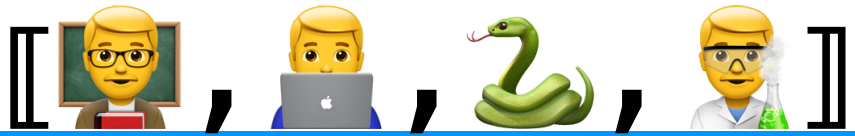
Lecture Notes for

Machine Learning in Python



Professor Eric Larson

Visualization and Dimensionality Reduction

Class Logistics and Agenda

- Welcome back!!!!
- Dimensionality Reduction
  - PCA
  - Sampling
  - Kernel Methods

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

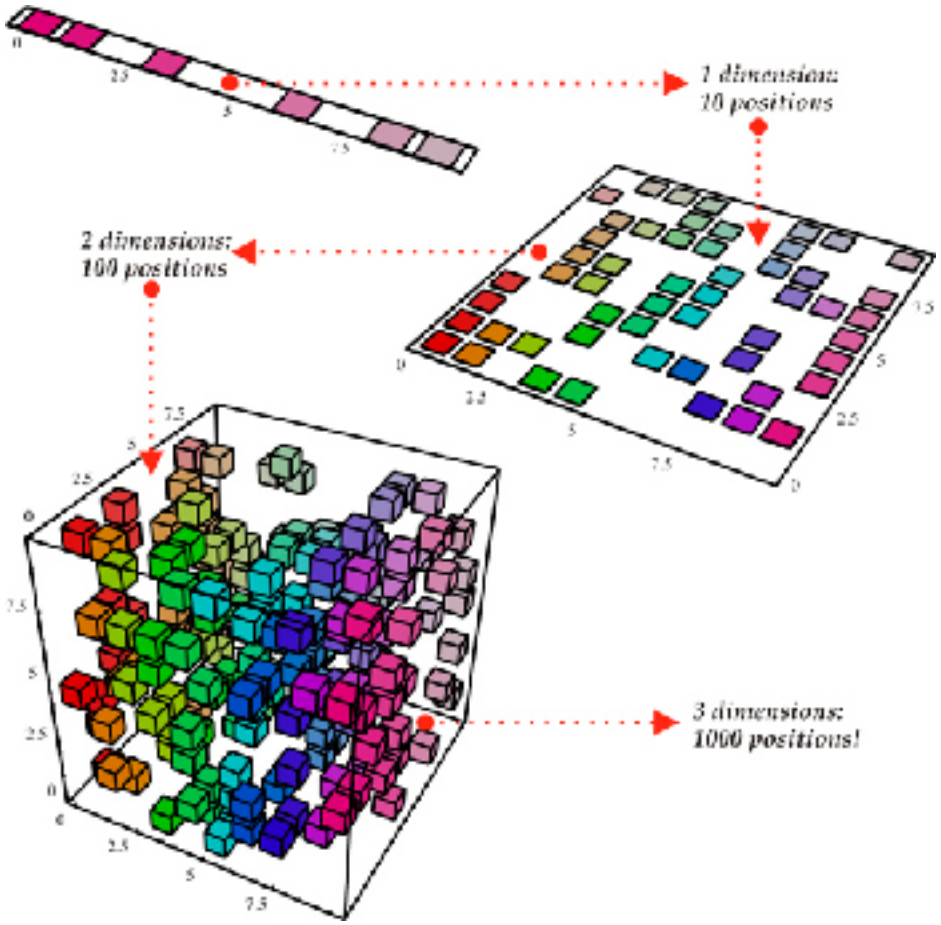


image source: http://www.iro.umontreal.ca/~bengioy/yoshua_en/research_files/CurseDimensionality.jpg

Dimensionality Reduction

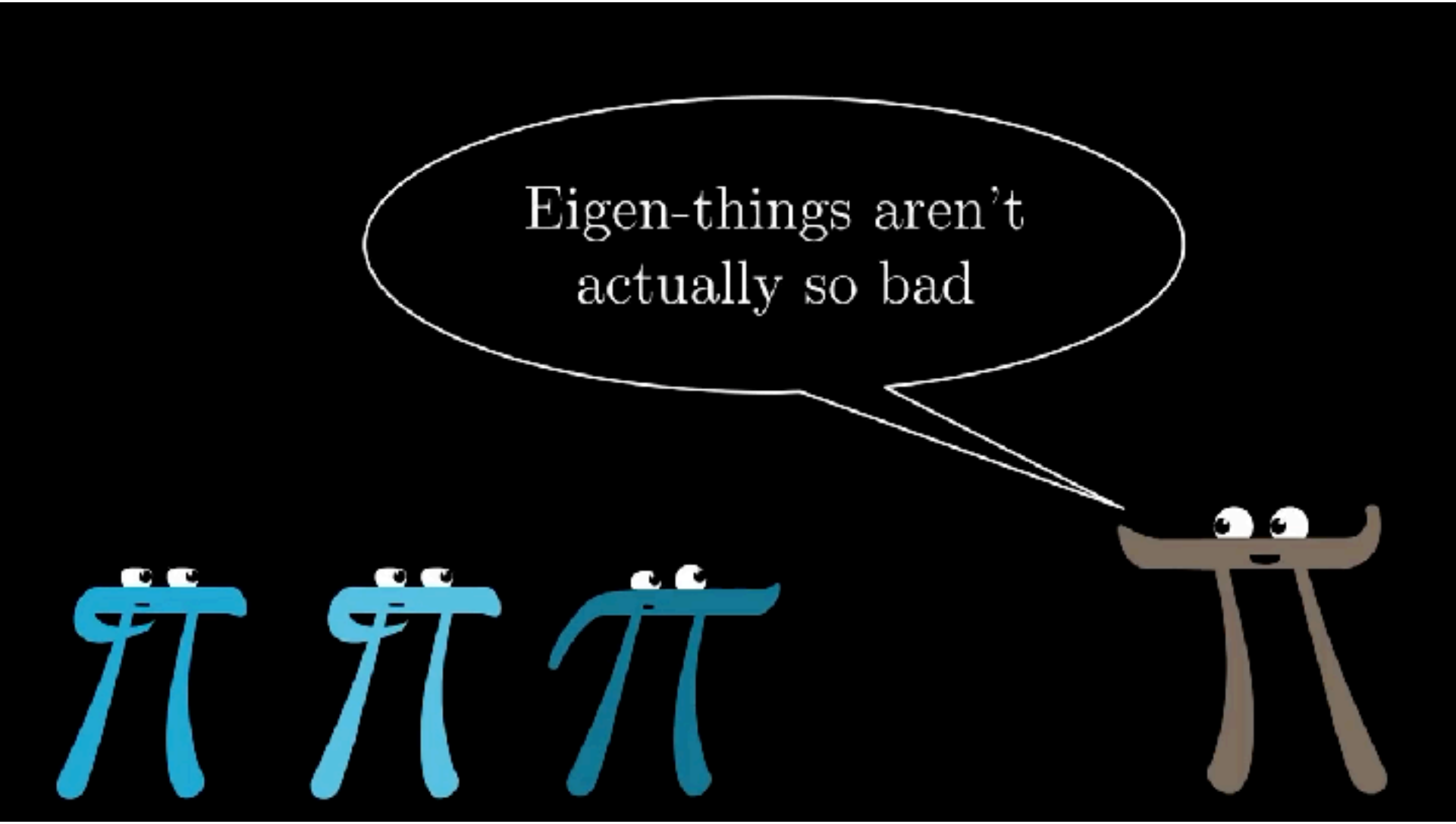
- Purpose:
  - Avoid curse of dimensionality
  - Select subsets of independent features
  - Reduce amount of time and memory required by data mining algorithms
  - Allow data to be more easily visualized
  - May help to eliminate irrelevant features or reduce noise

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

I invented PCA…
and *Social Darwinism*

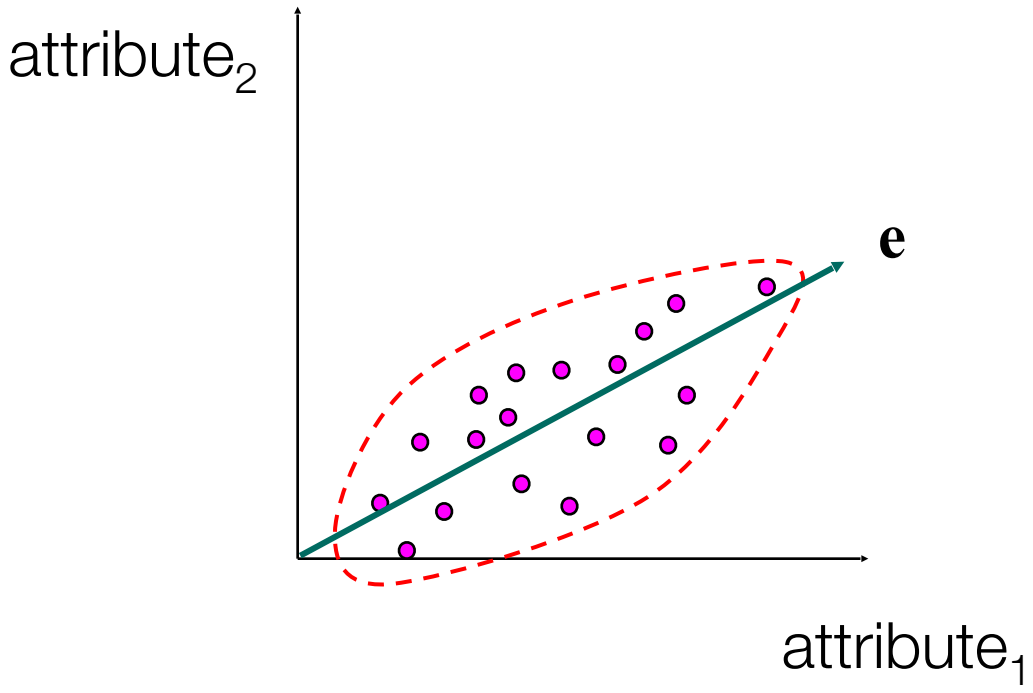
Aside: Eigen Vectors are your friend!

