Lecture Notes for Machine Learning in Python

Professor Eric Larson

Visualization and Dimensionality Reduction

Class Logistics and Agenda

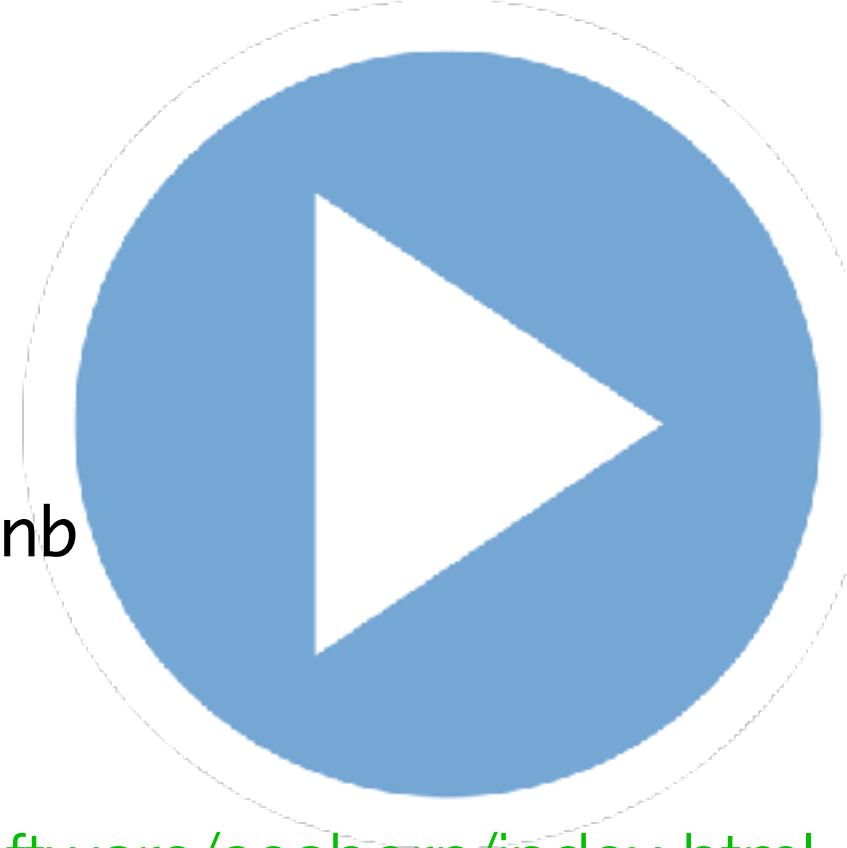
- Finish Visualization Demo
- Dimensionality Reduction
  - PCA and LDA
  - Kernel Methods

What did we talk about last time?

Demo

Visualization

- Matplotlib
- Seaborn
- Plotly



`03.Data Visualization.ipynb`

Other Tutorials:

https://t.co/zNzD8Q8w5E

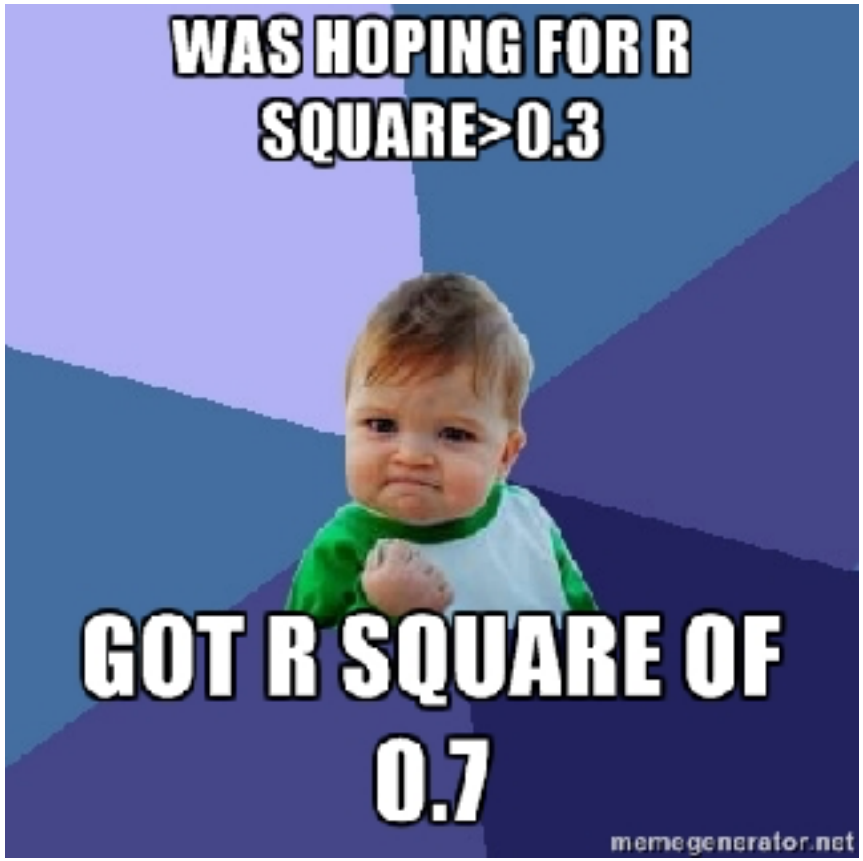
http://stanford.edu/~mwaskom/software/seaborn/index.html

http://pandas.pydata.org/pandas-docs/stable/visualization.html

http://matplotlib.org/examples/index.html

http://nbviewer.ipython.org/github/mwaskom/seaborn/blob/master/examples/plotting_distributions.ipynb

