Lecture Notes for

Machine Learning in Python

[👨‍🏫, 👨‍💻, 🐍, 👨‍🔬]

Professor Eric Larson

Visualization and Dimensionality Reduction

Class Logistics and Agenda

- Dimensionality Reduction
    - PCA
    - Randomized PCA
    - Images

Dimensionality Reduction: PCA

Curse of Dimensionality

- 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

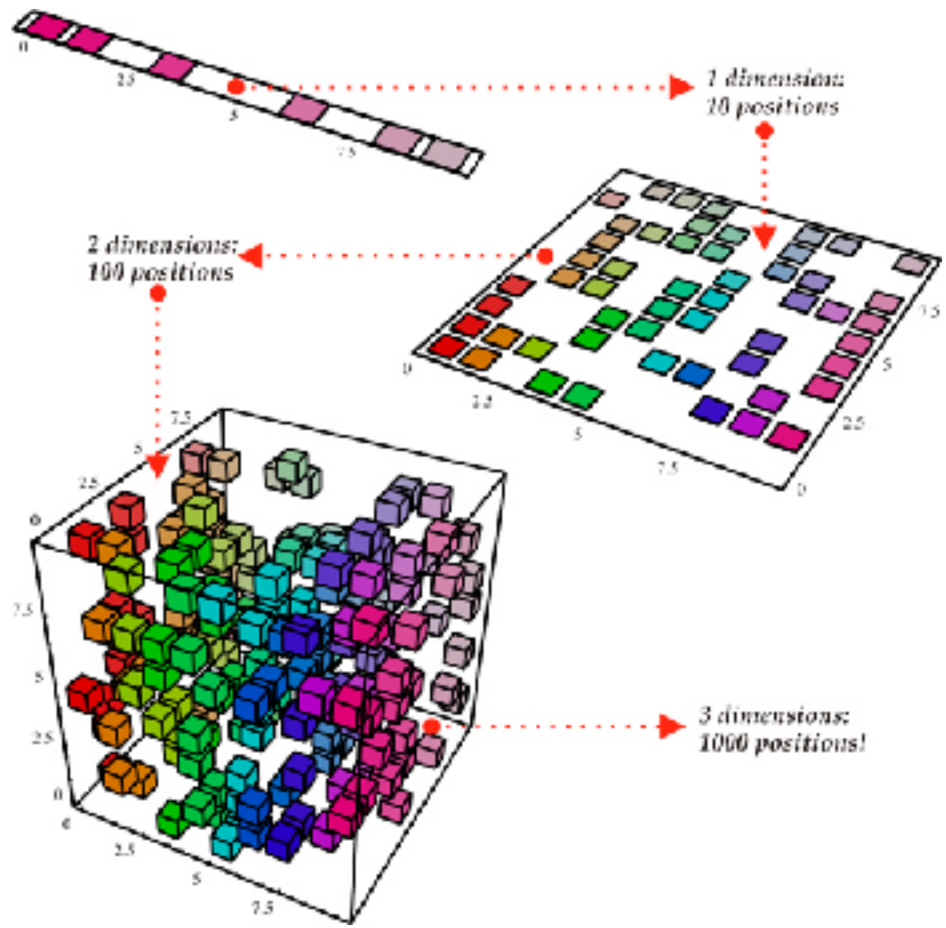


image source: http://www.iro.umontreal.ca/~bengioy/yoshua_en/research_files/CurseDimensionality.jpg

Dimensionality Reduction

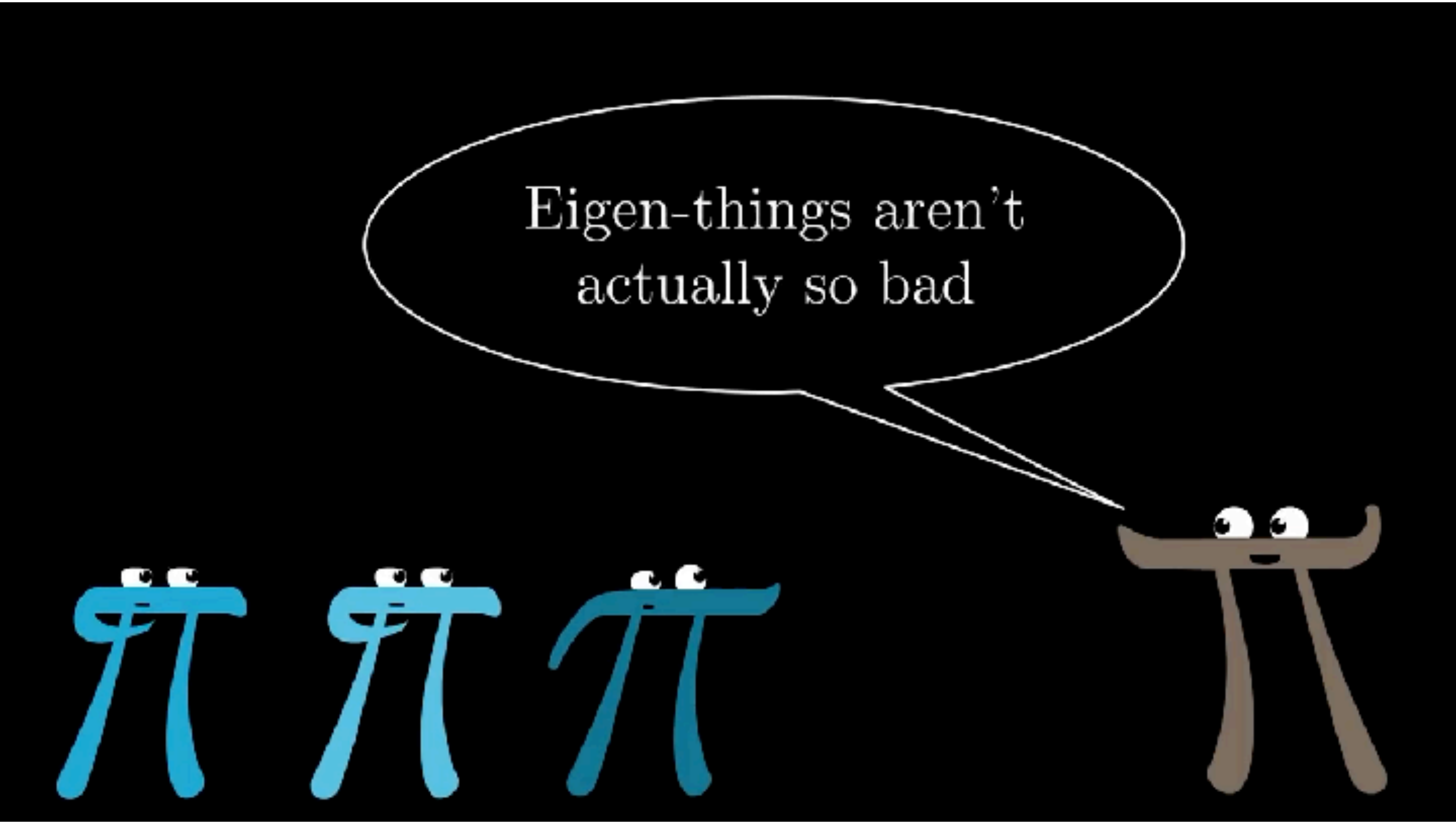
- Purpose:
  - Avoid curse of dimensionality
  - Select subsets of independent features
  - Reduce amount of time and memory required by data mining algorithms
  - Allow data to be more easily visualized
  - May help to eliminate irrelevant features or reduce noise

- Techniques
  - Principle Component Analysis
  - Non-linear PCA
  - Stochastic Neighbor Embedding

I invented PCA…
and *Social Darwinism*

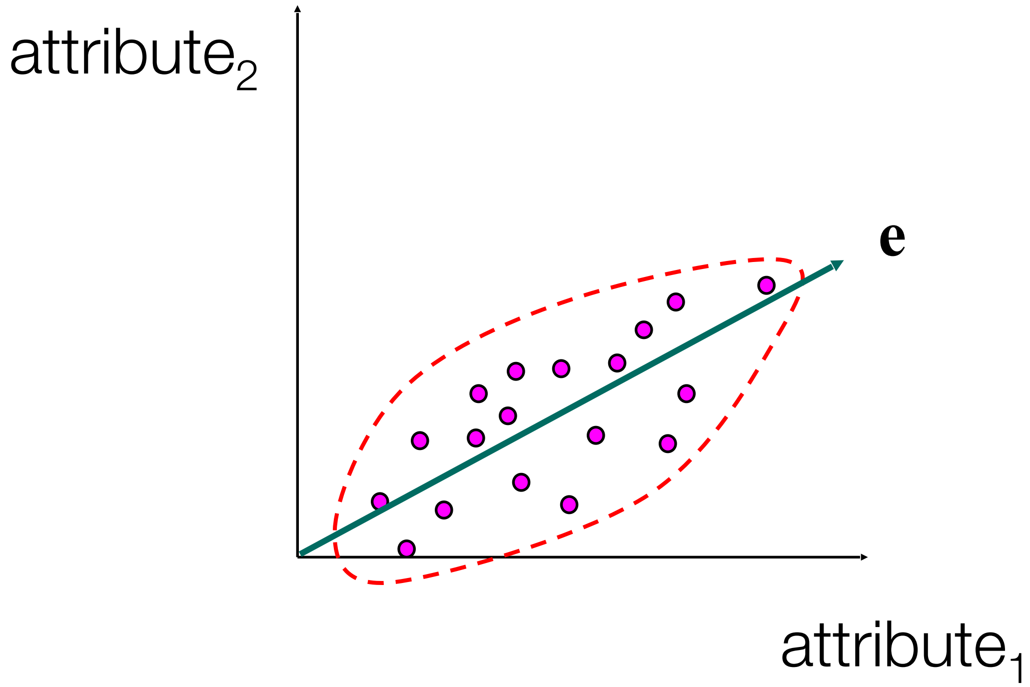
Aside: Eigen Vectors are your friend!