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



Dimensionality Reduction: PCA

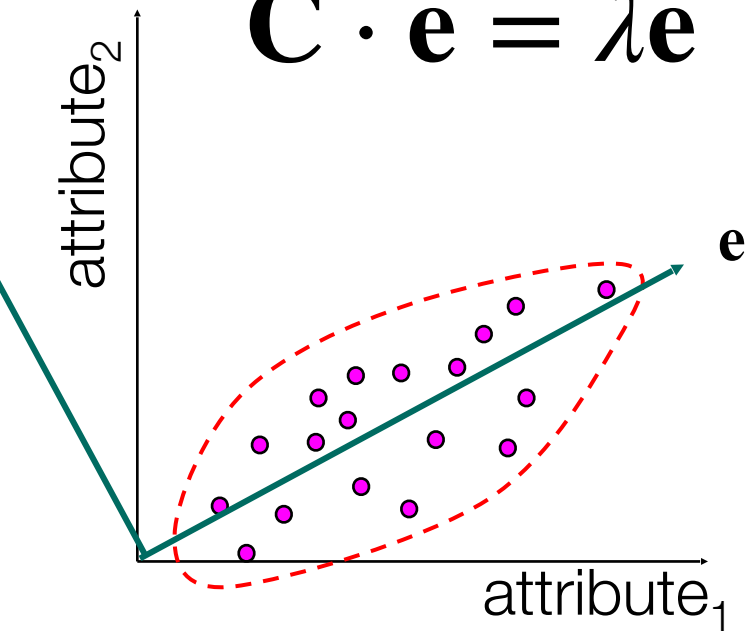
- Goal is to find a projection that captures the largest amount of variation in data



