9

Image Representation, Features

Problem: need to represent image as table data

- need a compact representation

Solution: row concatenation (vectorizing)

Row 1	1	4	2	5	6	9	1	4	2	5	5	9	1	4	2	8	8	7	3
Row 2	1	4	2	8	8	7	3	4	3	9	9	8	1	4	2	5	5	9	1

…

Row N	9	4	6	8	8	7	4	1	3	9	2	1	1	5	2	1	5	9	1

Self test: 3a-1

- When vectorizing images into table data, each "feature column" corresponds to:
  - a. the value (color) of a pixel
  - b. the spatial location of a pixel in the image
  - c. the size of the image
  - d. the spatial location and color channel of a pixel in an image

Row N	9	4	6	8	8	7	4	1	3	9	2	1	1	5	2	1	5	9	1

Dimension Reduction with Images **Demo**

Images Representation
in PCA and
Randomized PCA

`04.Dimension Reduction and Images.ipynb`

For Next Lecture

- Next Lecture:
  - Finish Dimension Reduction Demo
  - Crash-course Image Feature Extraction