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



Dimensionality Reduction: PCA

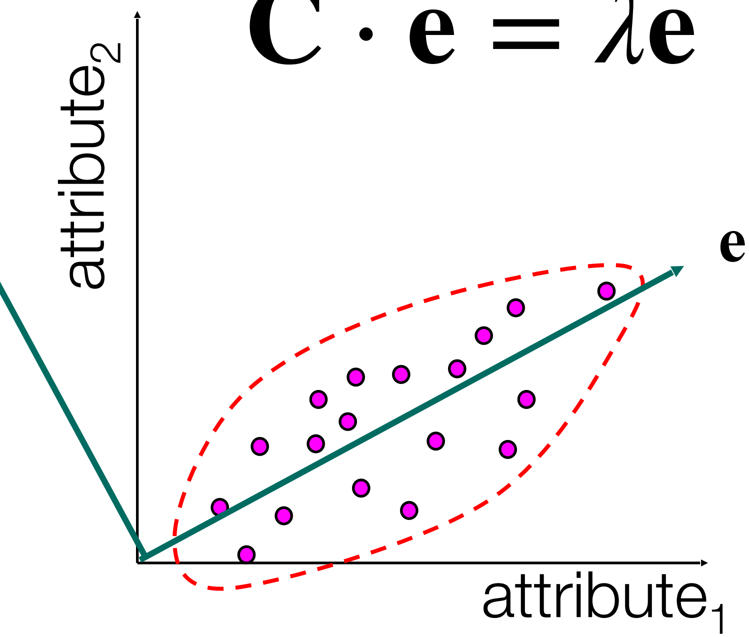
- Goal is to find a projection that captures the largest amount of variation in data