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

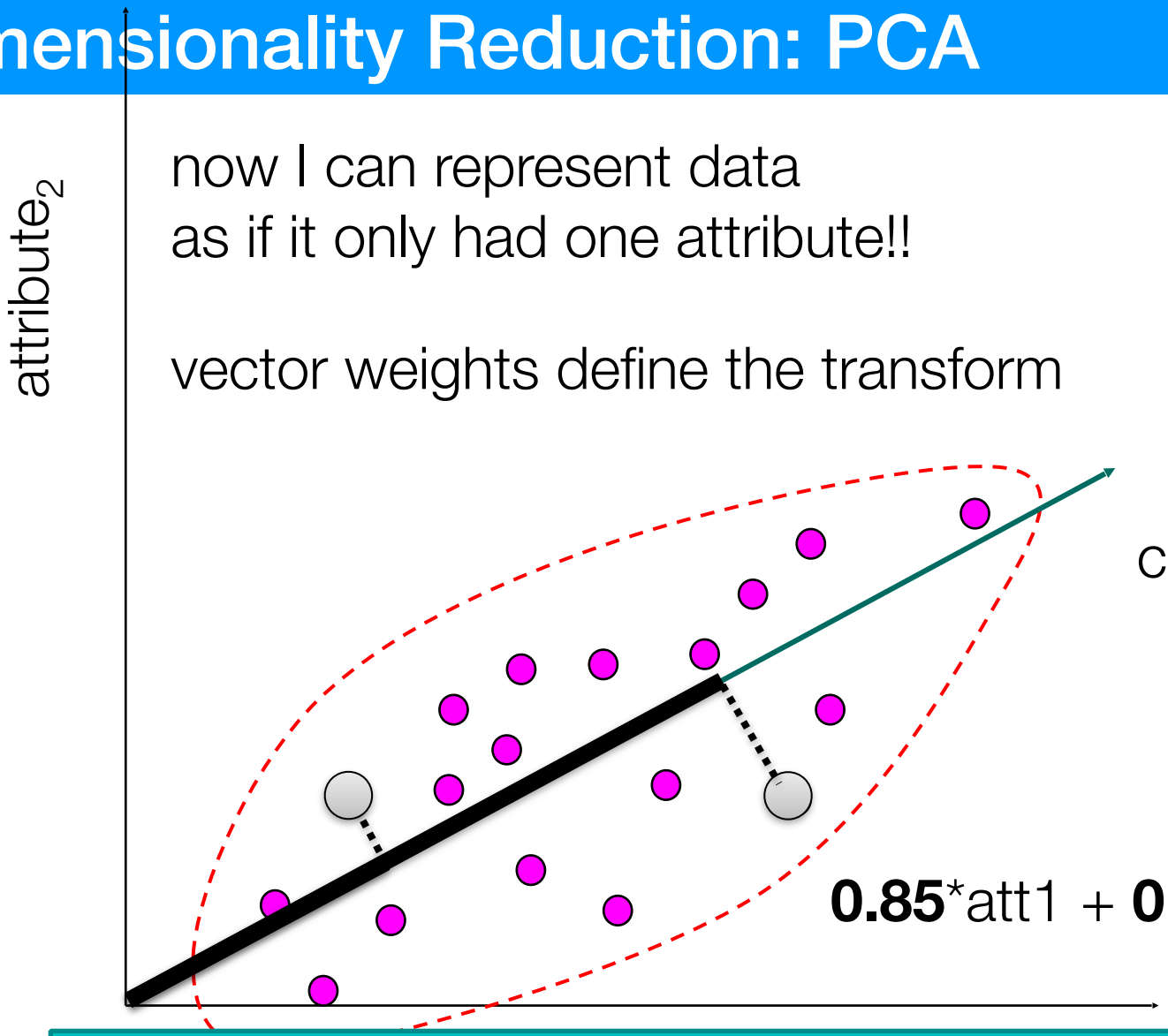
37.1	-6.7
-6.7	43.9

	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)**

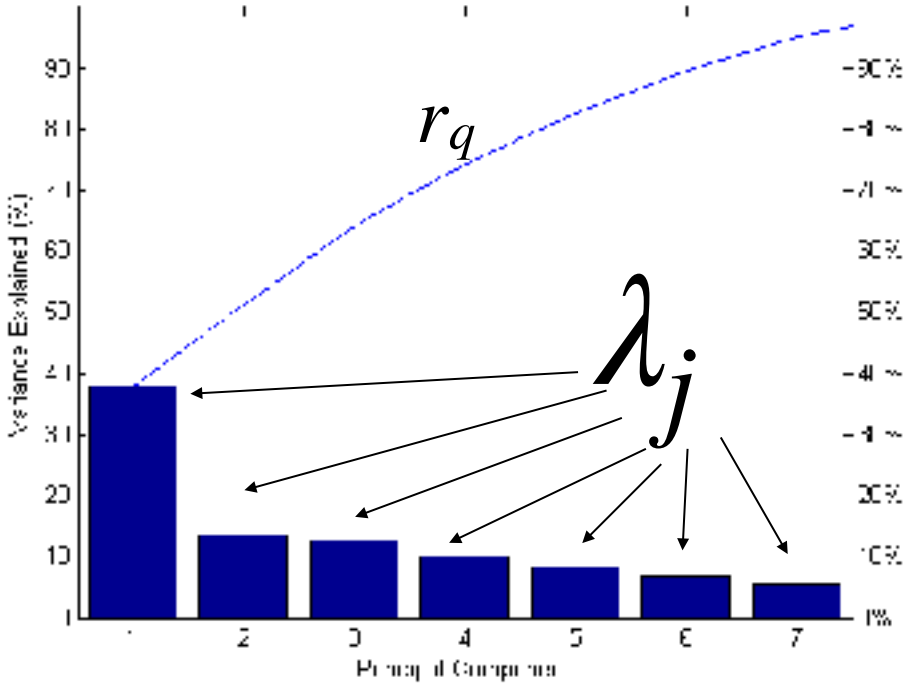
Explained Variance

- 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

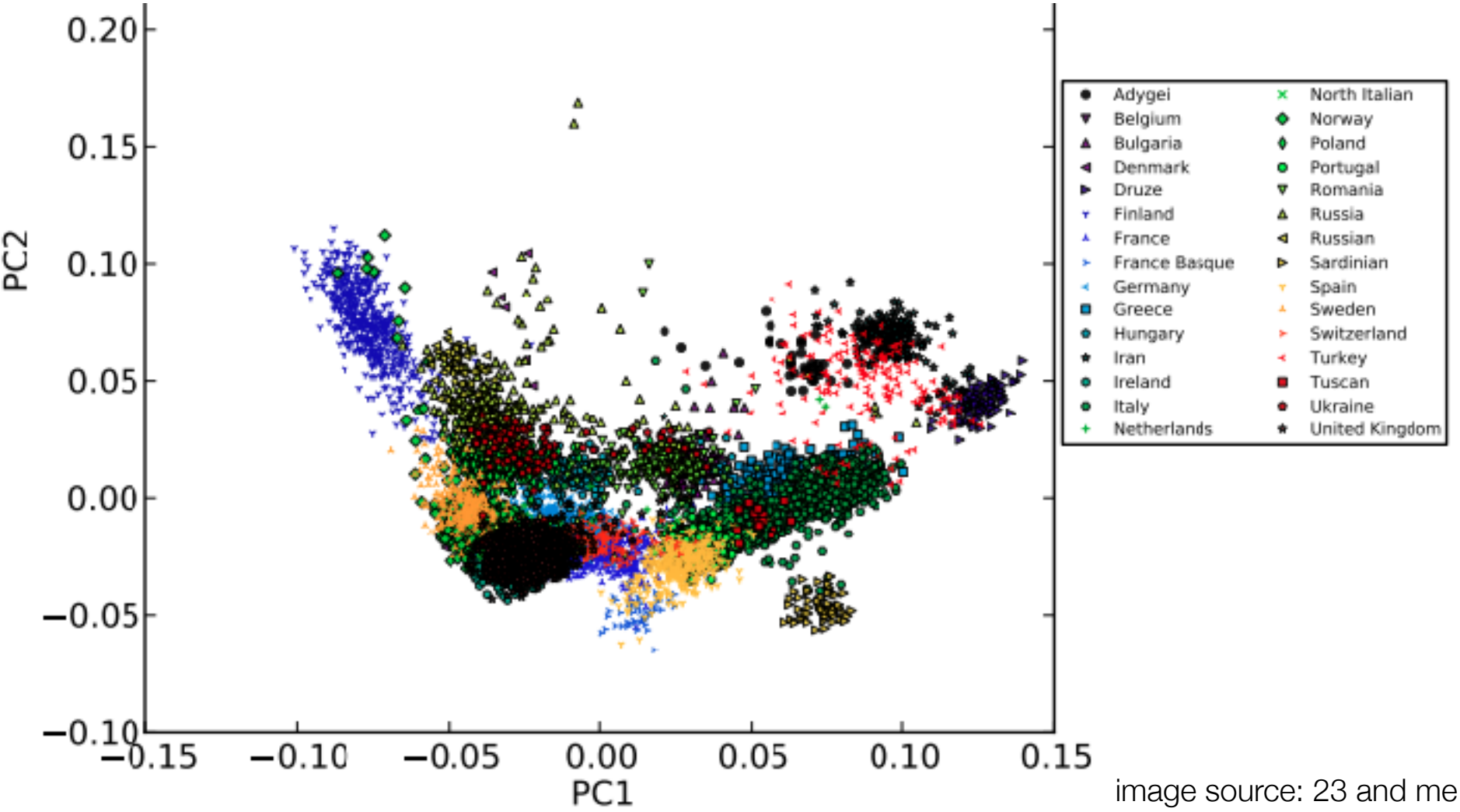


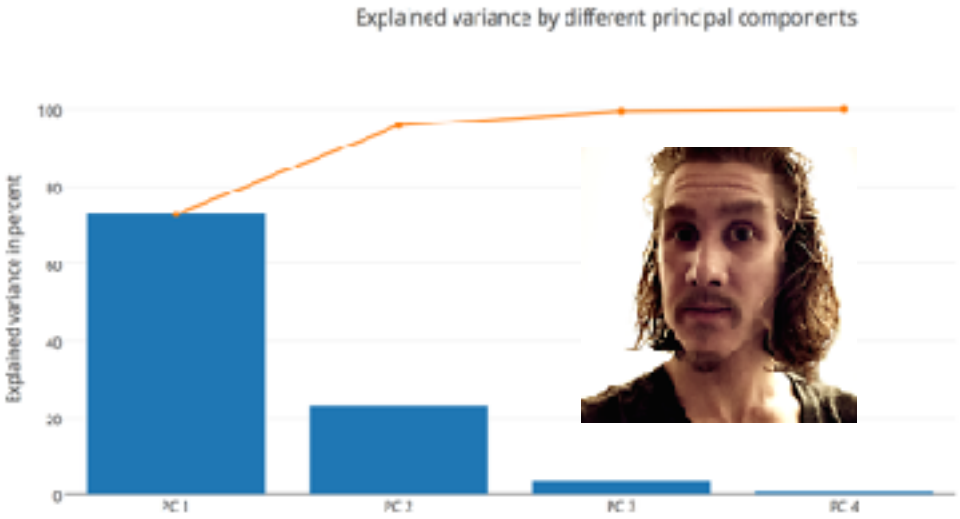
image source: 23 and me

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

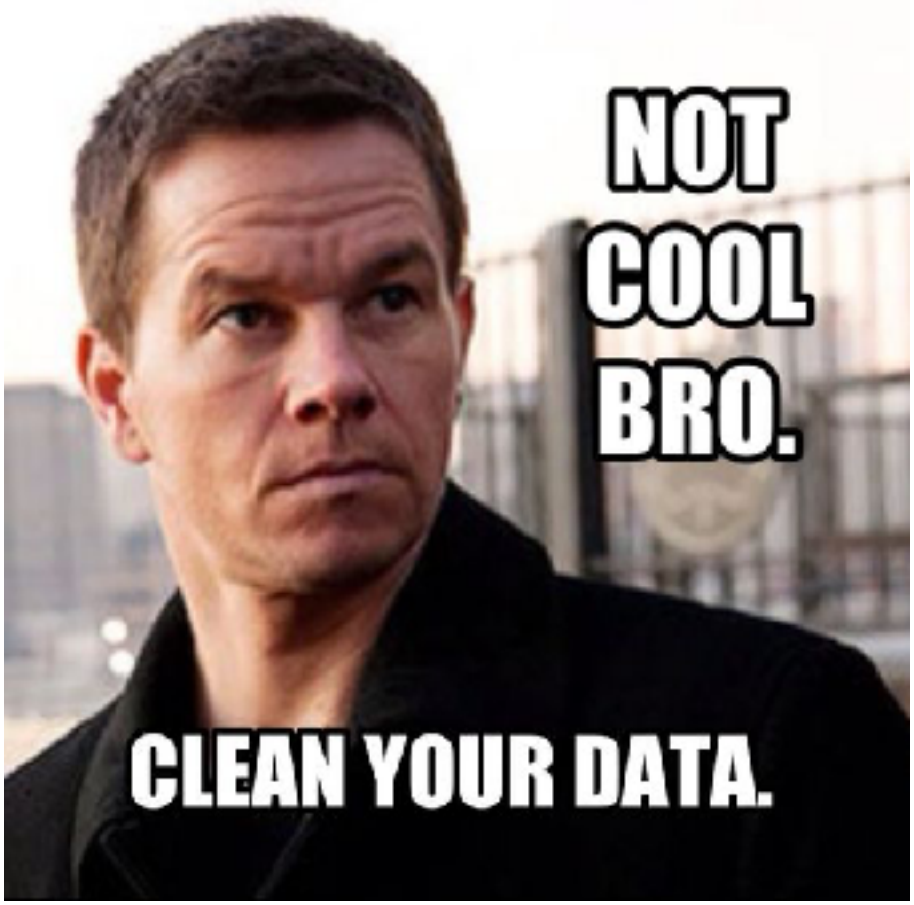
- **Problem**: PCA on all that data can take a while to compute
  - What if the number of instances is gigantic?
  - What if the number of dimensions is gigantic?

- What if we partially construct the covariance matrix with a lower rank matrix?
  - By **randomly sampling** from the dataset and projecting, we can get something **representative** of **covariance matrix**, but with **lower rank**
  - Gives a matrix with typically good enough precision of actual eigenvectors. One example:

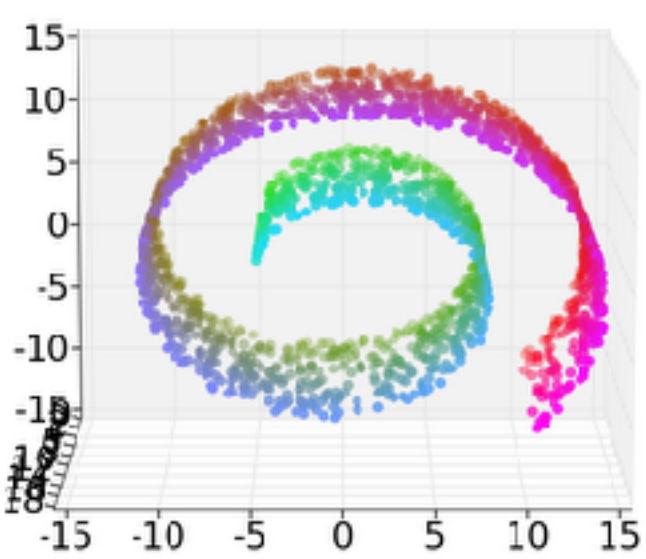
$$\|\boldsymbol{A} - \boldsymbol{Q}\boldsymbol{Q}^*\boldsymbol{A}\| \leq \left[1 + 11\sqrt{k+p} \cdot \sqrt{\min\{m,n\}}\right] \sigma_{k+1}$$

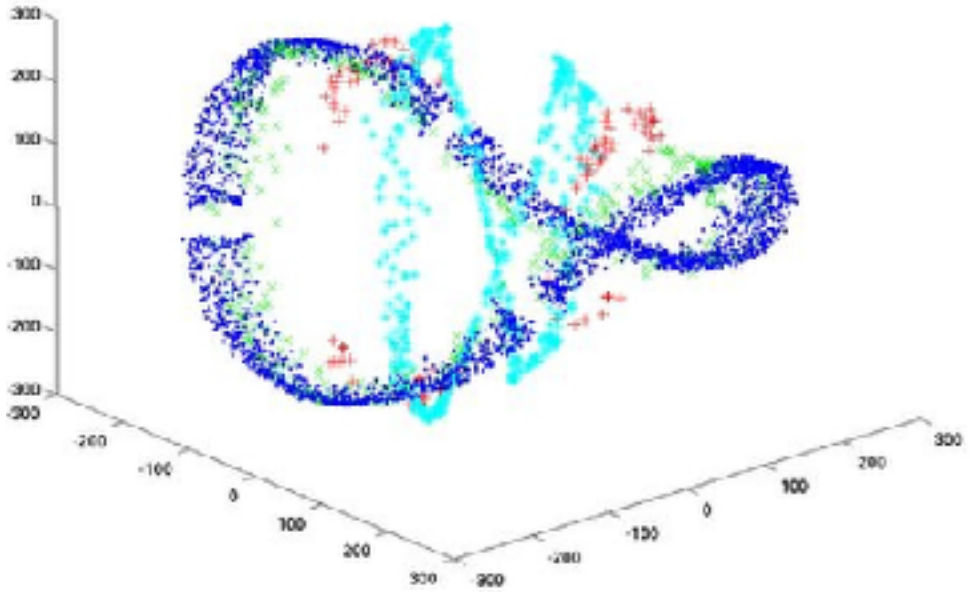
Halko, et al., (2009) Finding structure with randomness: Stochastic algorithms for constructing approximate matrix decompositions. https://arxiv.org/pdf/0909.4061.pdf

Non-linear Dimensionality Reduction



Dimensionality Reduction: non-linear

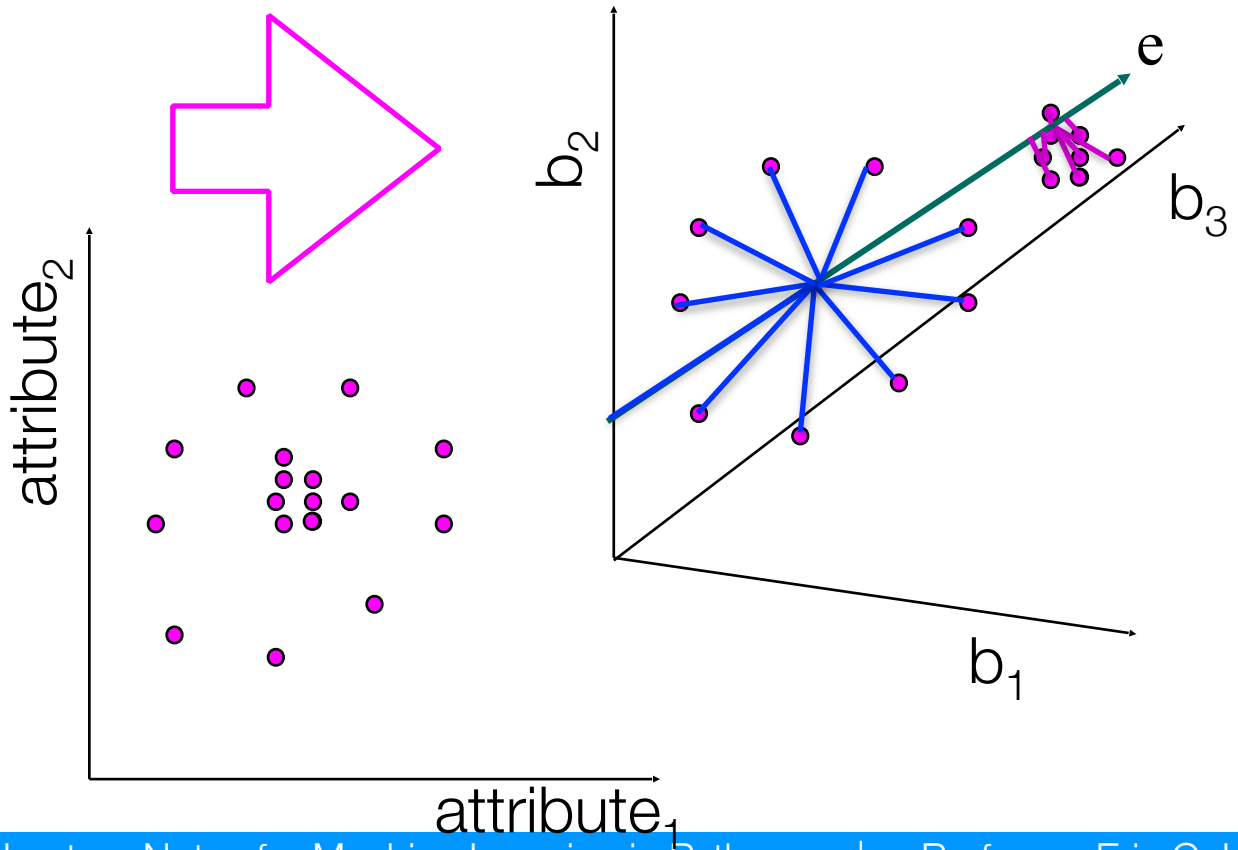




- Sometimes a **linear transform** is not enough
- A powerful non-linear transform has seen a resurgence in past decade: **kernel PCA**

Kernel PCA

- Estimate Covariance in nonlinear **transformed space**
- **Eigenvectors** appear **nonlinear** when transformed back
- Projecting onto these can be understood as principle components from a "higher dimensional" space



$\Phi(A1)\cdot\Phi(A1)$	$\Phi(A2)\cdot\Phi(A1)$
$\Phi(A2)\cdot\Phi(A1)$	$\Phi(A2)\cdot\Phi(A2)$

	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*

Kernel PCA

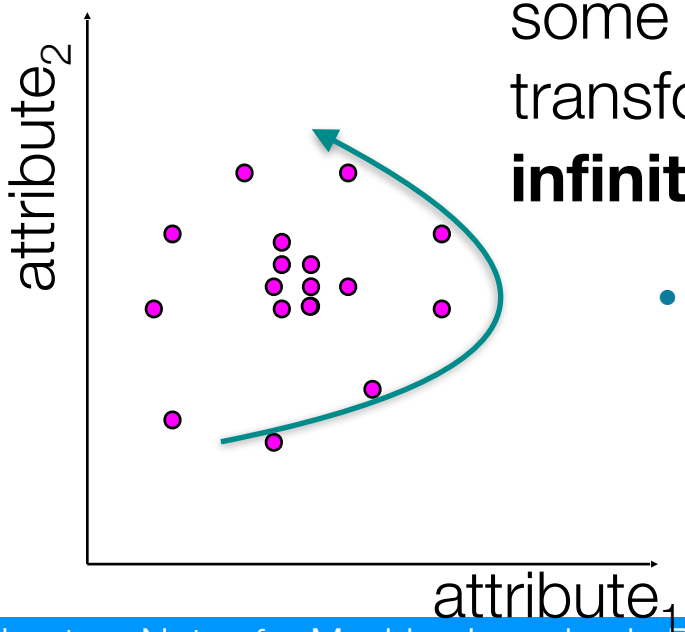
- **Key insight**: don't need to know the actual principle components, just the projections

$\kappa(A1,A1)$	$\kappa(A2,A1)$
$\kappa(A1,A2)$	$\kappa(A2,A2)$

$\phi(A1)\cdot\phi(A1)$	$\phi(A2)\cdot\phi(A1)$
$\phi(A2)\cdot\phi(A1)$	$\phi(A2)\cdot\phi(A2)$

kernel: defines what the dot product is in nonlinear space

some kernels, κ, have transformations, ϕ, with **infinite dimensions**!!