Dimensionality Reduction: PCA and LDA



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

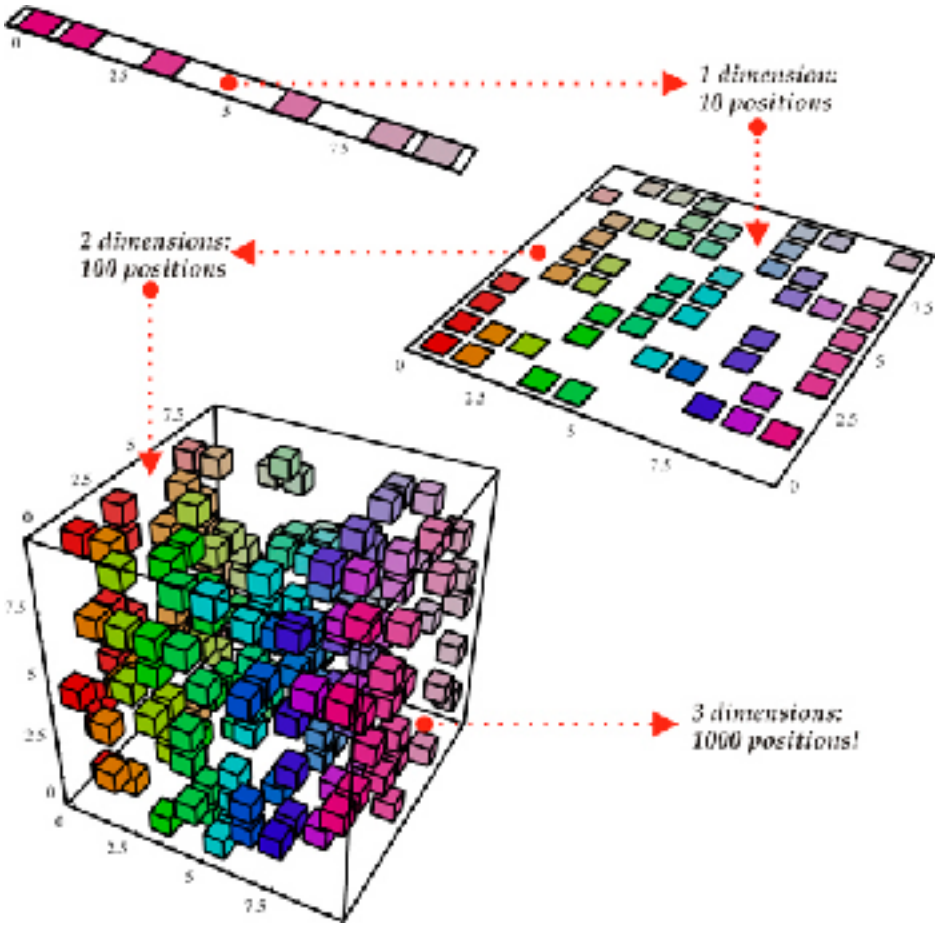


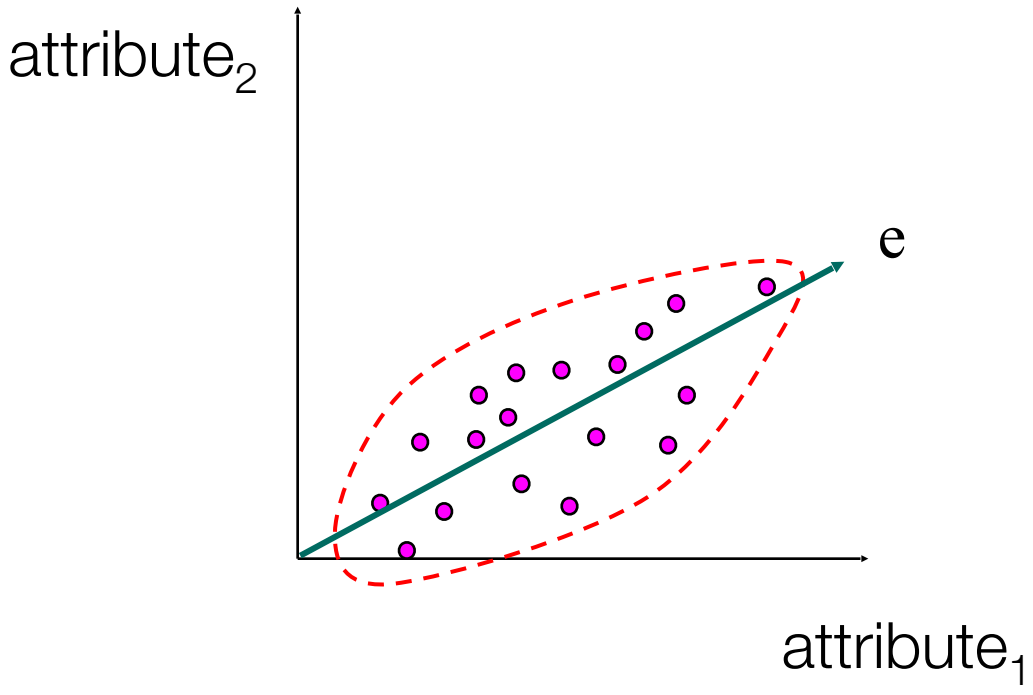
image source: http://www.iro.umontreal.ca/~bengioy/yoshua_en/research_files/CurseDimensionality.jpg

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
  - Discriminant Analysis
  - Others: supervised and non-linear techniques