Dimensionality Reduction: PCA

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

$$\mathbf{C} \cdot \mathbf{e} = \lambda \mathbf{e}$$



E1	E2
0.85	0.85
0.52	-0.52

covariance

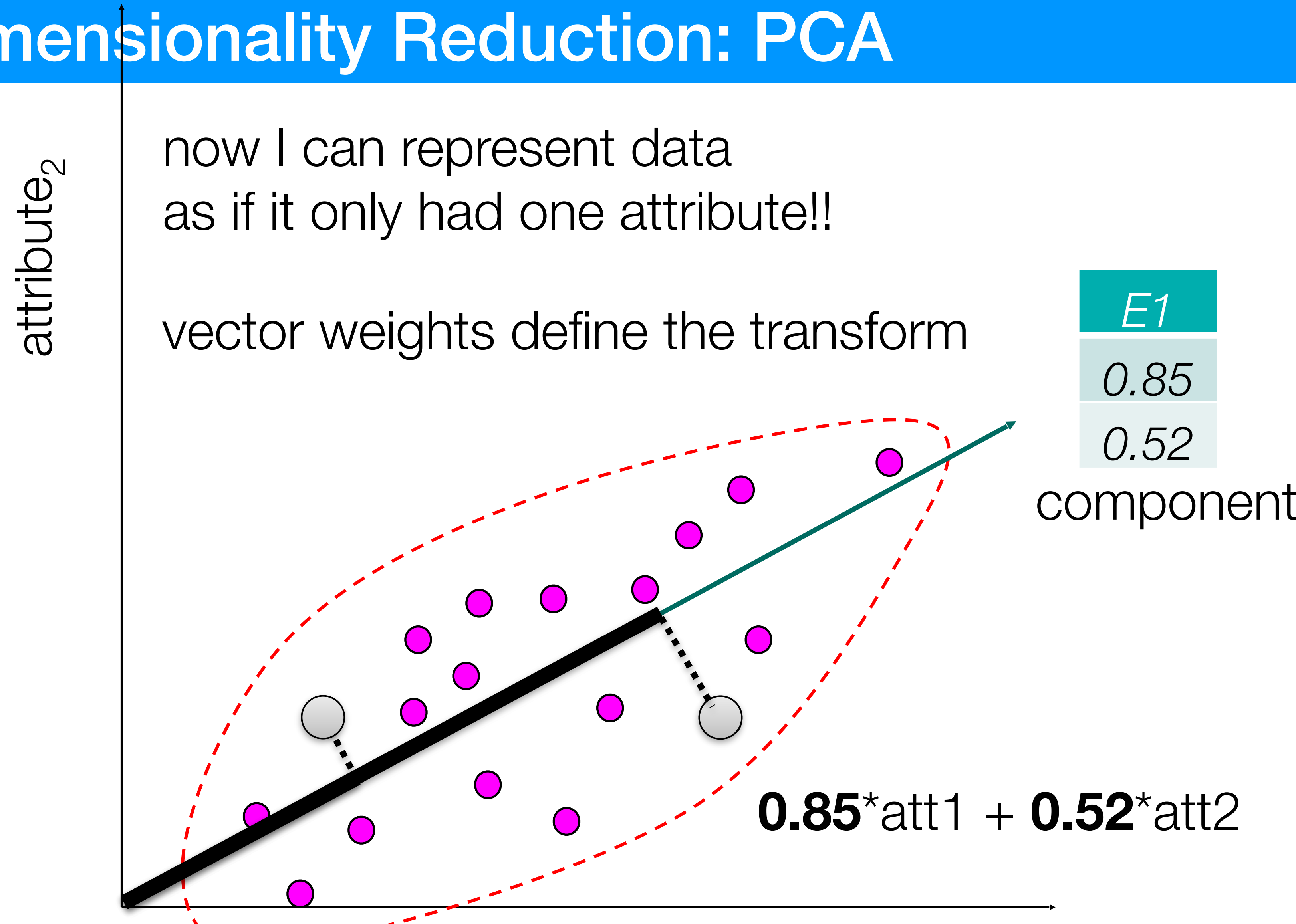
37.1	-6.7
-6.7	43.9

	A1	A2
1	66	33.6
2	54	26.6
3	69	23.3
4	73	28.1
5	61	43.1
6	62	25.6

	A1	A2
1	1.83	3.55
2	-10.1	-3.45
3	4.83	-6.75
4	8.83	-1.95
5	-3.17	13.05
6	-2.17	-4.45

zero mean

Dimensionality Reduction: PCA



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

Dimensionality Reduction: PCA

	A1	A2
1	1.83	3.55
2	-10.1	-3.45
3	4.83	-6.75
4	8.83	-1.95
5	-3.17	13.05
6	-2.17	-4.45

zero mean

0.85*att1 + **0.52***att2

	P1
1	3.4015
2	-10.379
3	0.5955
4	6.4915
5	4.0915
6	-4.1585

First Principle Component

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

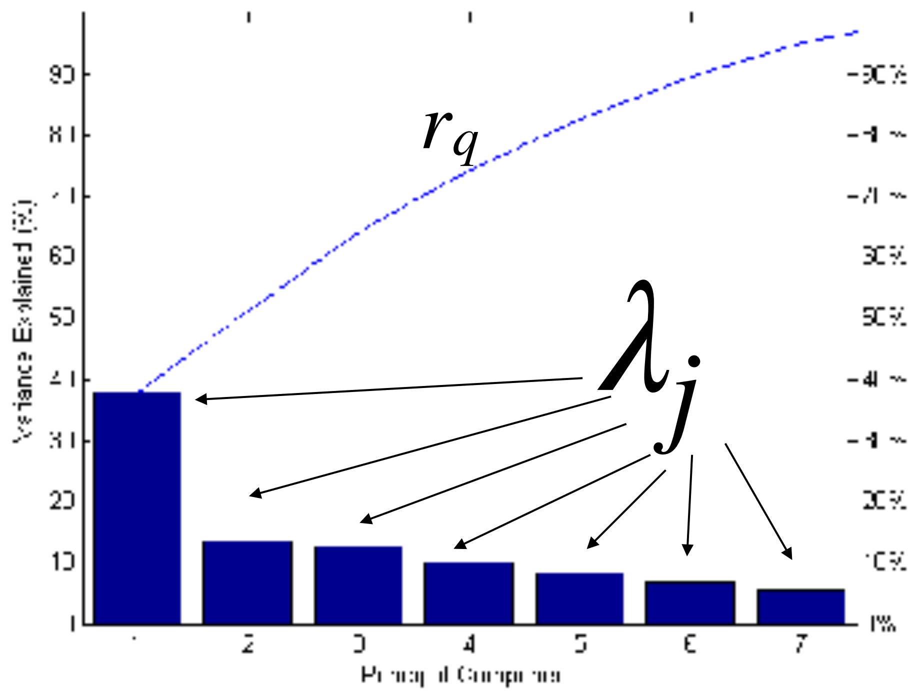
Explained Variance

- 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

$$r_q = \frac{\sum_{j=1}^{q} \lambda_j}{\sum_{j=1}^{p} \lambda_j}$$

sum of all eigenvalues



Dimensionality Reduction: PCA

- Genetic profiles distilled to 2 components

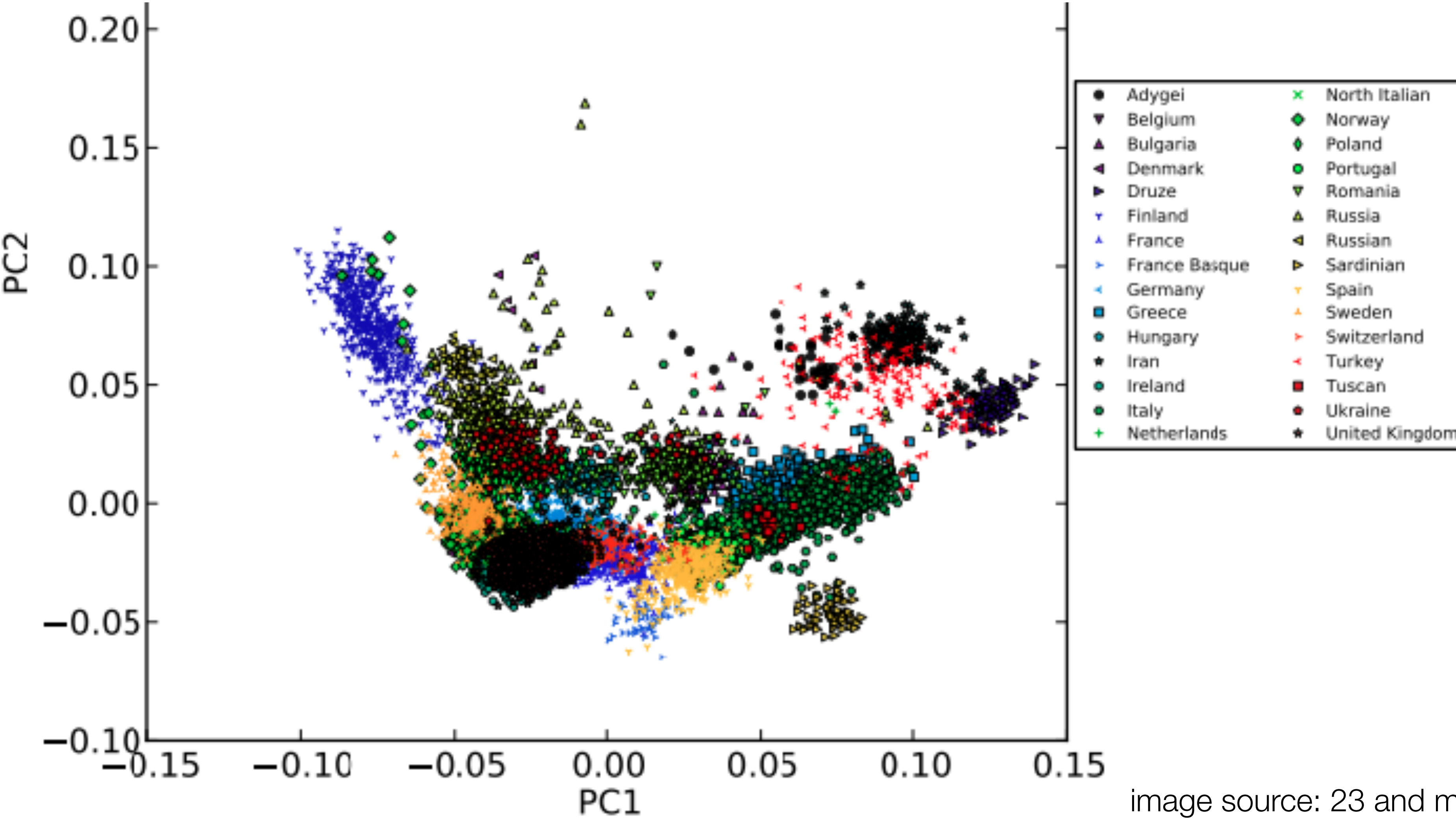


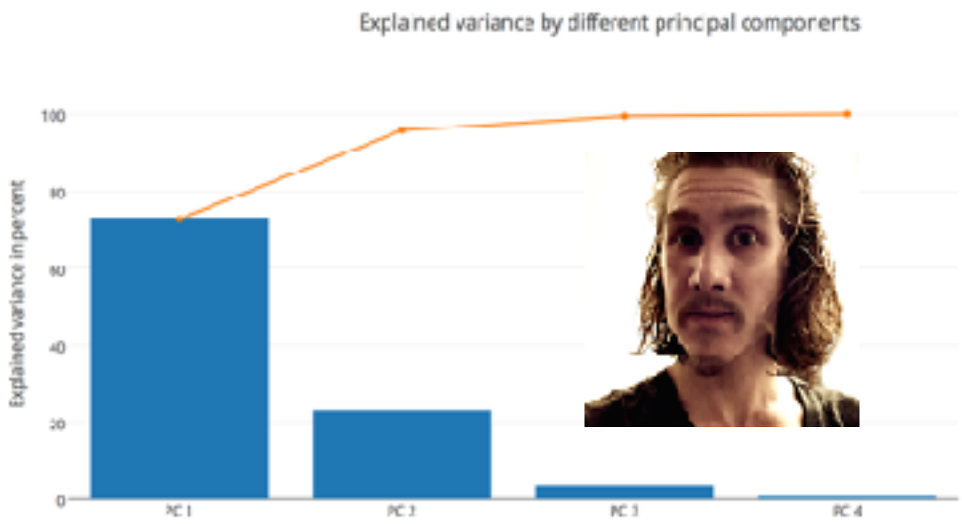
image source: 23 and me

Dimensionality Reduction: PCA

- Need more help with the PCA algorithm (and python)?
  - check out Sebastian Raschka's notebooks:

http://nbviewer.ipython.org/github/rasbt/pattern_classification/blob/master/dimensionality_reduction/projection/principal_component_analysis.ipynb

Or check out PCA for dummies:
https://georgemdallas.wordpress.com/2013/10/30/principal-component-analysis-4-dummies-eigenvectors-eigenvalues-and-dimension-reduction/



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

Dimensionality Reduction: Randomized PCA

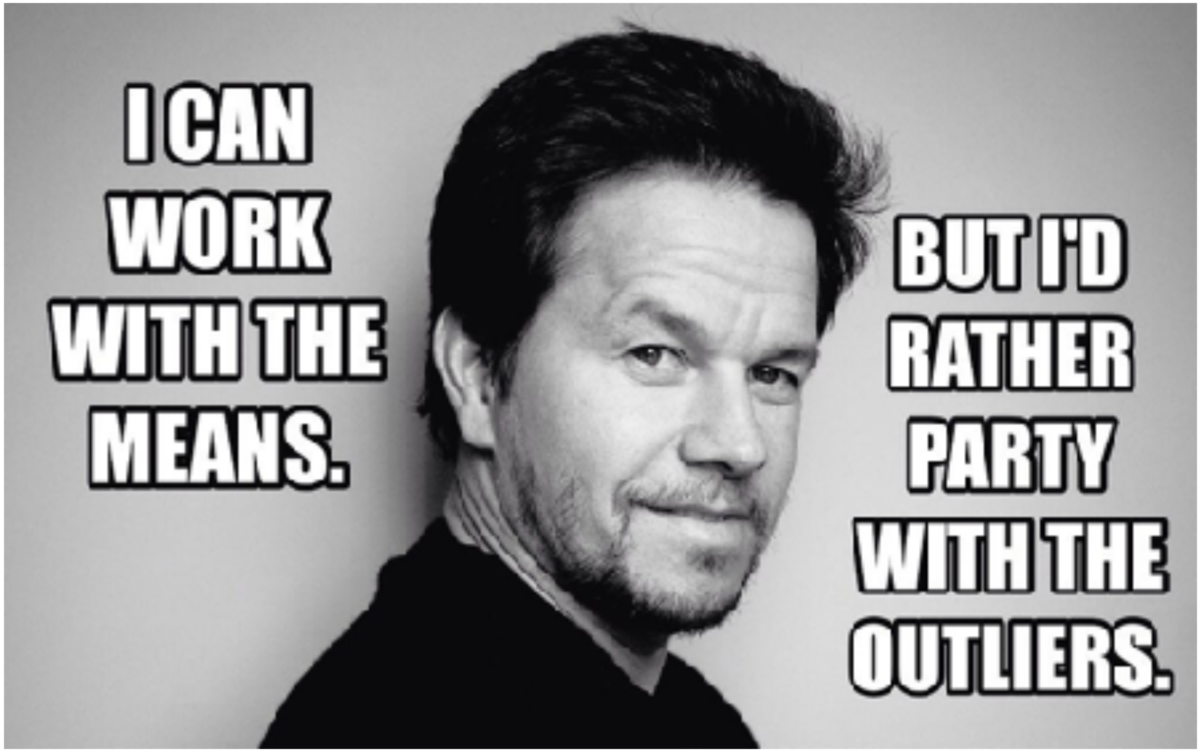
- **Problem**: PCA on all that data can take a while to compute
  - What if the number of instances is gigantic?
  - What if the number of dimensions is gigantic?
- What if we partially construct the covariance matrix with a lower rank matrix?
  - By **transforming** our table data, A, with another orthogonal matrix, 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. $\boldsymbol{QQ}^{\mathrm{T}}\boldsymbol{A}$ is surrogate

Example Objective

$$\|\boldsymbol{A} - \boldsymbol{QQ}^*\boldsymbol{A}\| \leq \left[1 + 11\sqrt{k+p} \cdot \sqrt{\min\{m, n\}}\right] \sigma_{k+1}$$