- **Never need** eigen vectors of **full** covariance matrix, just how much the vectors co-vary in higher space!

	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

Kernel PCA

- **Key insight**: don't need to know the actual principle components, just the projections

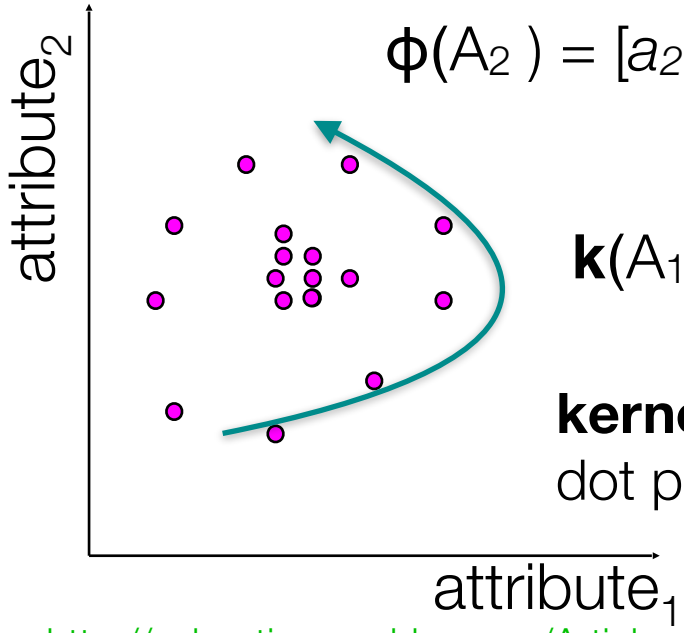
$\Phi(A1)\cdot\Phi(A1)$	$\Phi(A2)\cdot\Phi(A1)$
$\Phi(A2)\cdot\Phi(A1)$	$\Phi(A2)\cdot\Phi(A2)$

$$A_1 = [a_{11}\ a_{12}]^T \qquad A_2 = [a_{21}\ a_{22}]^T$$

$$\Phi(A_1) = [a_{11} \quad a_{12} \quad a_{11}*a_{12} \quad a_{11}^2 \quad a_{11}*a_{12}^3 \cdots]^T$$

$$\Phi(A_2) = [a_{21} \quad a_{22} \quad a_{21}*a_{22} \quad a_{21}^2 \quad a_{21}*a_{22}^3 \cdots]^T$$

	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



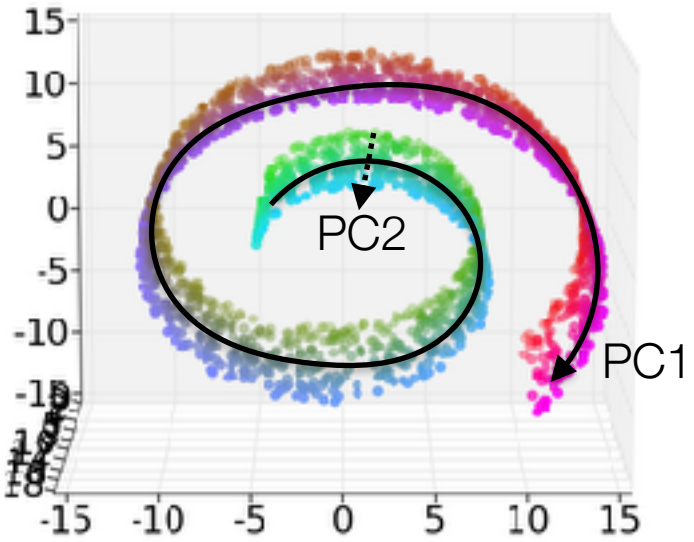
$$\Phi(A_1)\Phi(A_2) = \mathbf{k}(A_1, A_2)$$

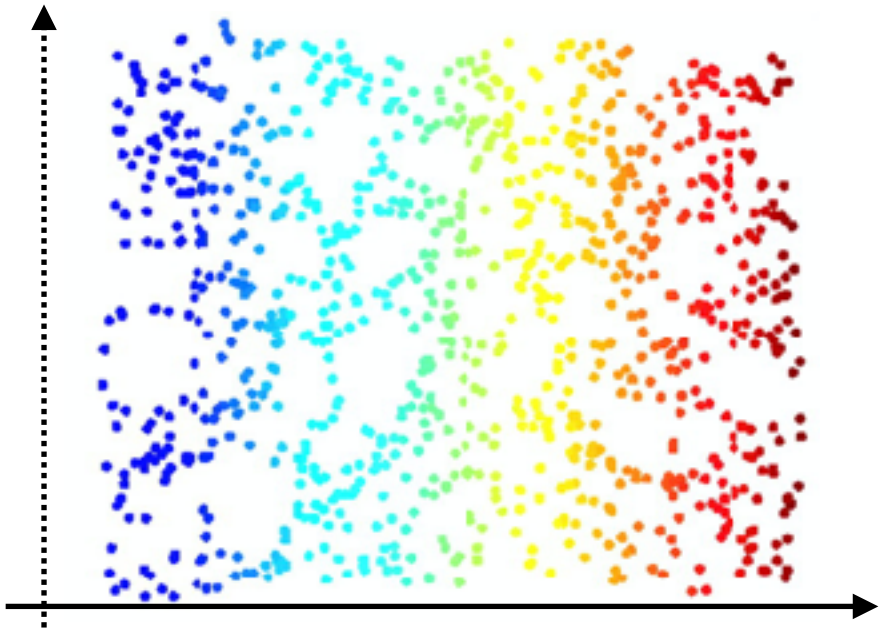
$$\mathbf{k}(A_1, A_2) = \exp(-\gamma \| A_1 - A_2 \|^2)$$

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

http://sebastianraschka.com/Articles/2014_kernel_pca.html#kernel-functions-and-the-kernel-trick

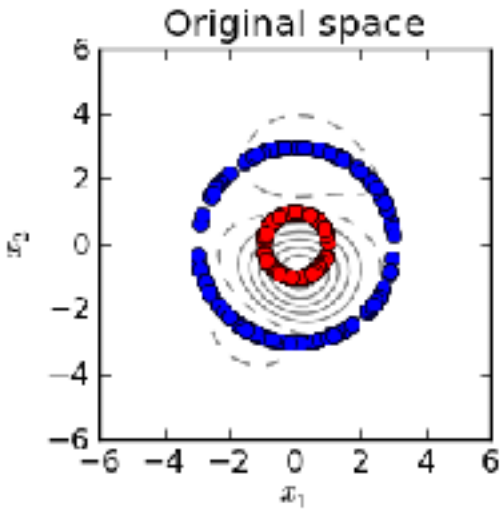
Kernel PCA as Manifold Learning

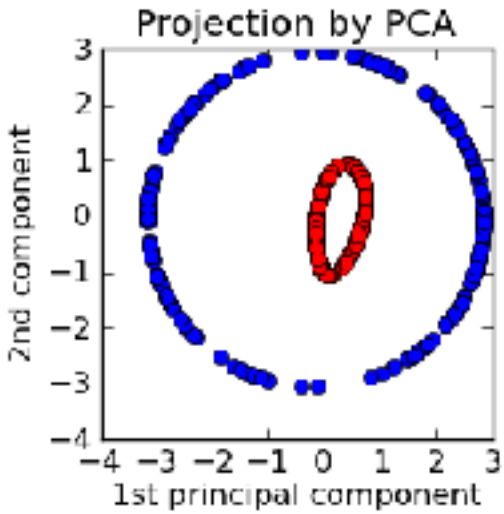


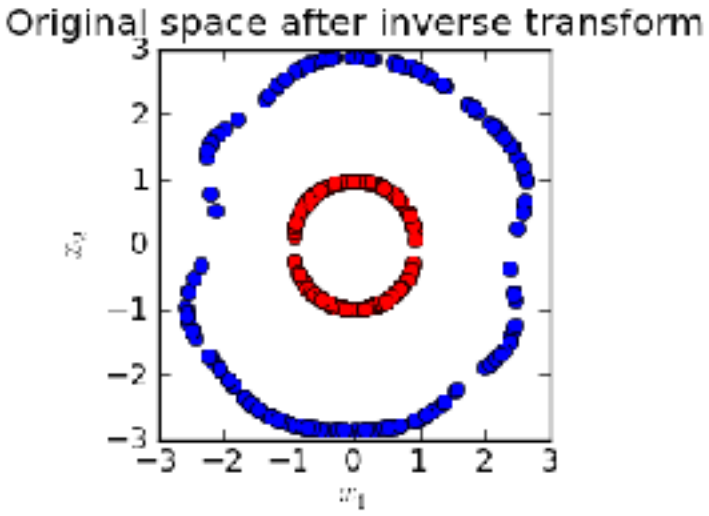


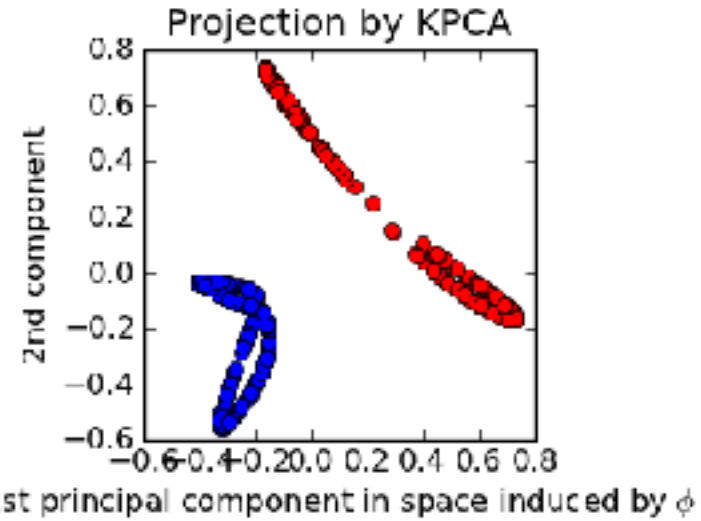
Kernel PCA

images: sklearn documentation









For Next Lecture

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

Lecture Notes for

Machine Learning in Python

Professor Eric Larson

Dimensionality Reduction and Images

Class Logistics and Agenda

- **Logistics**:
  - Lab due soon!
  - Turn in one per team (HTML), please use team names as specified on 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