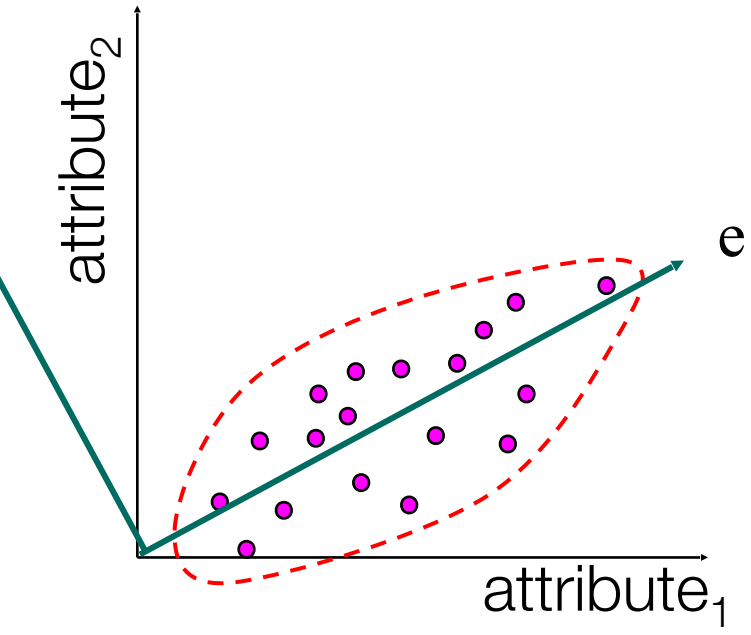
Dimensionality Reduction: PCA

- 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



E1	E2
0.85	0.85
0.52	-0.52

covariance

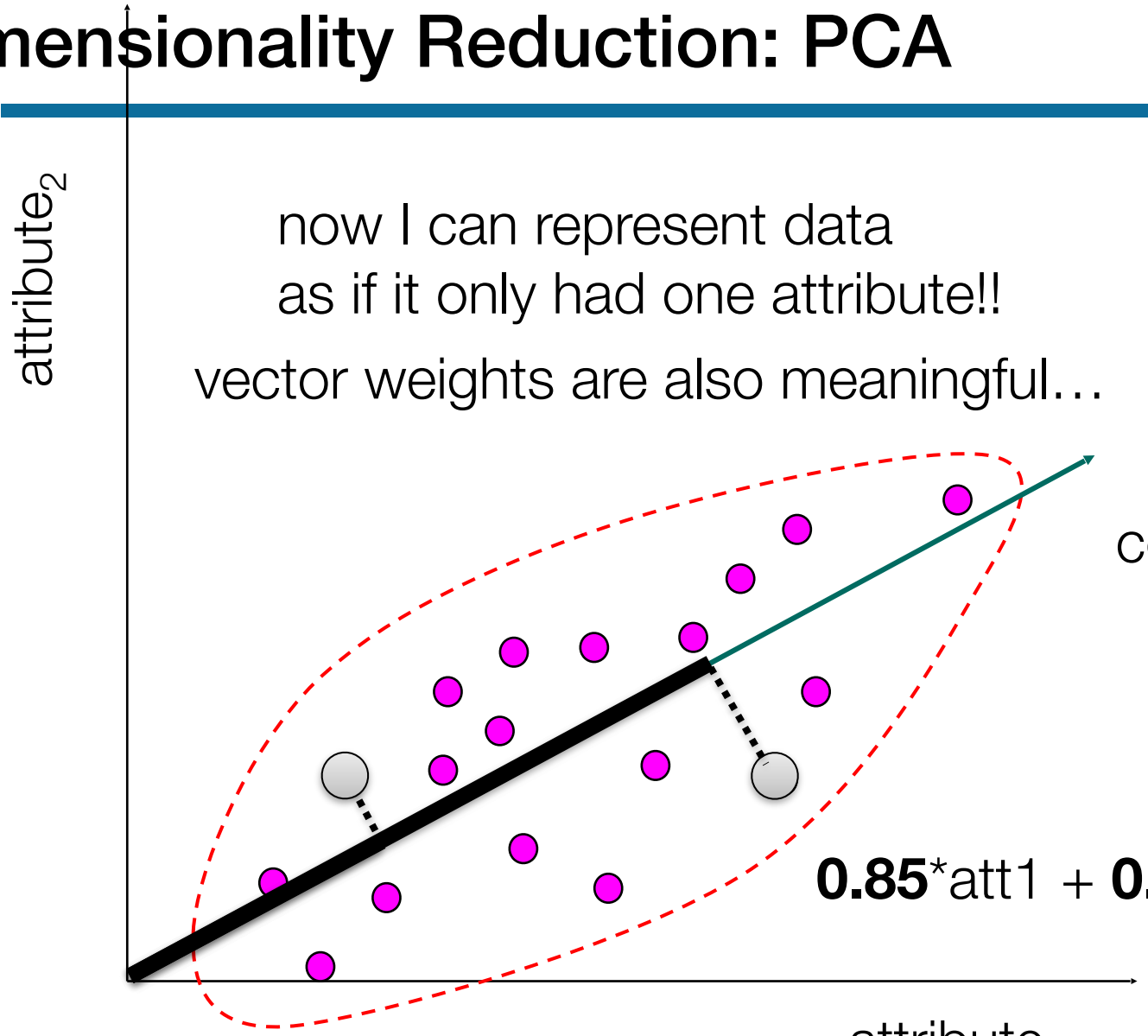
37.1	-6.7
-6.7	43.9

	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



now I can represent data
as if it only had one attribute!!