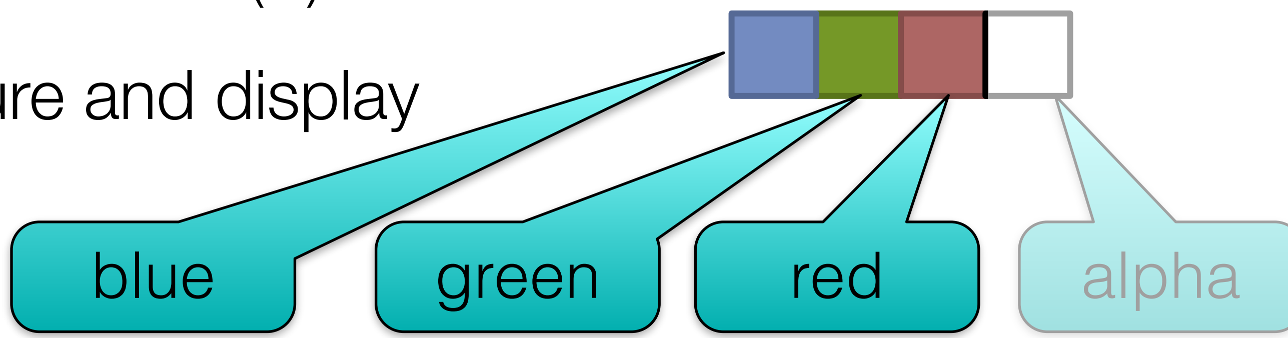
Halko, et al., (2009) Finding structure with randomness: Stochastic algorithms for constructing approximate matrix decompositions. https://arxiv.org/pdf/0909.4061.pdf

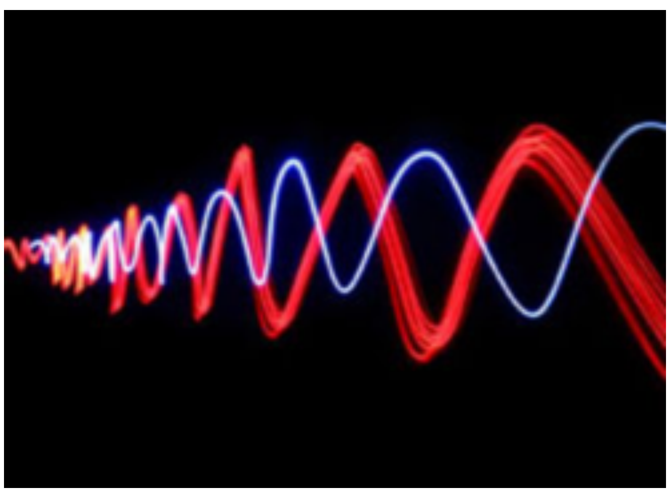
Image Processing and Representation

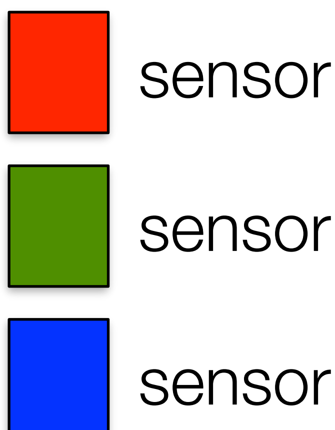


Images as data

- 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







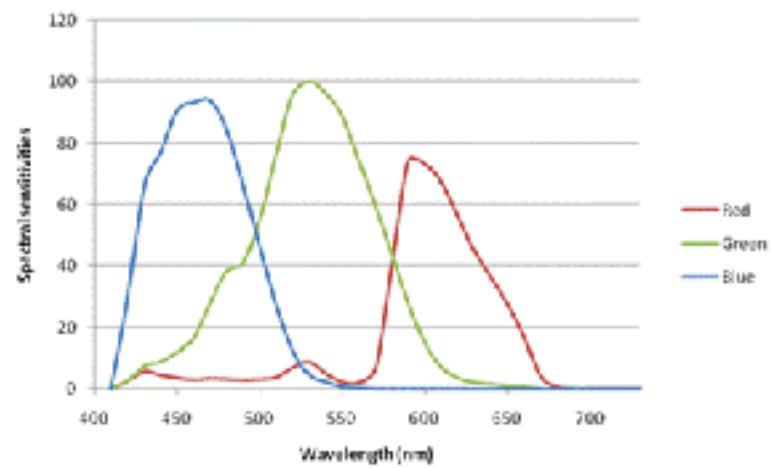


Image Representation

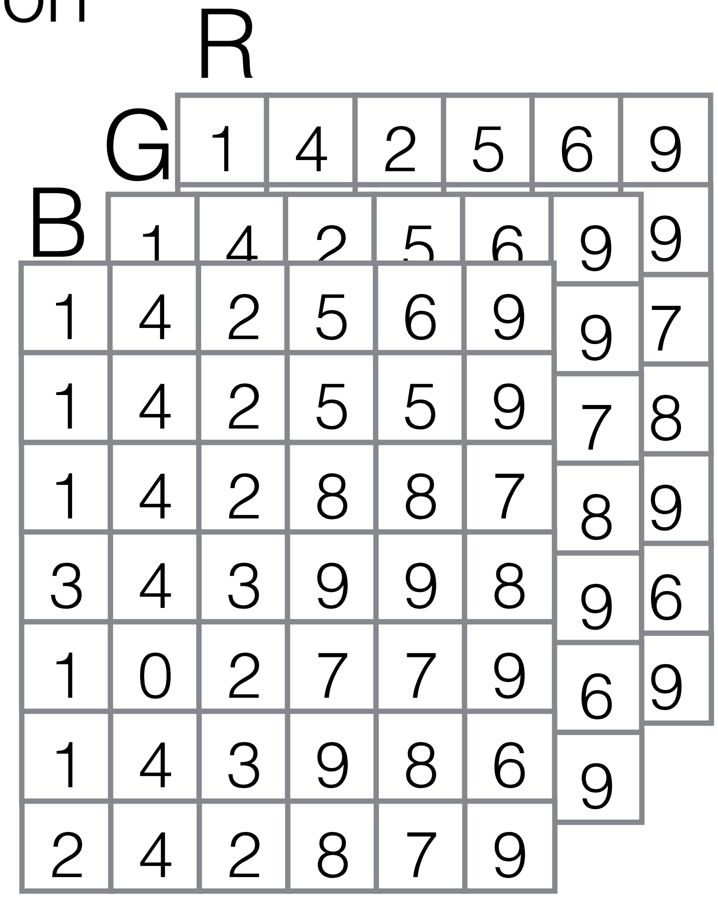
- need a compact representation

- **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 (also, 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 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

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

Lecture Notes for

Machine Learning in Python

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Professor Eric Larson

Dimensionality Reduction and Images

Class Logistics and Agenda

- **Logistics**:
  - Lab due soon!
  - Next Time: Flipped Module
  - Turn in one per team (HTML), please include team member names from canvas
- **Agenda**
  - Common Feature Extraction Methods for Images
  - Begin Town Hall, if time

Last time…

E1	E2
0.85	0.85
0.52	-0.52

37.1	-6.7
-6.7	43.9

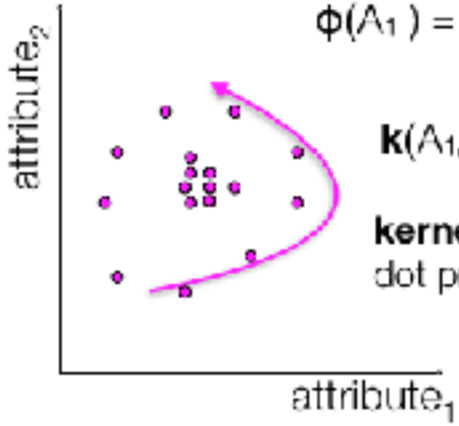
	A1	A2
1	66	33.6
2	54	26.6
3	69	23.3
4	73	28.1
5	61	43.1
6	62	25.6

	A1	A2
1	1.83	3.55
2	-10.1	-3.45
3	4.83	-6.75
4	8.83	-1.95
5	-3.17	13.05
6	-2.17	-4.45

zero mean

$A_1 = [a_1\ a_2]^T$

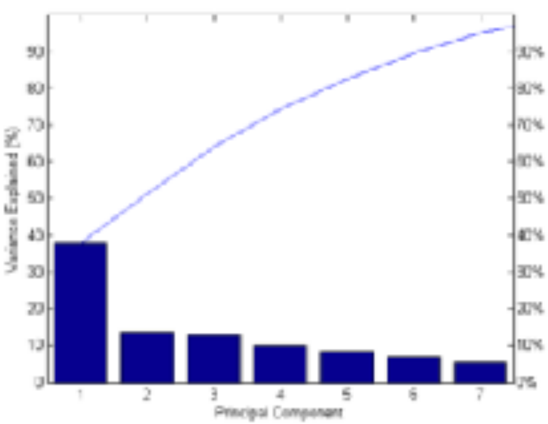
$\phi(A_1) = [a_1\quad a_2\quad a_1 \cdot a_2\quad a_1^2\quad a_1 \cdot a_2^3 \cdots]^T$