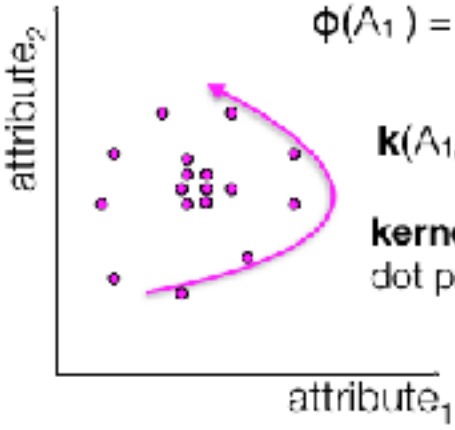
zero mean

$$A_1 = [a_1\ a_2]^T$$

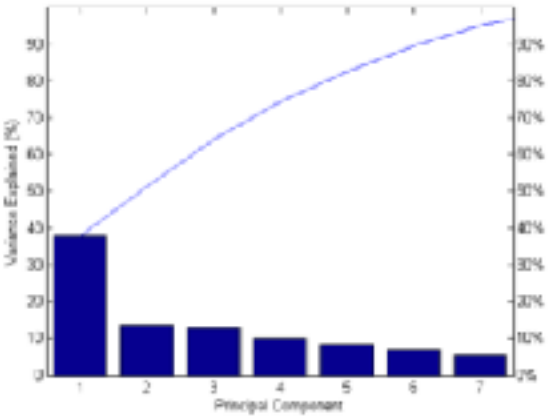
$$\Phi(A_1) = [a_1 \quad a_2 \quad a_1 a_2 \quad a_1^2 \quad a_1 a_2^3 \cdots]^T$$

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

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



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



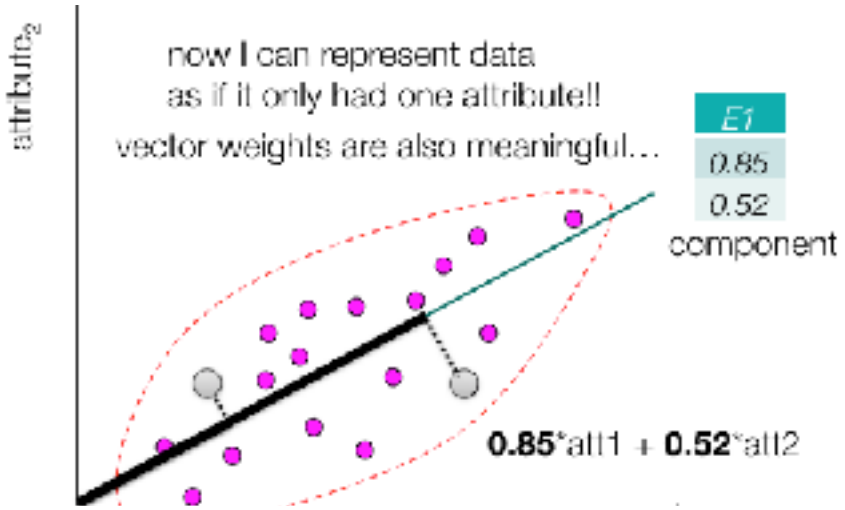
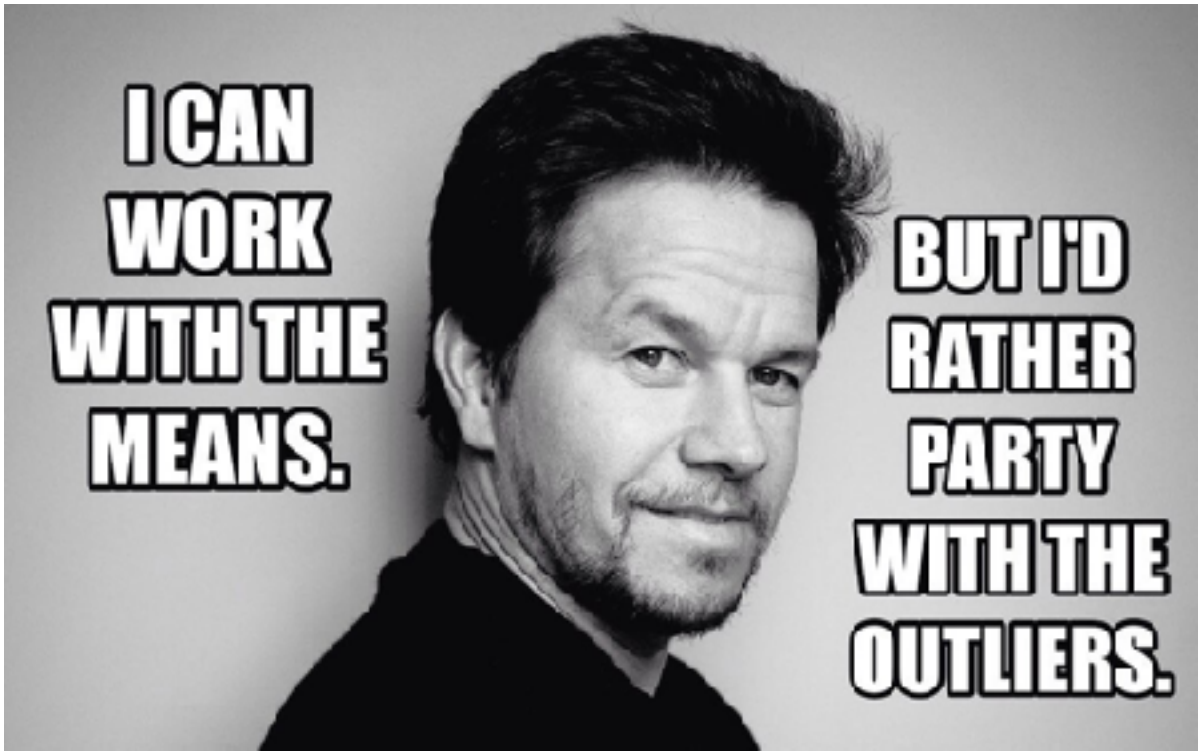
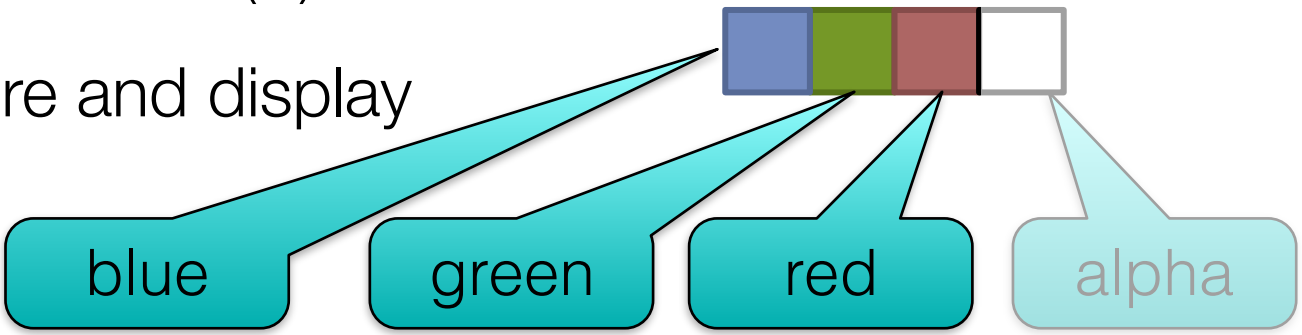


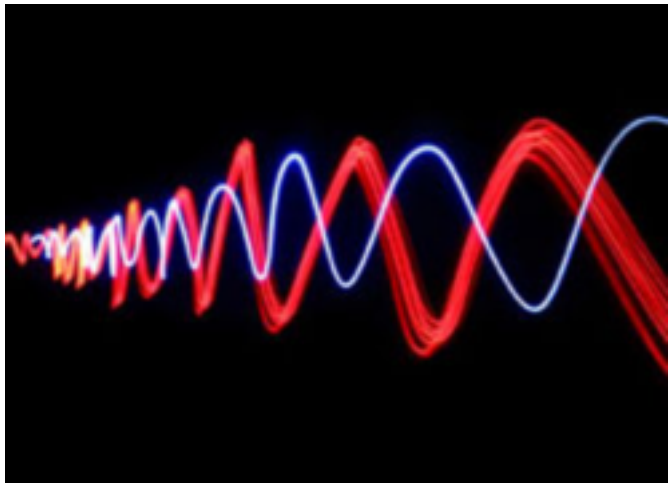
Image Processing and Representation

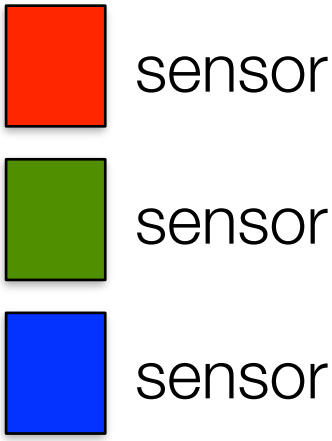


Images as data

- 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







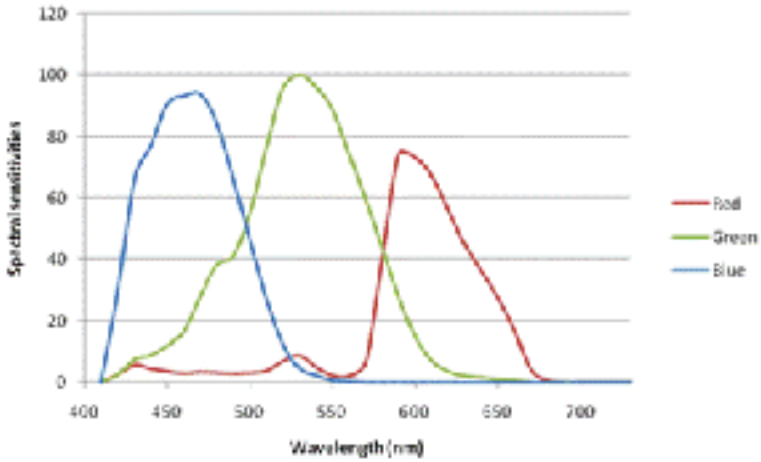


Image Representation

- need a compact representation

- **grayscale**

  0.3**R*+0.59**G*+0.11**B*,

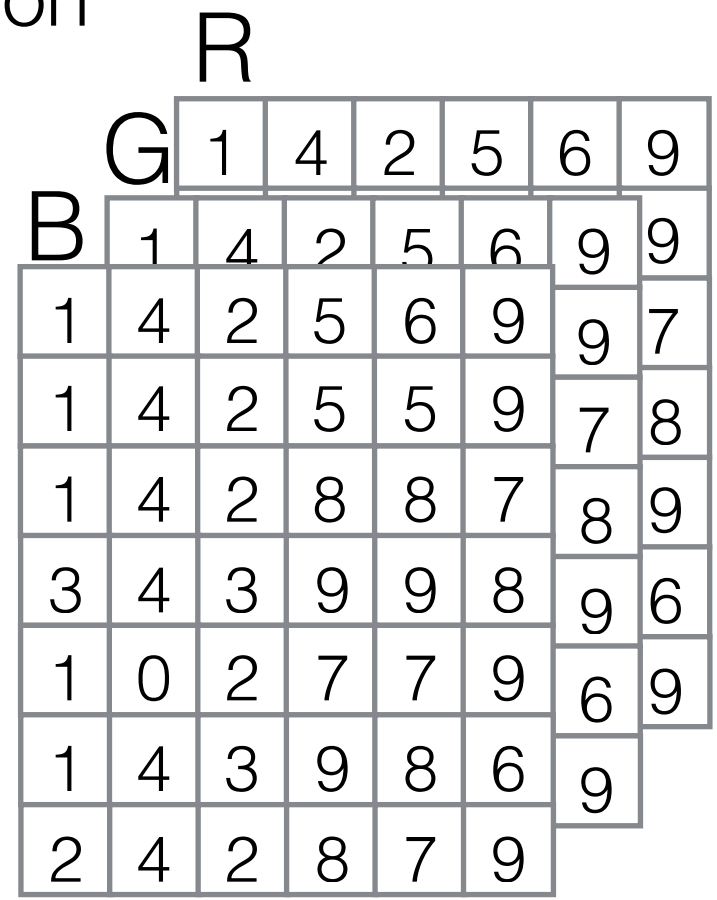
  "luminance"