vector weights are also meaningful…

E1
0.85
0.52

component

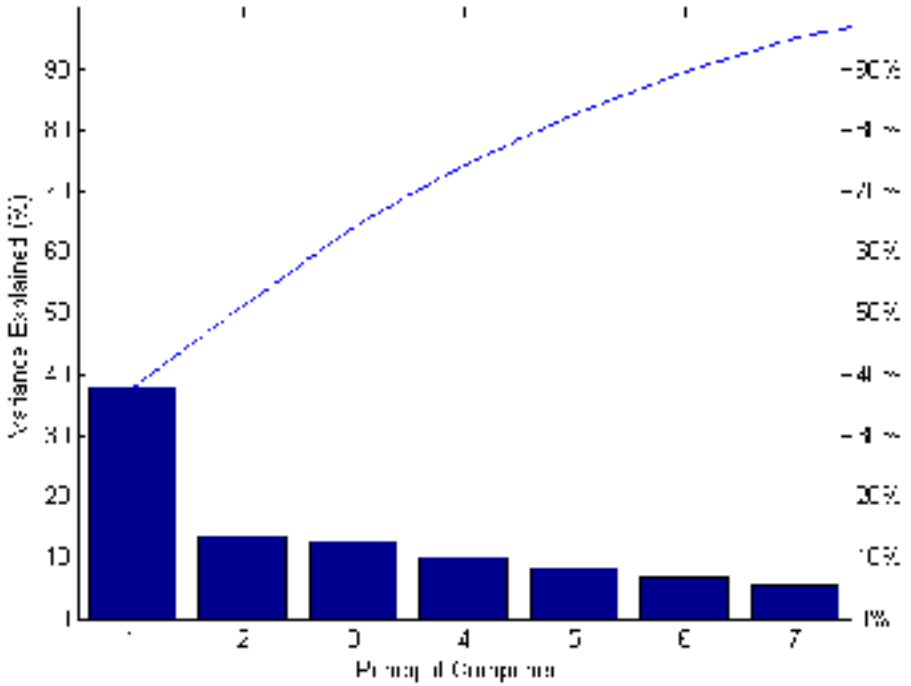
0.85*att1 + **0.52***att2

This projection is called a "Transform"
known as the **Karhunen-Loève Transform**