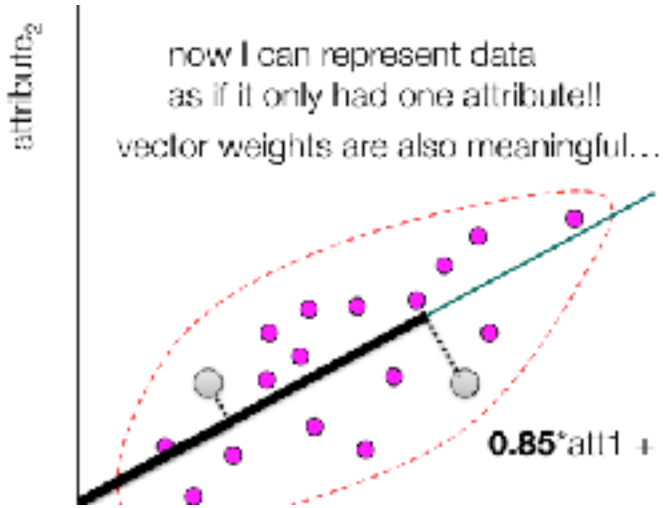


k$(A_1, A_2) = \exp(-\gamma \| A_1 - A_2 \|^2)$

kernel: radial basis function (rbf)
dot product in higher dimensional space

$$r_q = \frac{\sum_{j=1}^{q} \lambda_j}{\sum_{j=1}^{p} \lambda_j}$$





E1
0.85
0.52

component

Dimension Reduction with Images

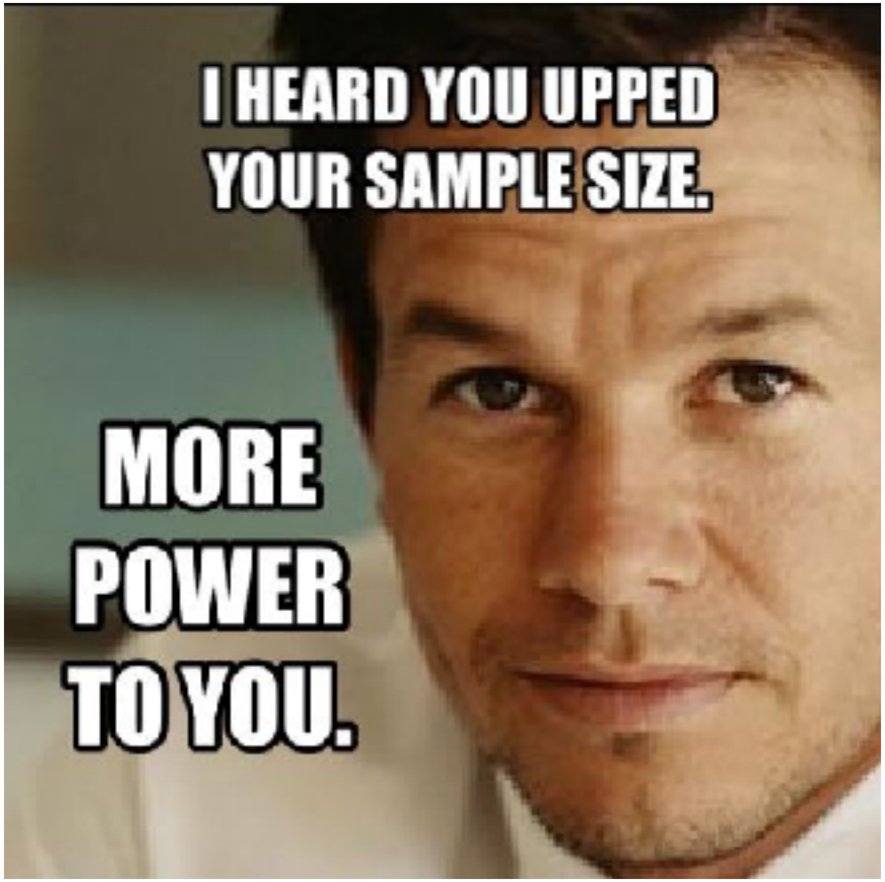
Demo

“Finish”

Images Representation in PCA and Randomized PCA

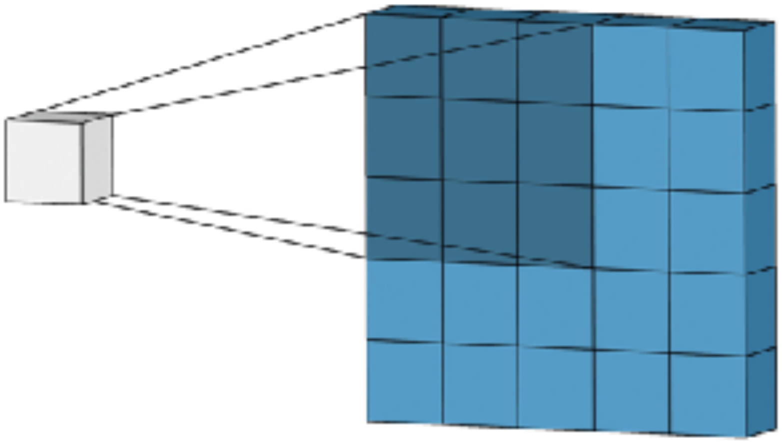
`04.Dimension Reduction and Images.ipynb`

Features of Images



Convolution

- For images:
  - kernel (matrix of values)
  - slide kernel across image,pixel by pixel
  - multiply and accumulate



This Example:
3x3 Kernel (dark)
Ignoring edges of input
Input Image is 5x5
Output is then 3x3

https://towardsdatascience.com/intuitively-understanding-convolutions-for-deep-learning-1f6f42faee1

Convolution

$$\mathbf{O}[i,j] = \sum \mathbf{I}\left[i-\frac{r}{2} : i+\frac{r}{2}, j-\frac{c}{2} : j+\frac{c}{2}\right] \cdot \mathbf{k}$$

output image at pixel i,j

input image at r x c range of pixels centered in i,j

kernel of size r x c usually r=c

Convolution of **Image** and **Kernel** Is **Multiplication** of their **Frequencies**

5	2	3	4	12	9	8	8
5	2	1	4	12	9	8	8
7	2	1	4	12	9	8	8
7	2	1	4	12	9	8	8
5	2	3	4	12	9	8	8
5	2	1	4	12	9	8	8
5	2	1	4	12	9	8	8

input image

1	2	1
2	4	2
1	2	1

kernel

output image

Convolution Examples

$*$

1	0	-1
2	0	-2
1	0	-1

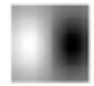
https://www.kdnuggets.com/2016/11/intuitive-explanation-convolutional-neural-networks.html/2

Common operations

- the gradient (2D derivative)