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

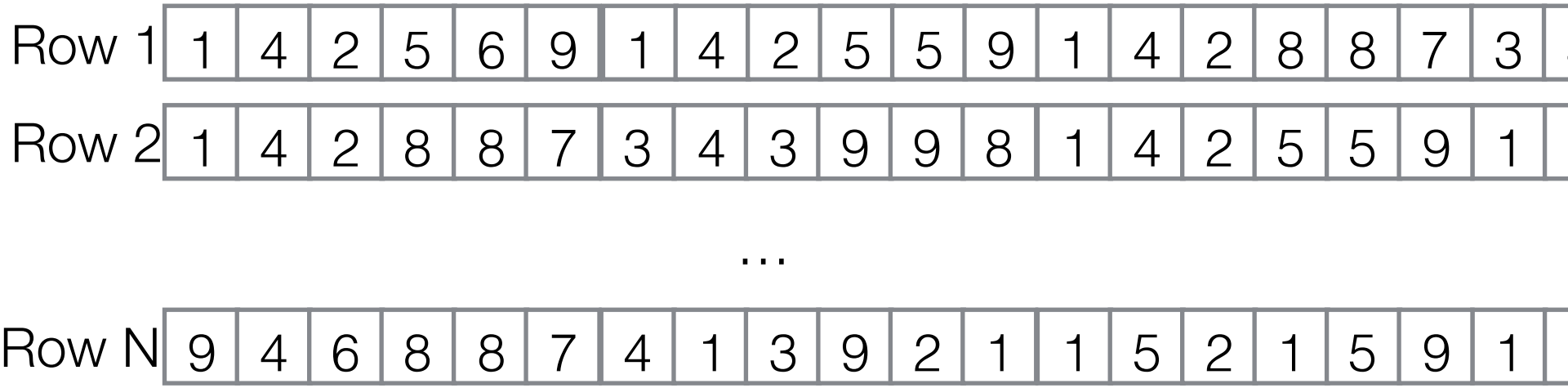
1	4	2	5	6	9
1	4	2	5	5	9
1	4	2	8	8	7
3	4	3	9	9	8
1	0	2	7	7	9
1	4	3	9	8	6
2	4	2	8	7	9

Image Representation, Features

Problem: need to represent image as table data

- need a compact representation

Solution: row concatenation (also, vectorizing)



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

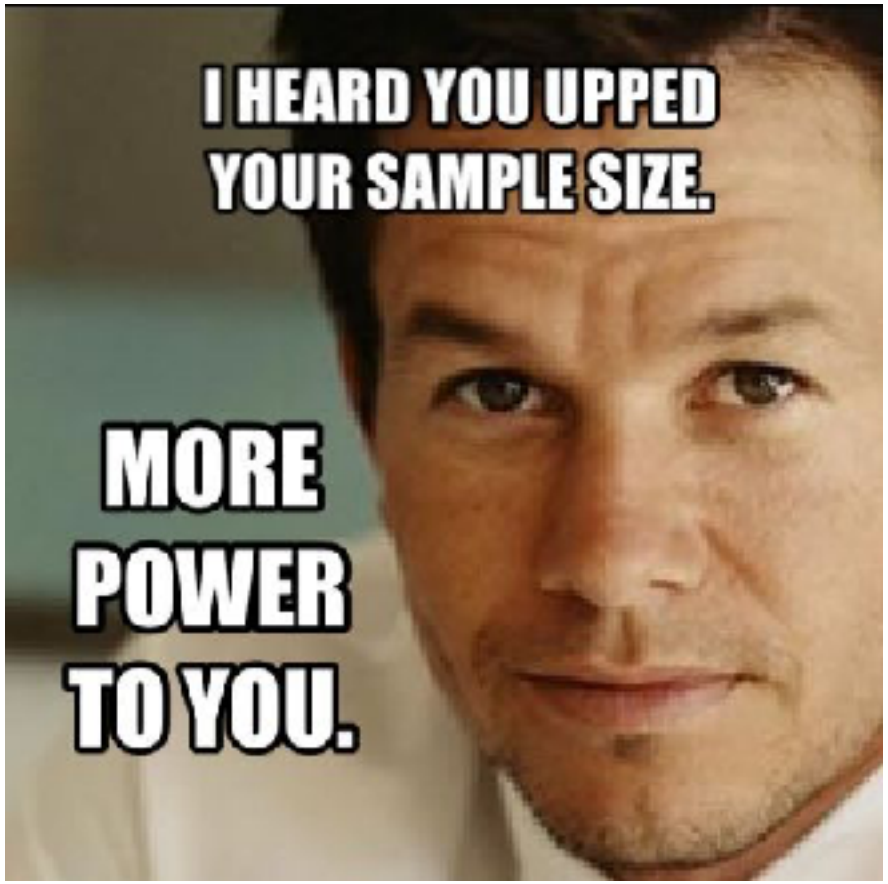
Dimension Reduction with Images

Demo

Images Representation
Randomized PCA
Kernel PCA

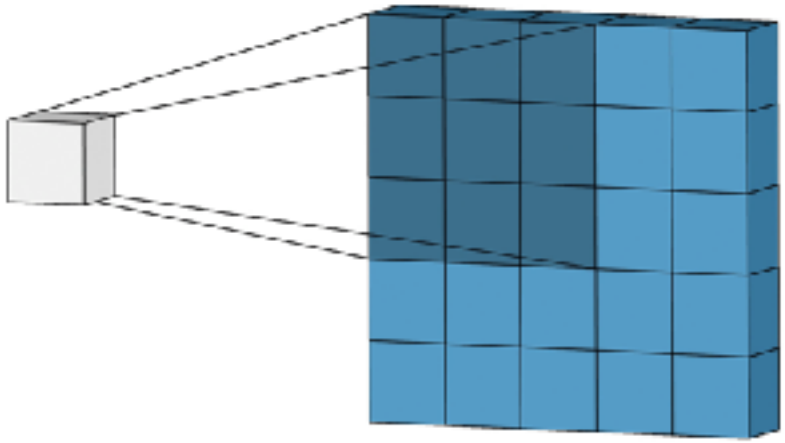
`04.Dimension Reduction and Images.ipynb`

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

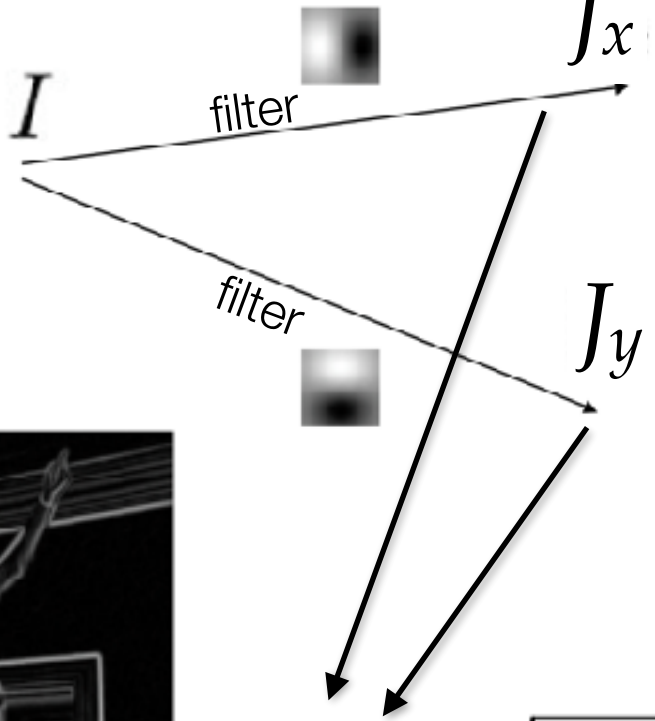
$*$

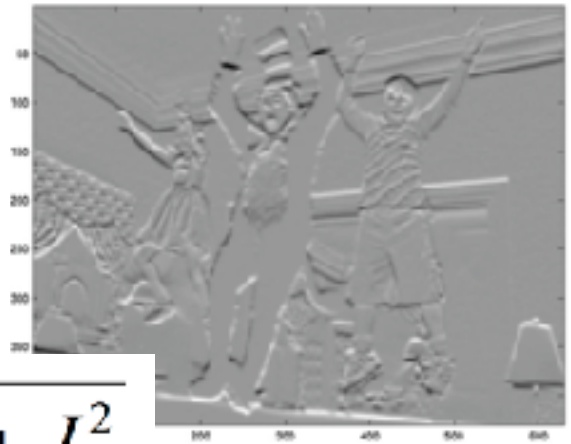
1	0	-1
2	0	-2
1	0	-1

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

Common operations

- the gradient (2D derivative)