Explained Variance

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

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



Dimensionality Reduction: PCA

- Genetic profiles distilled to 2 components

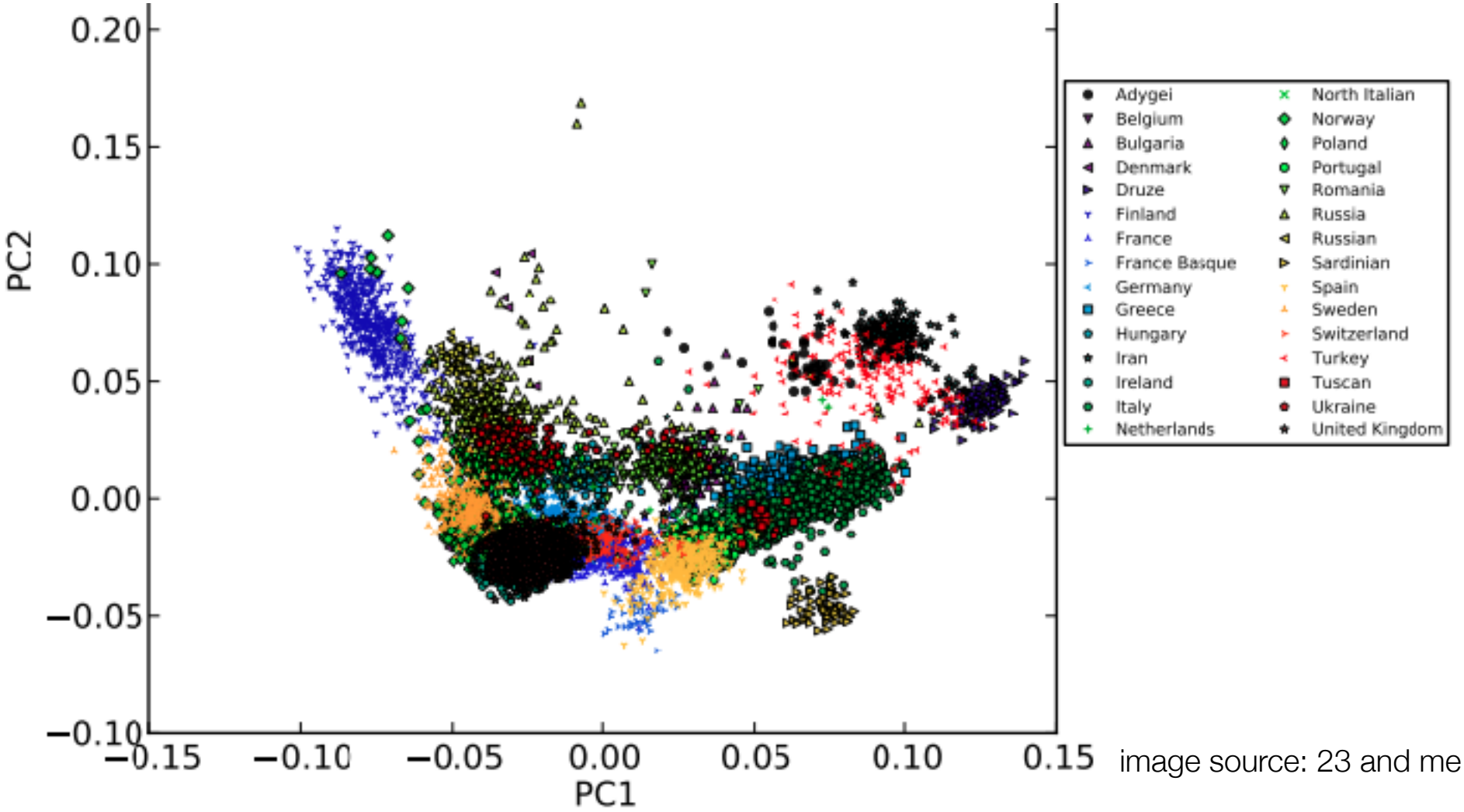


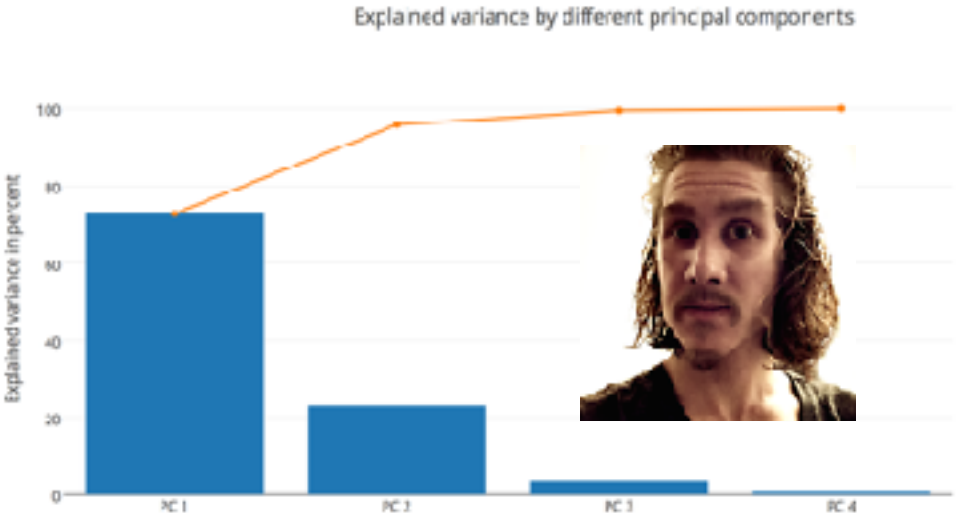
image source: 23 and me

Dimensionality Reduction: PCA

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

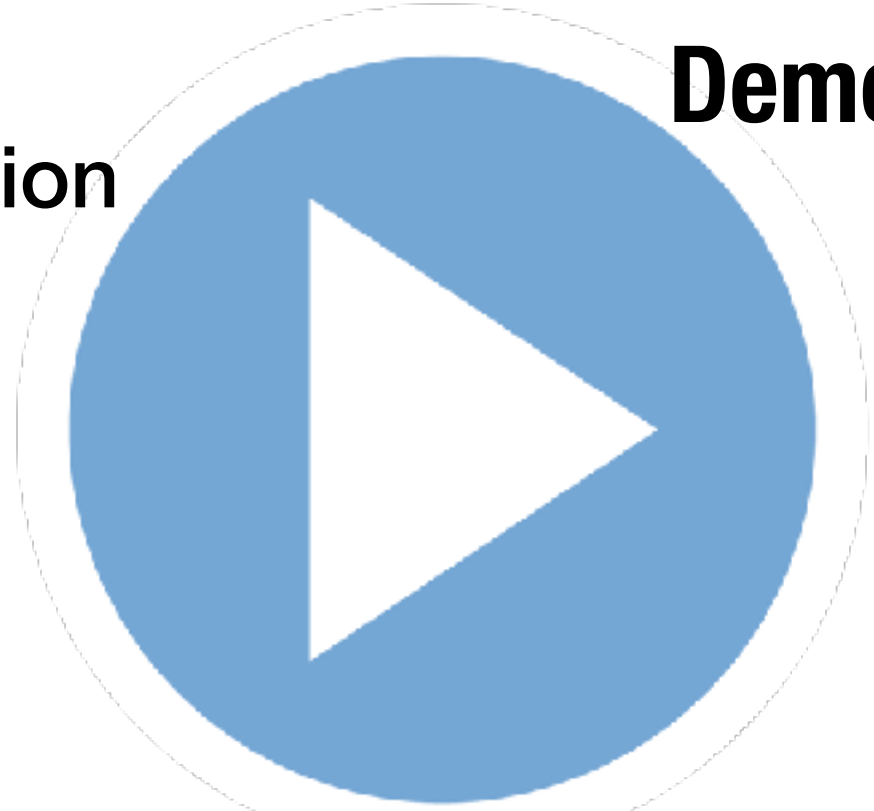
http://nbviewer.ipython.org/github/rasbt/pattern_classification/blob/master/dimensionality_reduction/projection/principal_component_analysis.ipynb

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



04.Dimension Reduction and Images.ipynb

Demo



Dimension Reduction

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

For Next Lecture

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

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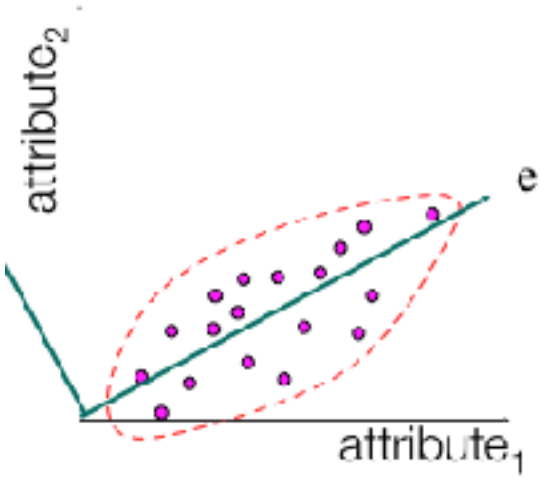
Dimensionality and Images

Class Logistics and Agenda

- **Logistics**:
  - Next lab due at the end of next week
- **Agenda**
  - Randomized
  - Kernel Methods
  - Common Feature Extraction Methods for Images