I

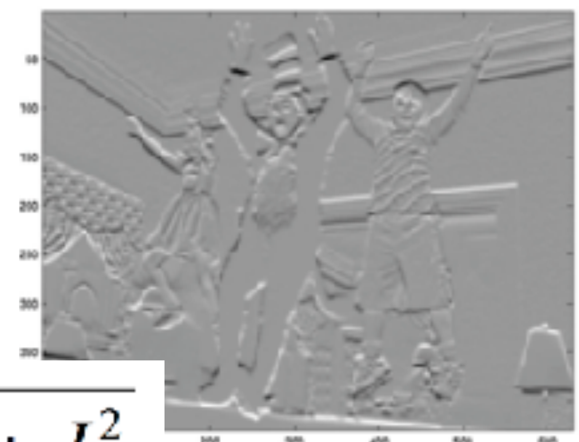
filter



J_x

filter

J_y

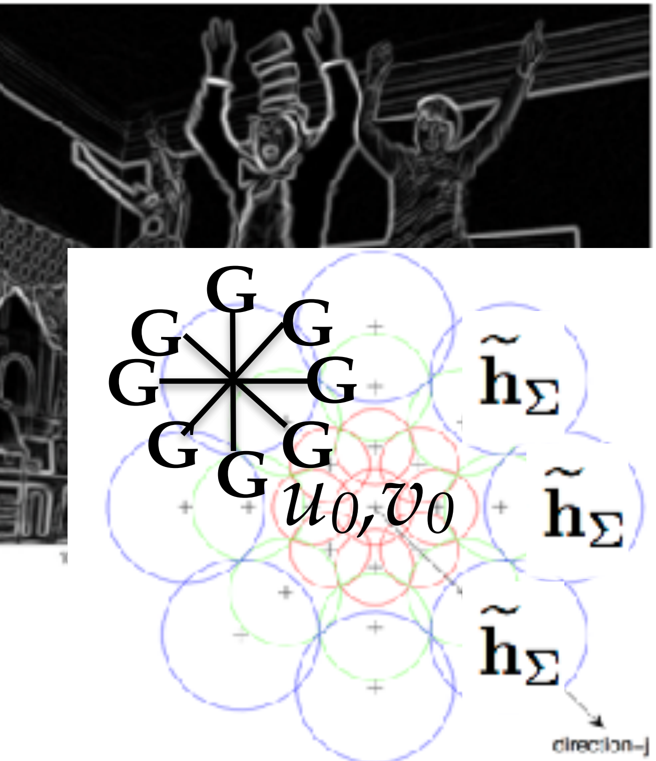


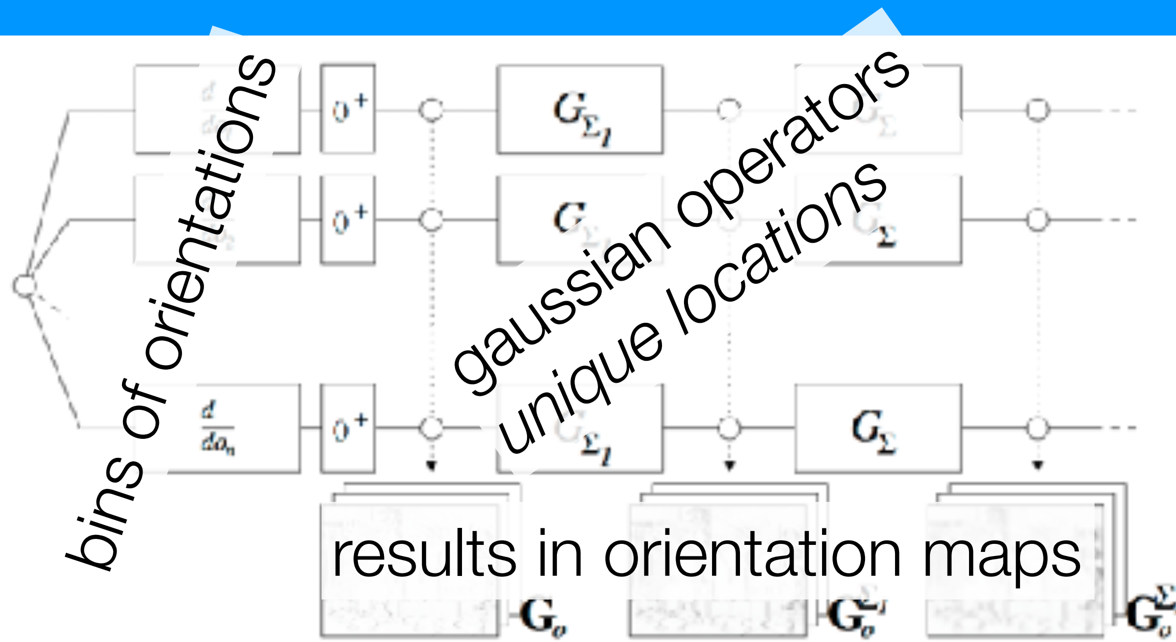
$$\|\nabla J\| = \sqrt{J_x^2 + J_y^2}$$

$$O = \tan^{-1}(Jx / Jy)$$

images: Jianbo Shi, Upenn

Common operations: DAISY





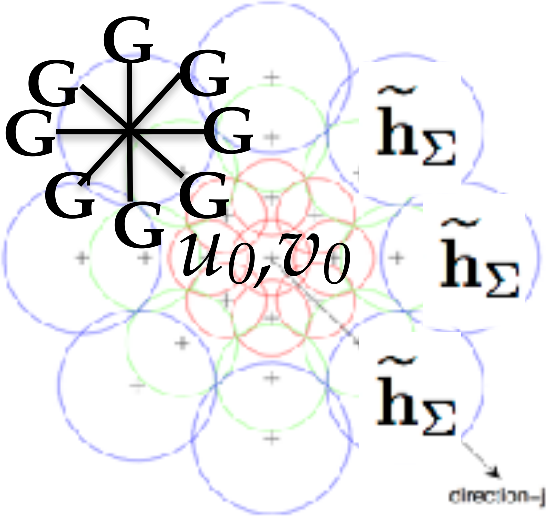
take normalized histogram at point u,v

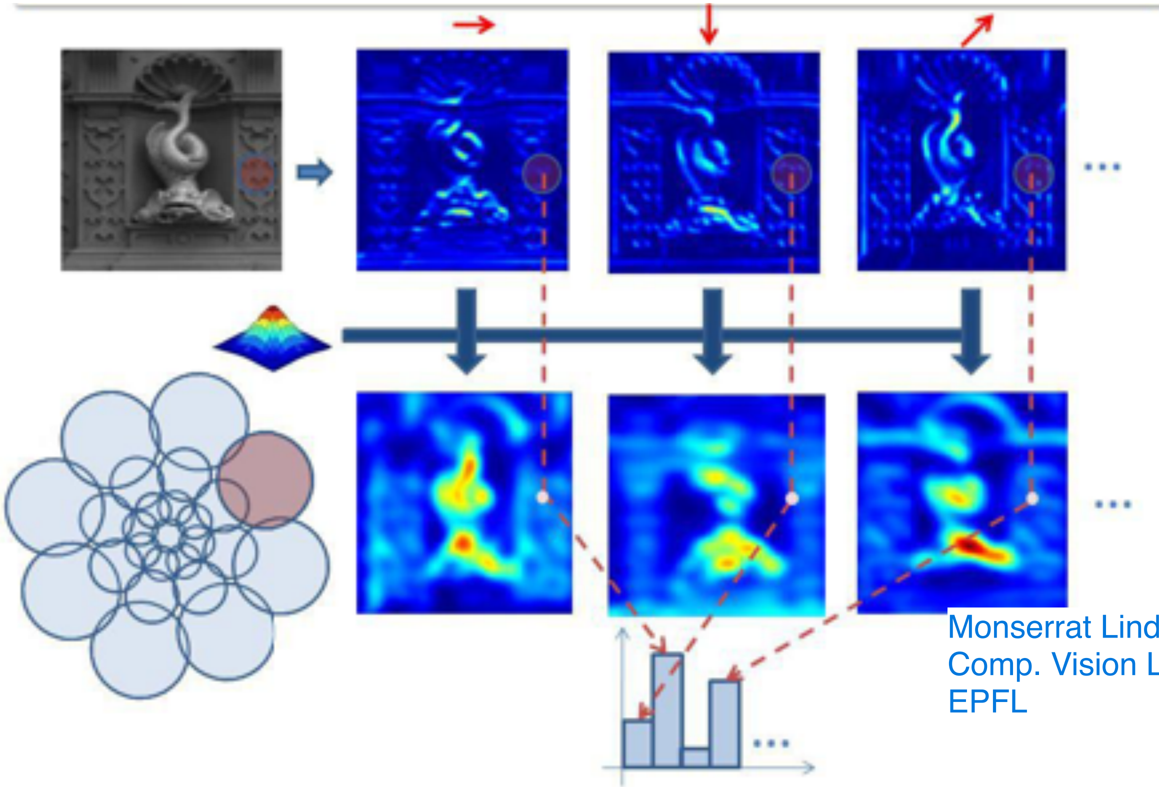
$$\tilde{\mathbf{h}}_\Sigma(u,v) = \left\| \left[\mathbf{G}_1^\Sigma(u,v), \ldots, \mathbf{G}_H^\Sigma(u,v)\right]^\top \right\|$$

$$\mathcal{D}(u_0,v_0) =$$
$$\Big[\ \tilde{\mathbf{h}}_{\Sigma_1}^\top(u_0,v_0),$$
$$\tilde{\mathbf{h}}_{\Sigma_1}^\top(\mathbf{l}_1(u_0,v_0,R_1)), \cdots, \tilde{\mathbf{h}}_{\Sigma_1}^\top(\mathbf{l}_T(u_0,v_0,R_1)),$$
$$\tilde{\mathbf{h}}_{\Sigma_2}^\top(\mathbf{l}_1(u_0,v_0,R_2)), \cdots, \tilde{\mathbf{h}}_{\Sigma_2}^\top(\mathbf{l}_T(u_0,v_0,R_2)),$$

Tola et al. "Daisy: An efficient dense descriptor applied to wide-baseline stereo." Pattern Analysis and Machine Intelligence, IEEE

Common operations: DAISY





Monserrat Lindley
Comp. Vision Lab
EPFL

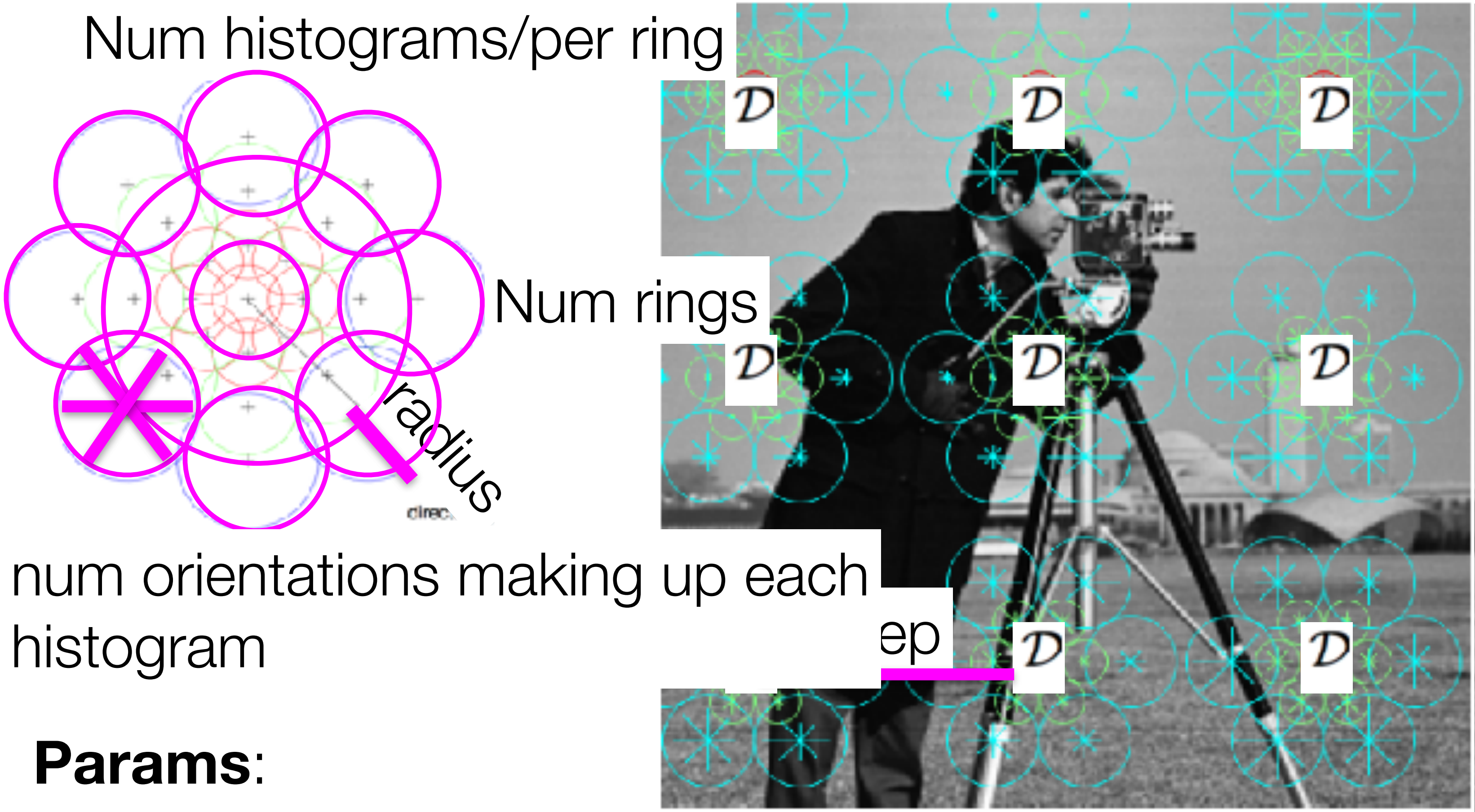
take normalized histogram at point u,v

$$\widetilde{\mathbf{h}}_\Sigma(u,v) = \left\|\left[\mathbf{G}_1^\Sigma(u,v),\ldots,\mathbf{G}_H^\Sigma(u,v)\right]^\top\right\|$$

$$\begin{aligned}\mathcal{D}(u_0,v_0) = \\ \Big[\ &\widetilde{\mathbf{h}}_{\Sigma_1}^\top(u_0,v_0),\\ &\widetilde{\mathbf{h}}_{\Sigma_1}^\top(\mathbf{l}_1(u_0,v_0,R_1)),\cdots,\widetilde{\mathbf{h}}_{\Sigma_1}^\top(\mathbf{l}_T(u_0,v_0,R_1)),\\ &\widetilde{\mathbf{h}}_{\Sigma_2}^\top(\mathbf{l}_1(u_0,v_0,R_2)),\cdots,\widetilde{\mathbf{h}}_{\Sigma_2}^\top(\mathbf{l}_T(u_0,v_0,R_2)),\end{aligned}$$