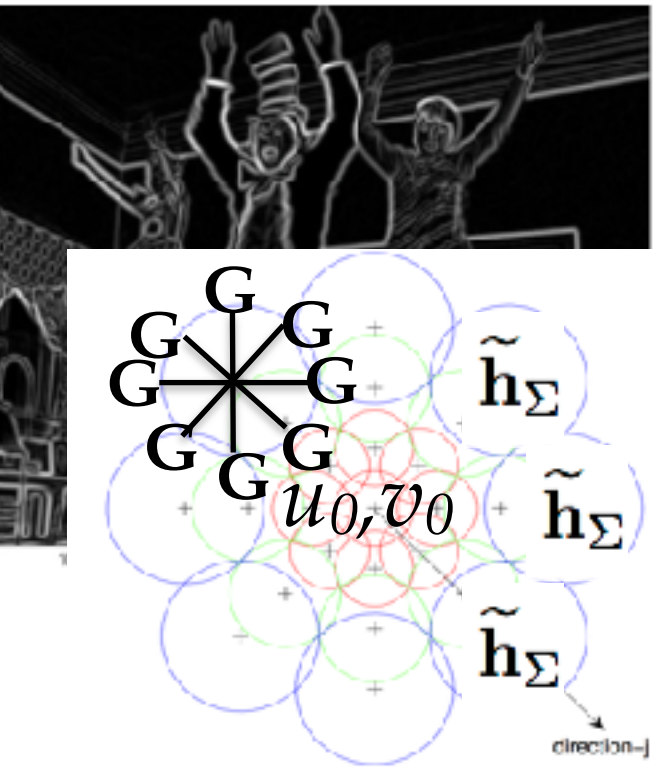


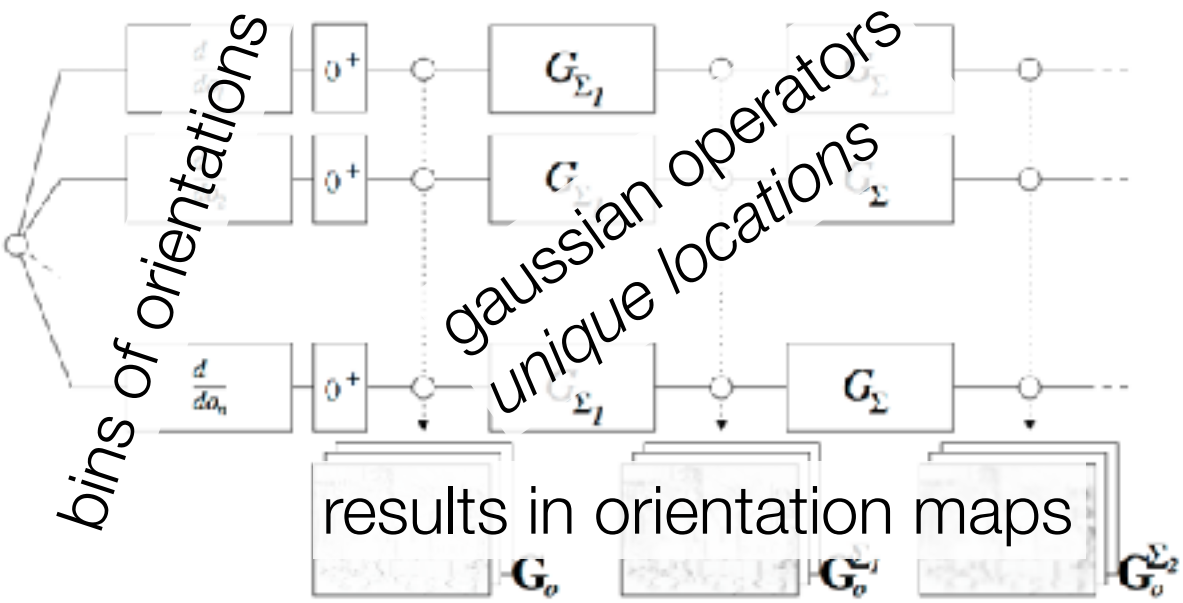
$$\|\nabla J\| = \sqrt{J_x^2 + J_y^2}$$

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

images: Jianbo Shi, Upenn

Common operations: DAISY





take normalized histogram at point u,v

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

$$\mathcal{D}(u_0, v_0) =$$

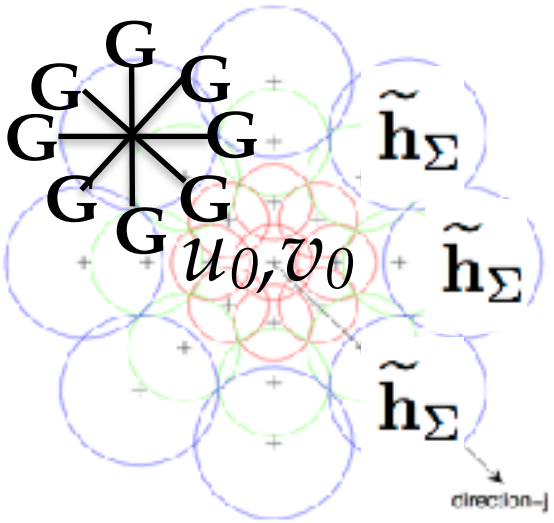
$$\Big[\tilde{\mathbf{h}}_{\Sigma_1}^\top(u_0, v_0),$$

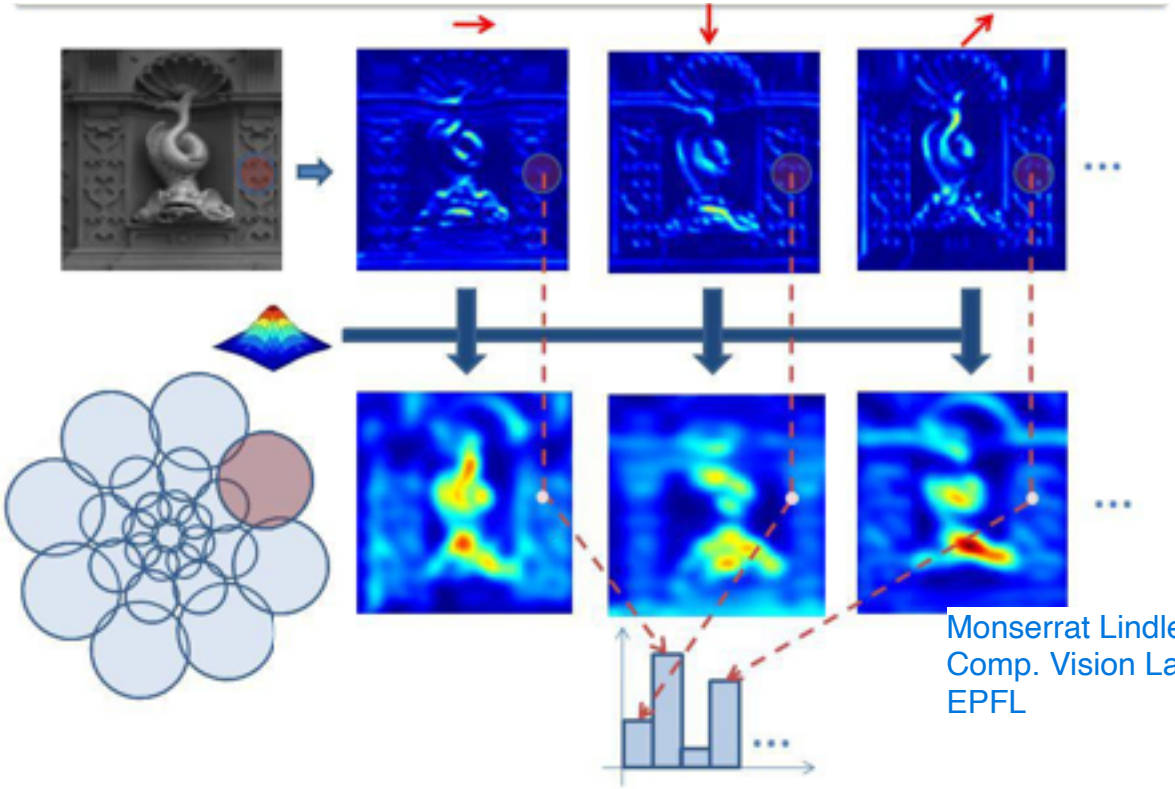
$$\tilde{\mathbf{h}}_{\Sigma_1}^\top(\mathbf{l}_1(u_0, v_0, R_1)), \cdots, \tilde{\mathbf{h}}_{\Sigma_1}^\top(\mathbf{l}_T(u_0, v_0, R_1)),$$

$$\tilde{\mathbf{h}}_{\Sigma_2}^\top(\mathbf{l}_1(u_0, v_0, R_2)), \cdots, \tilde{\mathbf{h}}_{\Sigma_2}^\top(\mathbf{l}_T(u_0, v_0, R_2)),$$

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

Common operations: DAISY





Monserrat Lindley
Comp. Vision Lab
EPFL

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

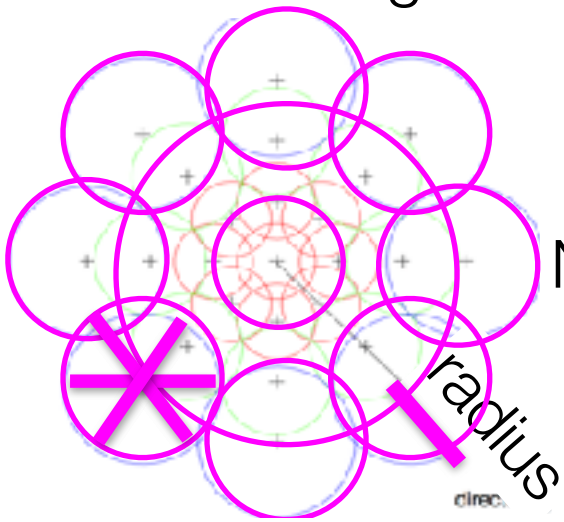
take normalized histogram at point u,v

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

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

Common operations: DAISY

Num histograms/per ring



Num rings

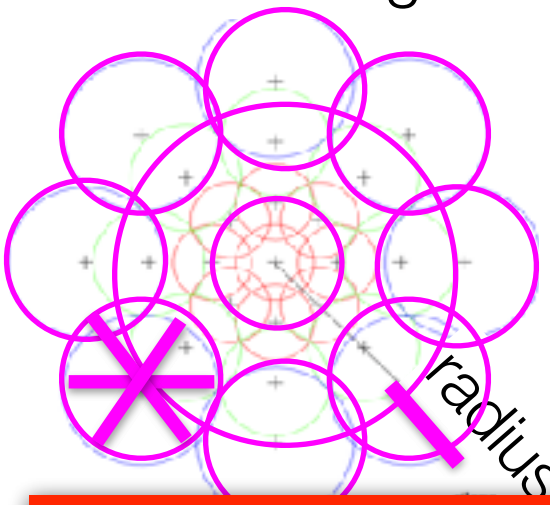
num orientations making up each histogram

ep

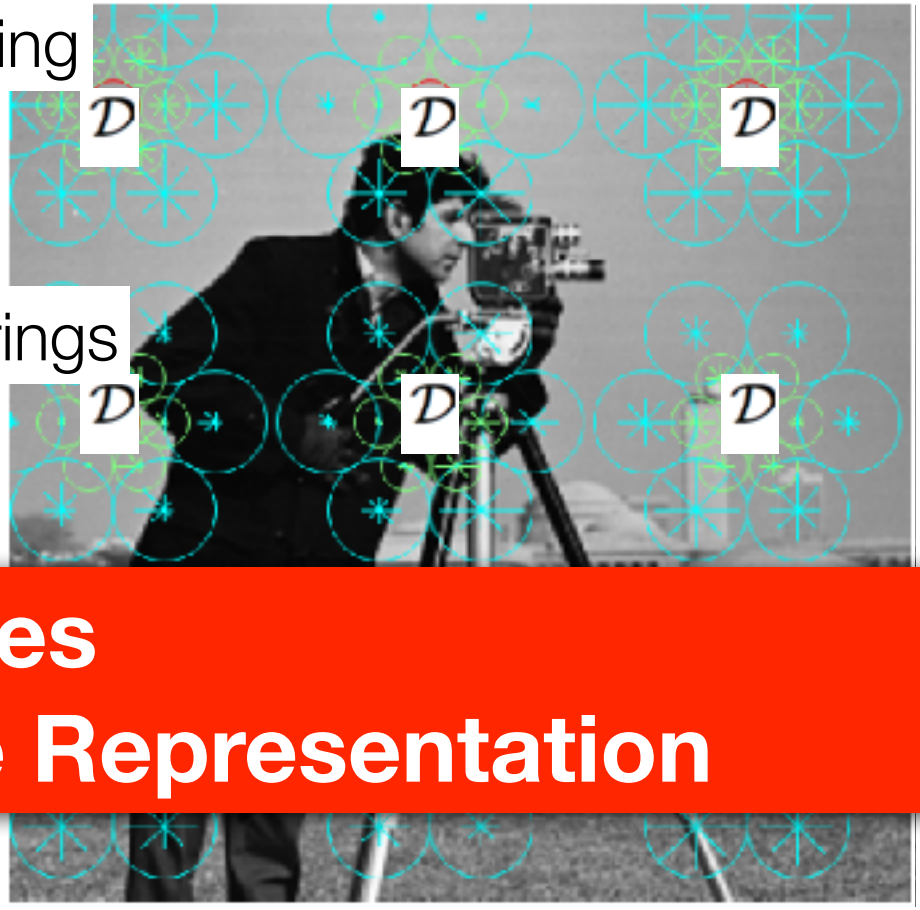
Params:
step, radius, num rings,
num histograms per ring,
orientations per histogram