Last time it was so linear…



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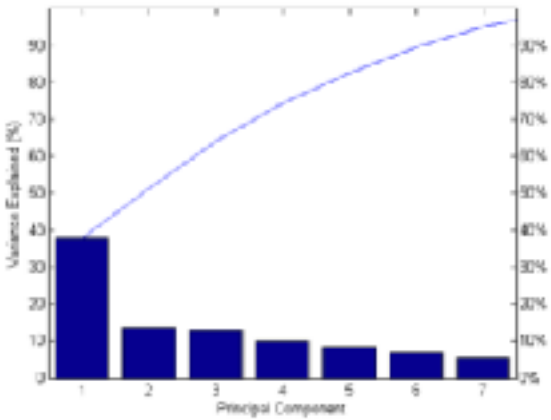
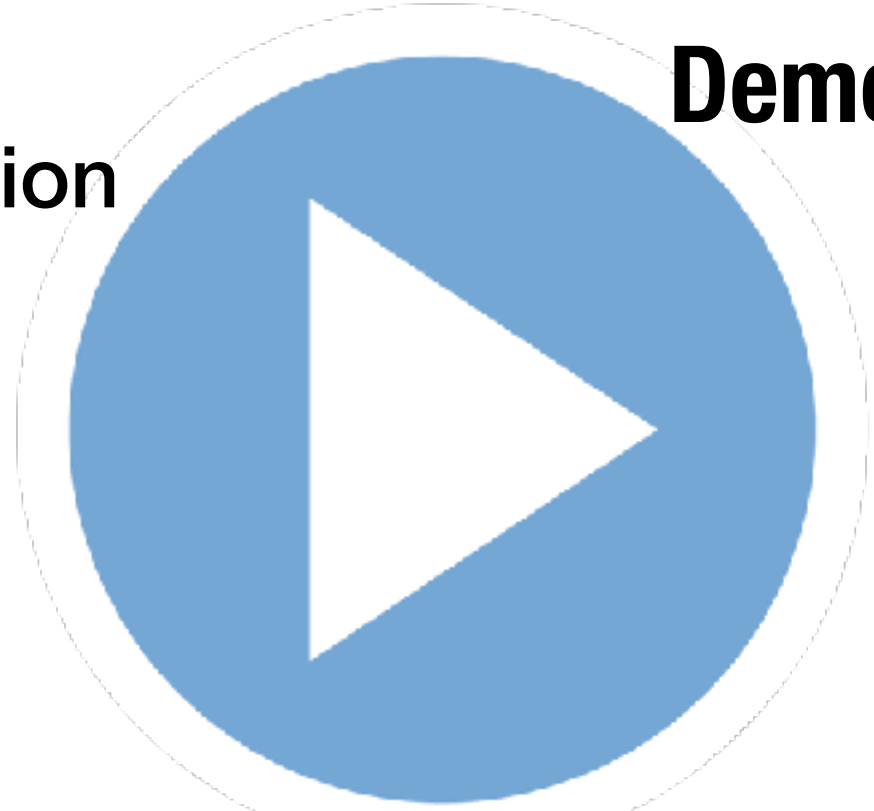
zero mean

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



04.Dimension Reduction and Images.ipynb

Demo



Dimension Reduction

PCA

biplots

Other Tutorials:

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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

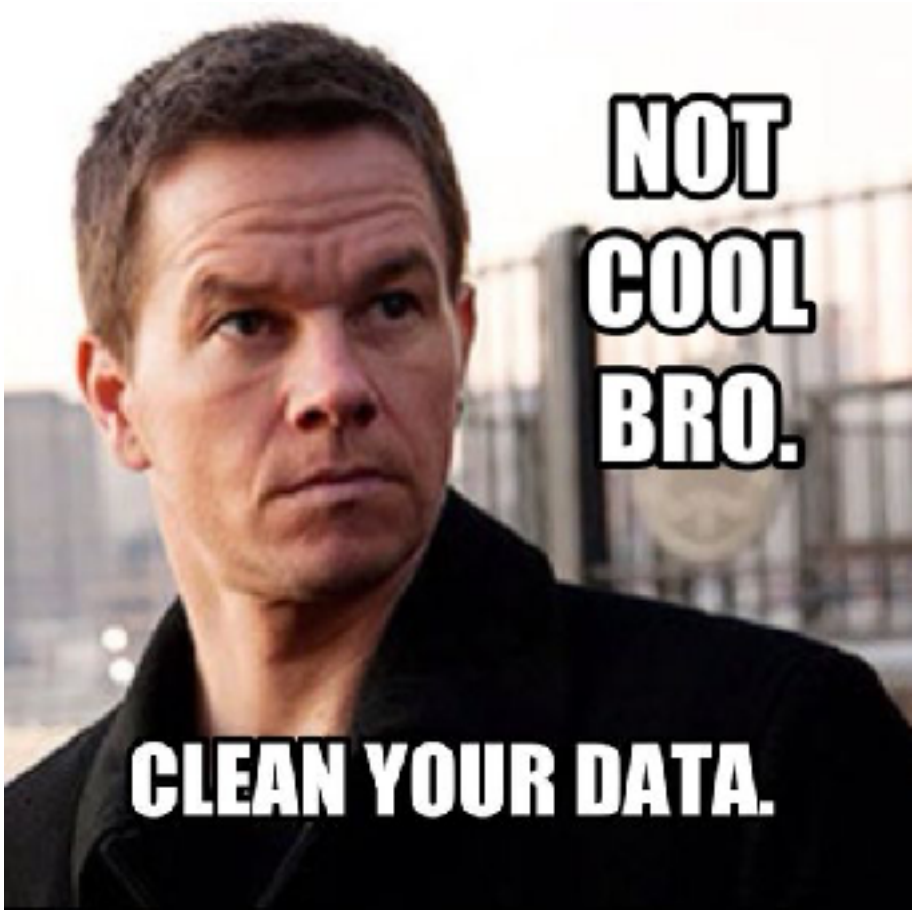
- **Problem**: PCA on all that data can take a while to compute
  - What if the number of instances is gigantic?
  - What if the number of dimensions is gigantic?