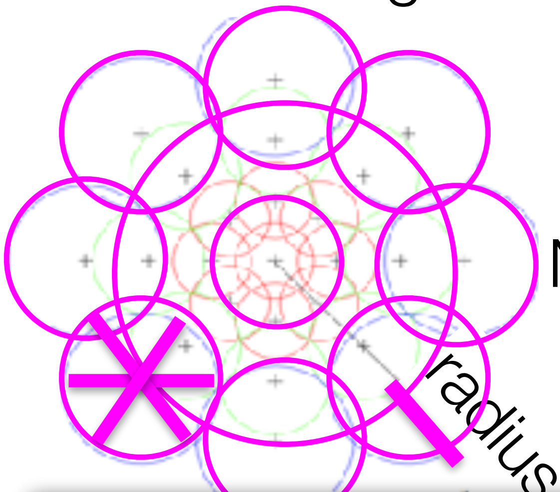
Tola et al. “Daisy: An efficient dense descriptor applied to wide-baseline stereo.” Pattern Analysis and Machine Intelligence, IEEE

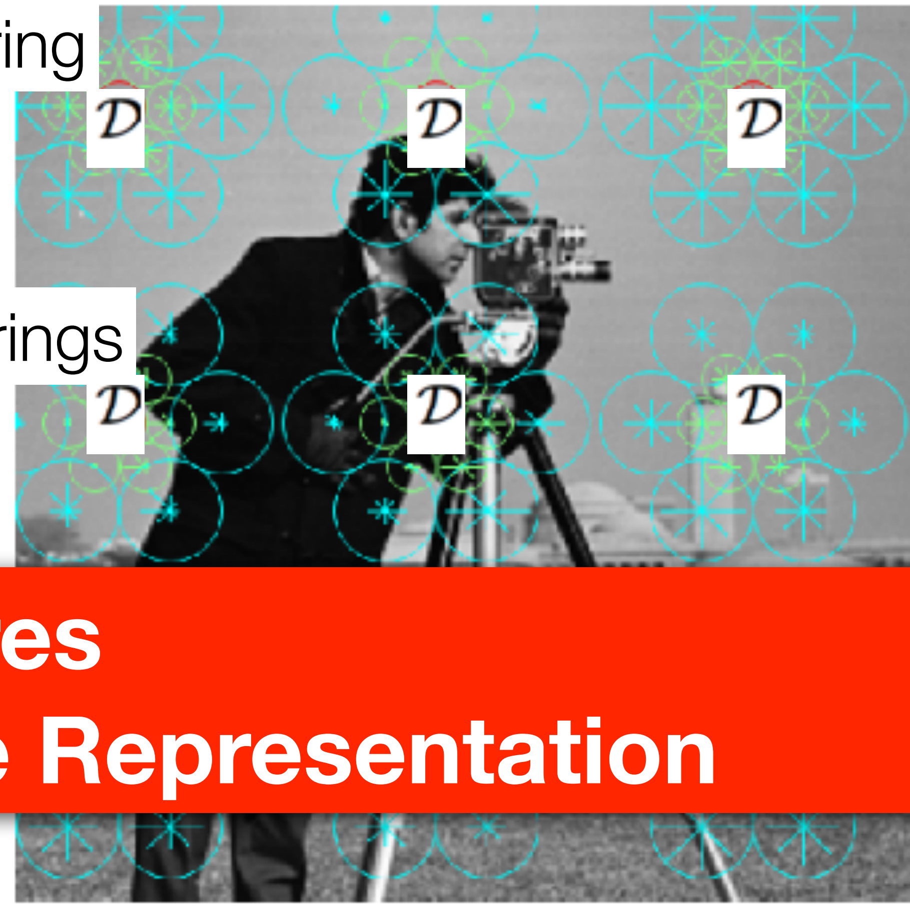
Common operations: DAISY



Params:
step, radius, num rings,
num histograms per ring,
orientations per histogram

Common operations: DAISY





Bag of Features
Image Representation

Params:
step, radius, num rings,
num histograms per ring,
orientations per histogram

More Image Processing

Demo

Gradients

DAISY

(if time)Gabor Filter Banks

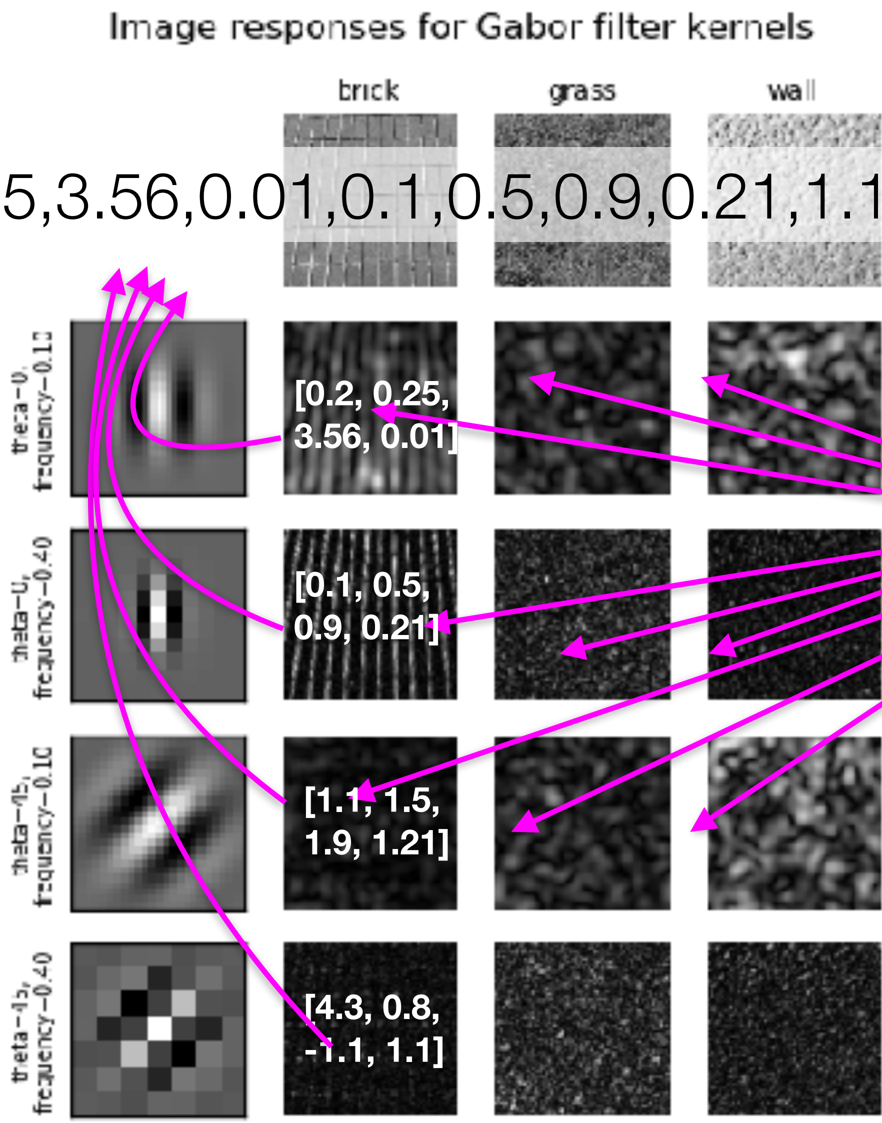
Other Tutorials:

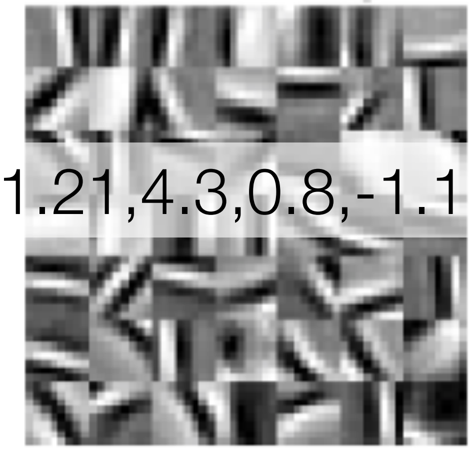
http://scikit-image.org/docs/dev/auto_examples/

Common operations: Gabor filter Banks (if time)

- common used for texture classification

[0.2,0.25,3.56,0.01,0.1,0.5,0.9,0.21,1.1,1.5,1.9,1.21,4.3,0.8,-1.1,1.1]