Common operations: DAISY

Num histograms/per ring



Num rings



Bag of Features Image Representation

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

More Image Processing

Demo

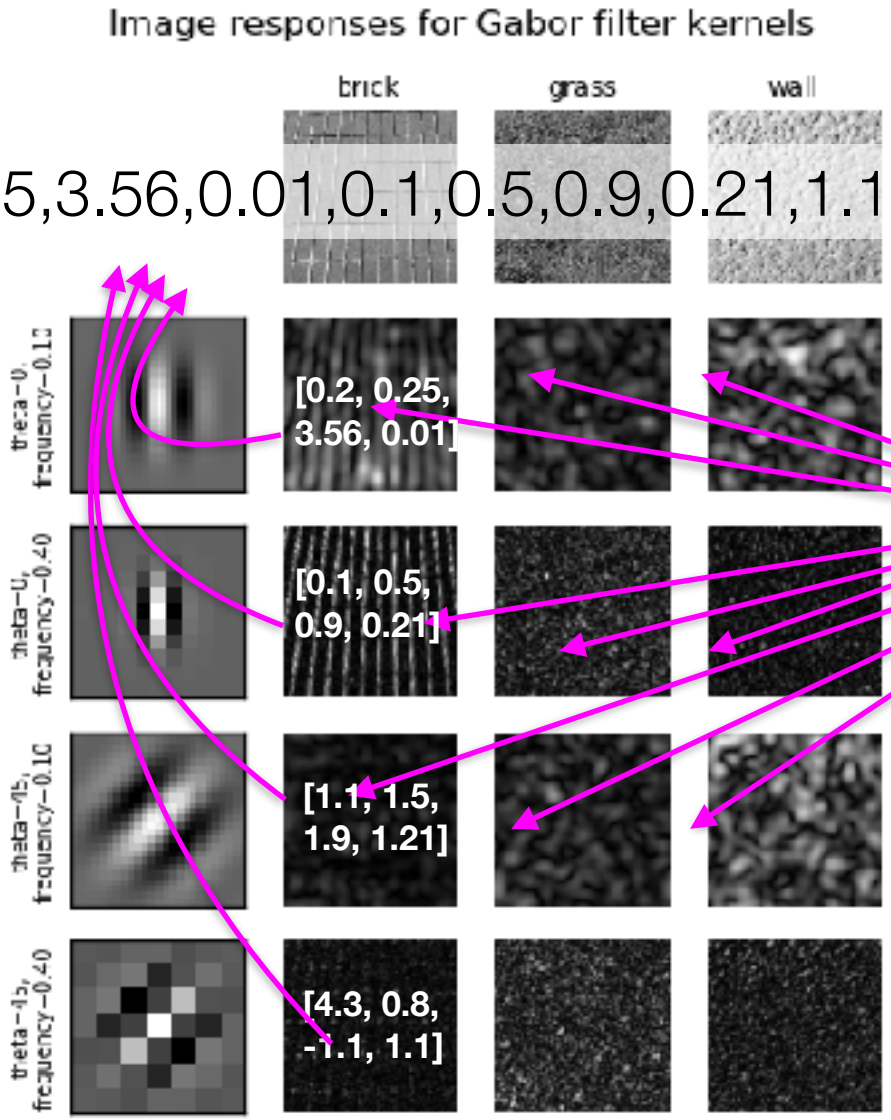
Gradients
DAISY
(if time)Gabor Filter Banks

Other Tutorials:

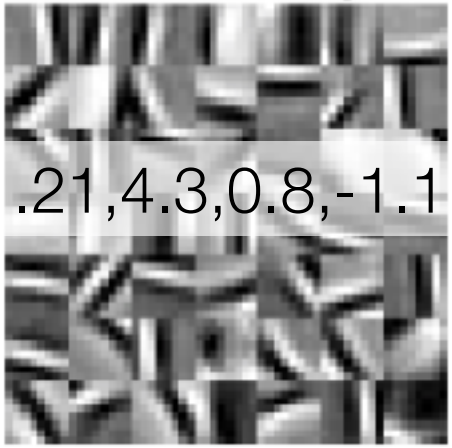
http://scikit-image.org/docs/dev/auto_examples/

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]

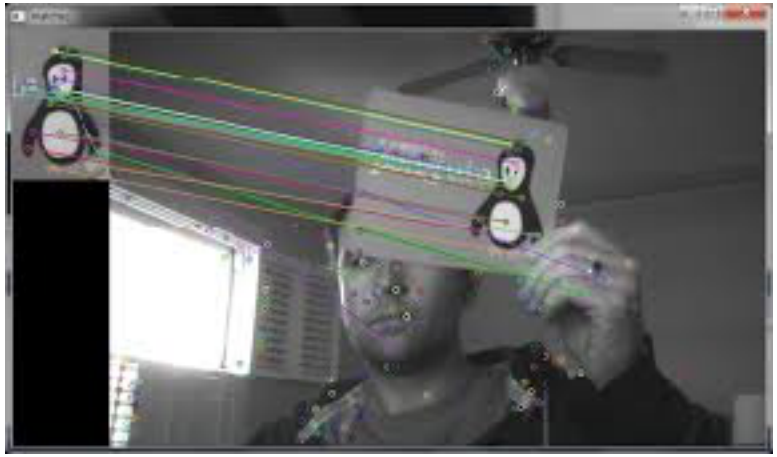


mean
std
skew
kurtosis

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

Town Hall for Lab 2, Images

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

Supplemental Slides

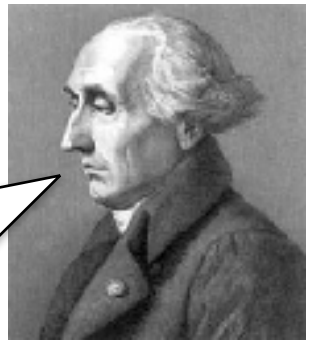
- Peruse these at your own leisure!
- These slides might assist you as additional visual aides
- **Slides courtesy of Tan, Steinbach, Kumar**
    - **Introduction to Data Mining**

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

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

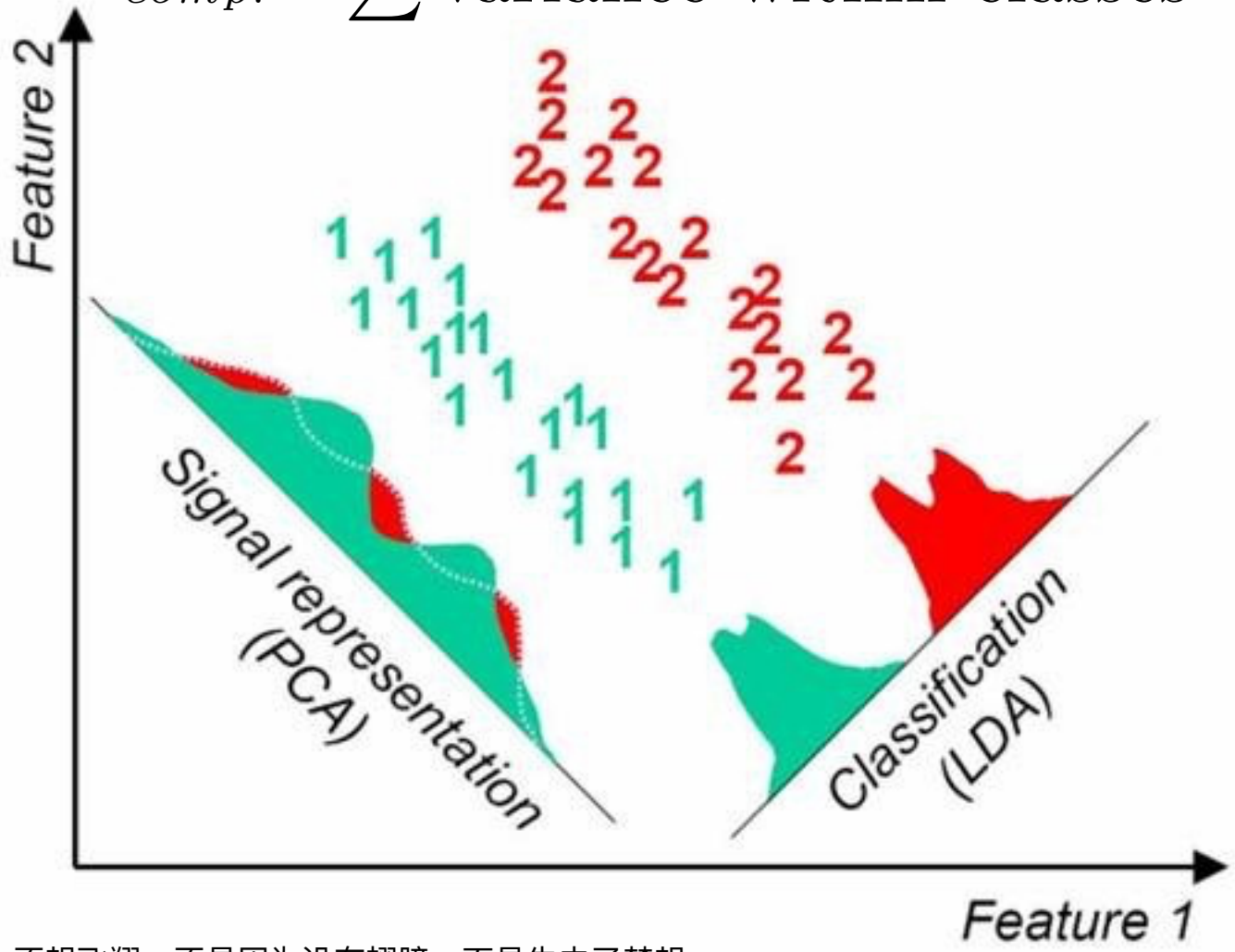
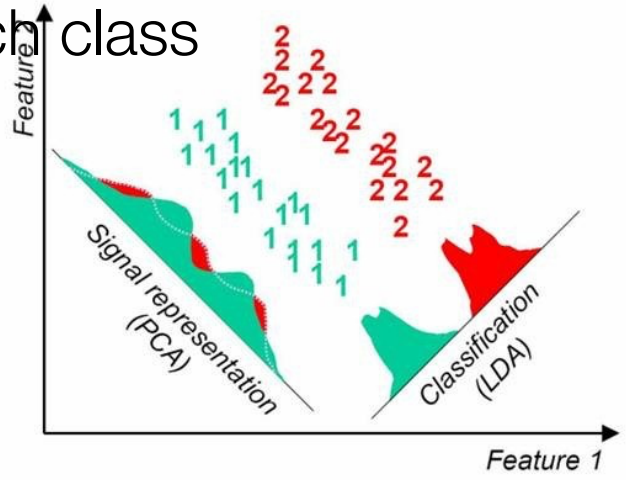


image source: 不想飞翔，不是因为没有翅膀，而是失去了梦想

Dimensionality Reduction: LDA versus QDA

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

- "*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