- 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

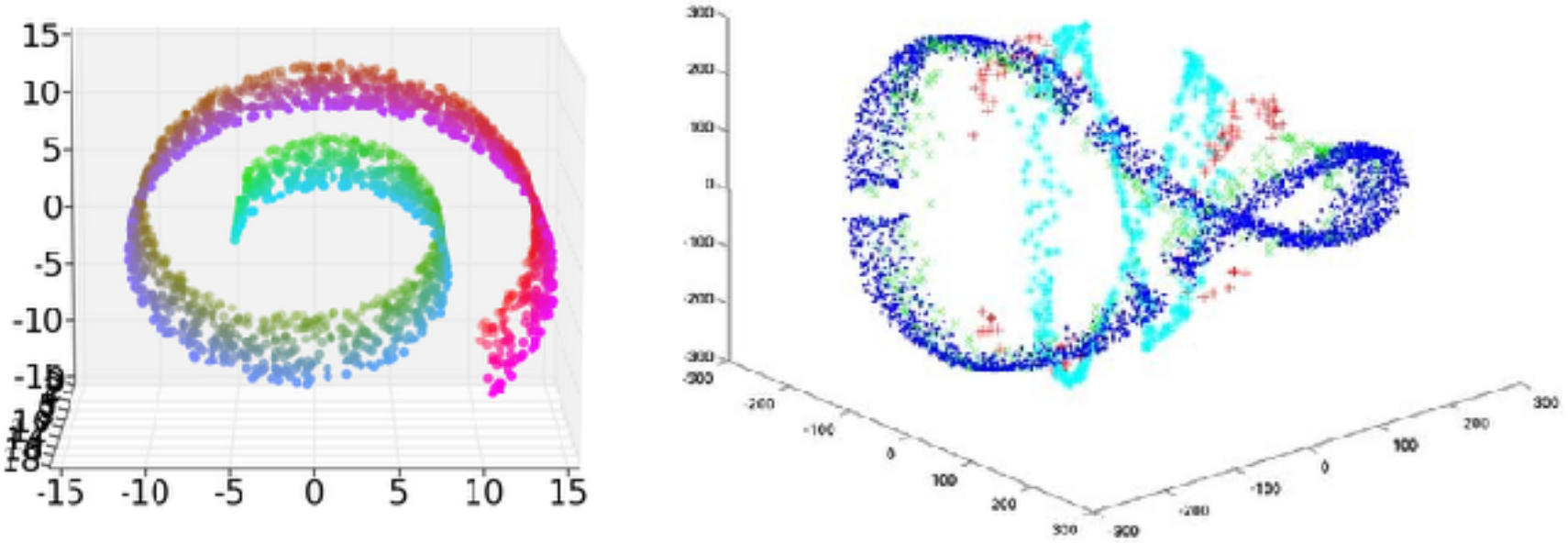
$$\|\boldsymbol{A} - \boldsymbol{Q}\boldsymbol{Q}^*\boldsymbol{A}\| \leq \left[1 + 11\sqrt{k+p} \cdot \sqrt{\min\{m,n\}}\right] \sigma_{k+1}$$