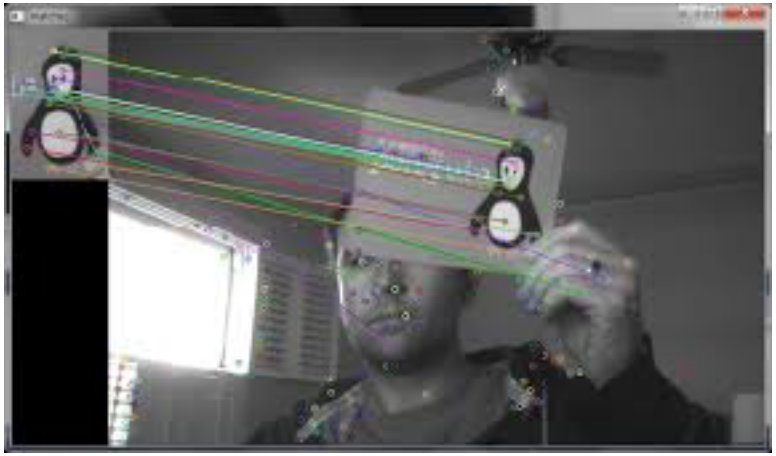


mean
std
skew
kurtosis

Concatenate statistics of different filters into one feature vector

Matching versus Bag of Features

- Not a difference of vectors, but a percentage of matching points

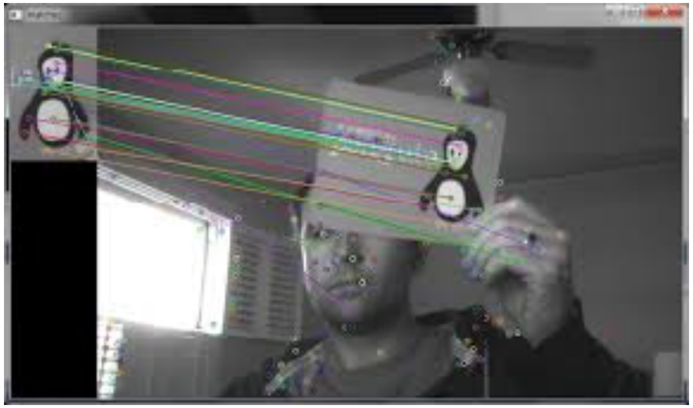


- SURF, ORB, SIFT, DAISY

Feature Matching

Matching test image to source dataset

1. Choose src image from dataset
2. Take keypoints of src image
3. Take keypoints of test image
4. For each kp in src:
    1. Match with closest kp in test
    2. How to define match?
5. Count number of matches between images
6. Determine if src and test are similar based on number of matches
7. Repeat for new src image in dataset
8. Once all images measured, choose best match as the target for the test image



Scikit-image Implementation

match_descriptors

`skimage.feature.match_descriptors(descriptors1, descriptors2, metric=None, p=2, max_distance=inf, cross_check=True, max_ratio=1.0)` [source]

Brute-force matching of descriptors.

For each descriptor in the first set this matcher finds the closest descriptor in the second set (and vice-versa in the case of enabled cross-checking).

Town Hall for Lab 2, Images

- **Quiz is live**: Image Processing!
- **Next Time**: Logistic Regression

Supplemental Slides

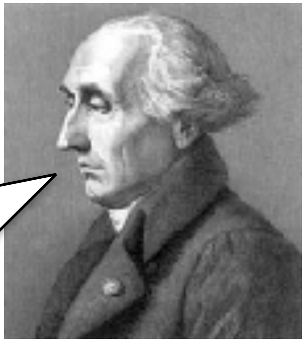
- Peruse these at your own leisure!
- These slides might assist you as additional visual aides
- **Slides courtesy of Tan, Steinbach, Kumar**
    - **Introduction to Data Mining**

Dimensionality Reduction: LDA

- PCA tell us variance explained by the data in different directions, but it ignores class labels
- Is there a way to find "components" that will help with **discriminate** between the classes?

$$\arg\max_{comp.} \frac{\sum \text{differences between classes}}{\sum \text{variance within classes}}$$

- called Fisher's discriminant
- …but we need to solve this using using *Lagrange multipliers* and gradient-based optimization
- which we haven't covered yet



I invented Lagrange multipliers… and …*nothing impresses me…*

Dimensionality Reduction: LDA versus QDA

$$\underset{comp.}{\arg\max} \frac{\sum \text{differences between classes}}{\sum \text{variance within classes}}$$

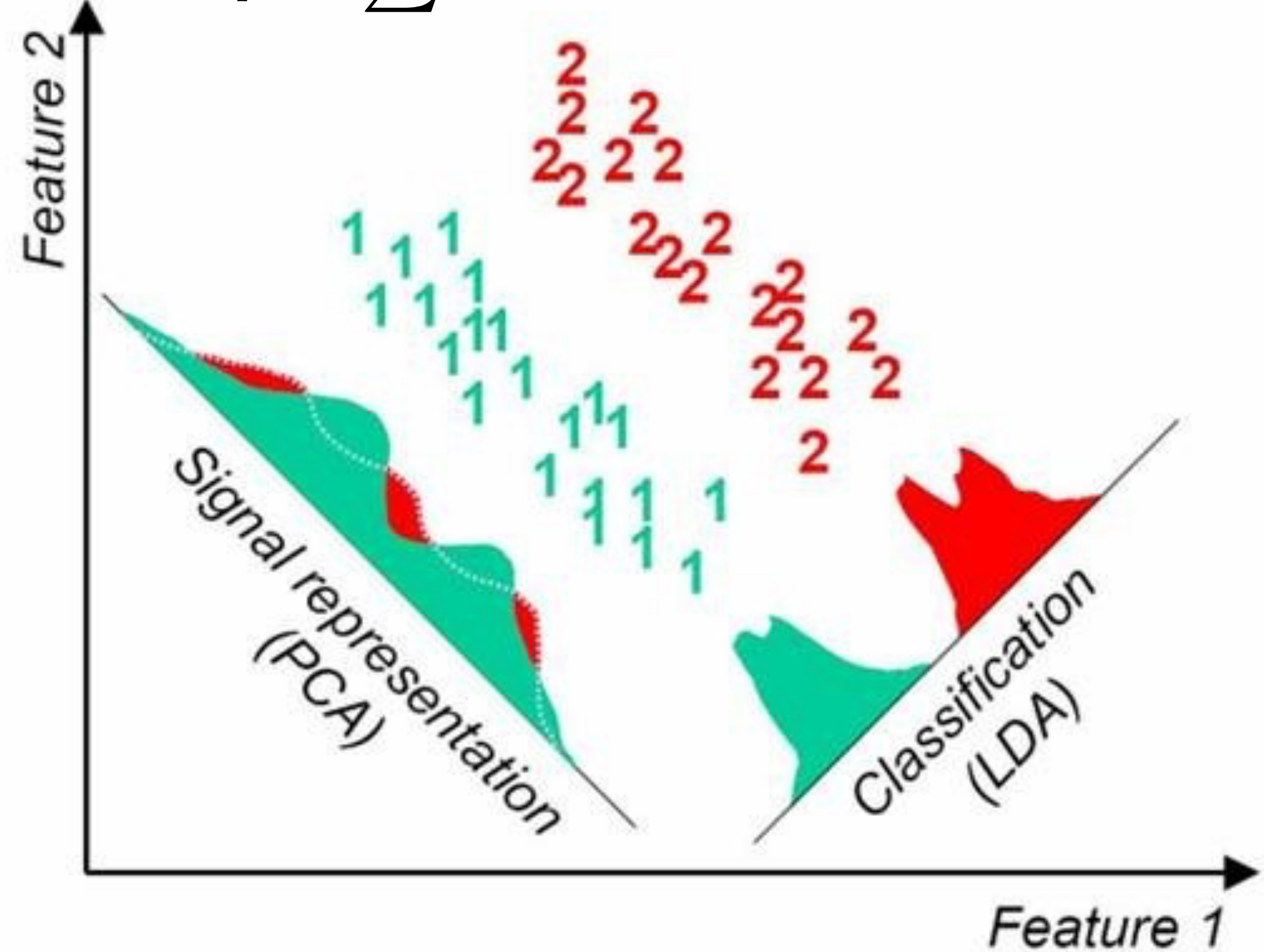
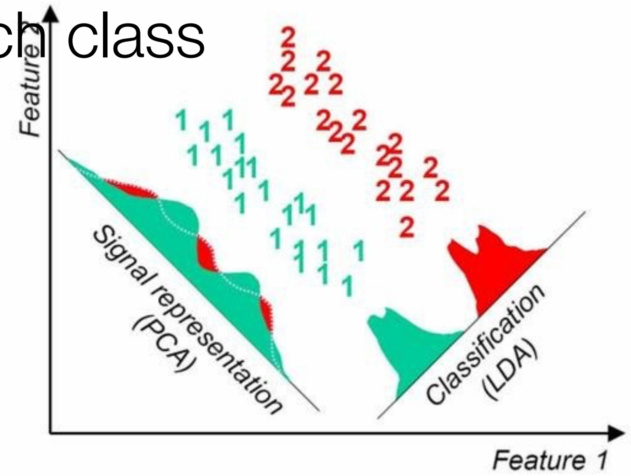


image source: 不想飞翔，不是因为没有翅膀，而是失去了梦想

Dimensionality Reduction: LDA versus QDA

$$\underset{comp.}{\arg\max} \frac{\sum \text{differences between classes}}{\sum \text{variance within classes}}$$

- "*differences between classes*" is calculated by trying to separate the **mean value** of each **feature** in each **class**
- Linear discriminant analysis:
  - assume the covariance in each class is the same
- Quadrature discriminant analysis:
  - estimate the covariance for each class



Self Test ML2b.2

LDA only allows as many components as there are unique classes in a dataset.

A. True
B. False

- Need more help with the PCA algorithm (and python)?
  - check out Sebastian Raschka's notebooks:

http://nbviewer.ipython.org/github/rasbt/pattern_classification/blob/master/dimensionality_reduction/projection/principal_component_analysis.ipynb