source: 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



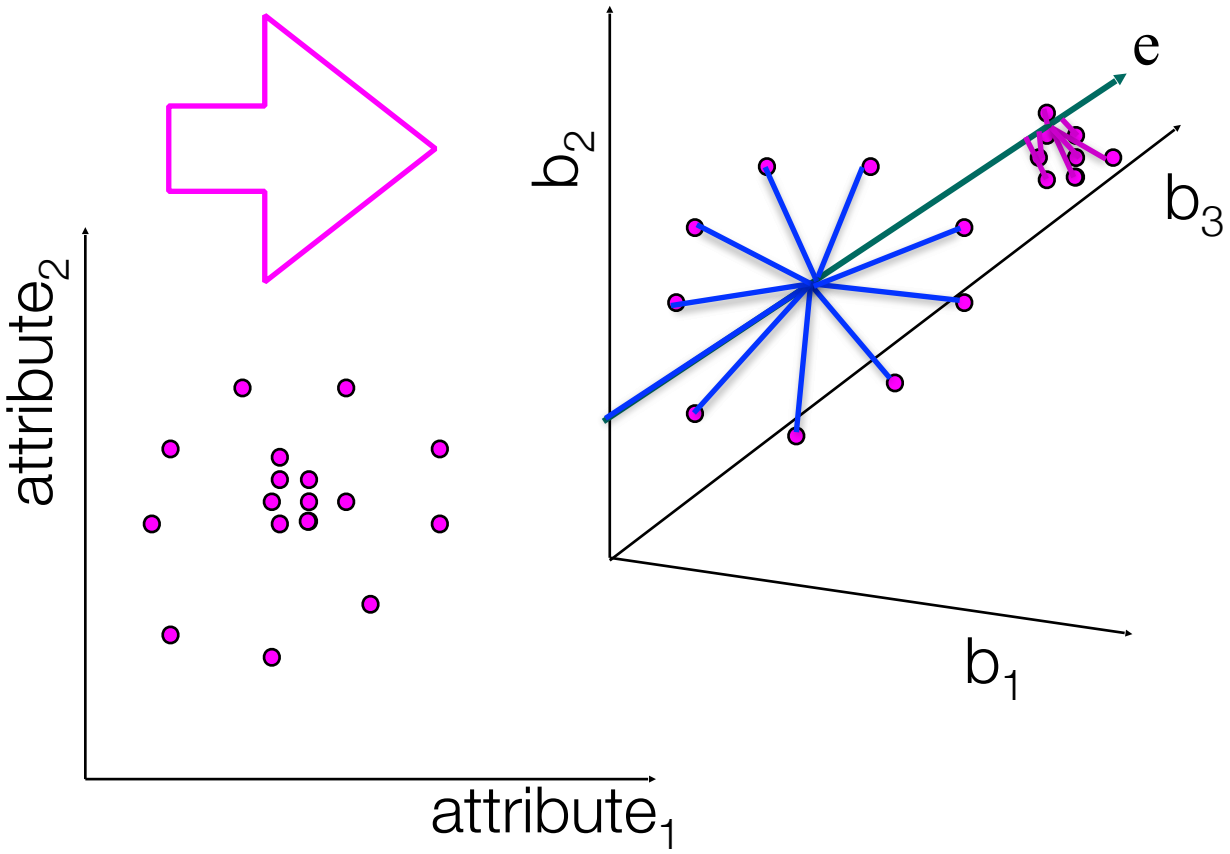
Dimensionality Reduction: non-linear



- 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 higher dimensional space
- Get eigen vectors from nonlinear dot product
- Projecting onto these can be understood as principle components from a higher dimensional space



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

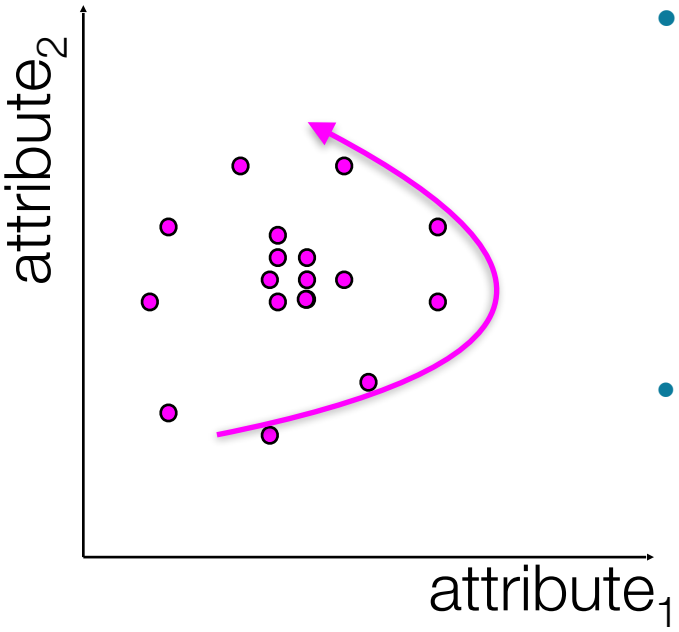
	A1	*A2*
1	*66*	*33.6*
2	*54*	*26.6*
3	*69*	*23.3*
4	*73*	*28.1*
5	*61*	*43.1*
6	*62*	*25.6*

Kernel PCA

kernel: defines what the dot product is in higher dimensional space

some kernels have corresponding transformations with **infinite dimensions**!!

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



- **Key insight**: don't need to know the actual principle components, just the projections
- **Never need** eigen vectors of full covariance matrix

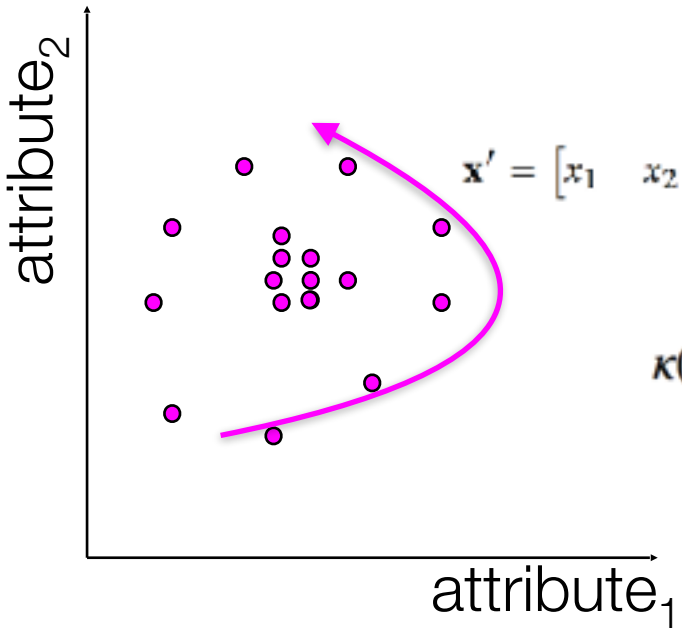
	A1	A2
1	66	33.6
2	54	26.6
3	69	23.3
4	73	28.1
5	61	43.1
6	62	25.6

Kernel PCA

kernel: defines what the dot product is in higher dimensional space

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

some kernels have corresponding transformations with **infinite dimensions**!!



$$\mathbf{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix}^T \qquad \mathbf{x} \in \mathbb{R}^d$$

$$\Downarrow \phi$$

$$\mathbf{x}' = \begin{bmatrix} x_1 & x_2 & x_1x_2 & x_1^2 & x_1x_2^3 & \dots \end{bmatrix}^T \qquad \mathbf{x} \in \mathbb{R}^k (k >> d)$$

$$\kappa(\mathbf{x_i}, \mathbf{x_j}) = exp\left(-\gamma \ \|\mathbf{x_i} - \mathbf{x_j}\|_2^2 \right)$$

kernel: radial basis function (rbf)

	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

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

Kernel PCA

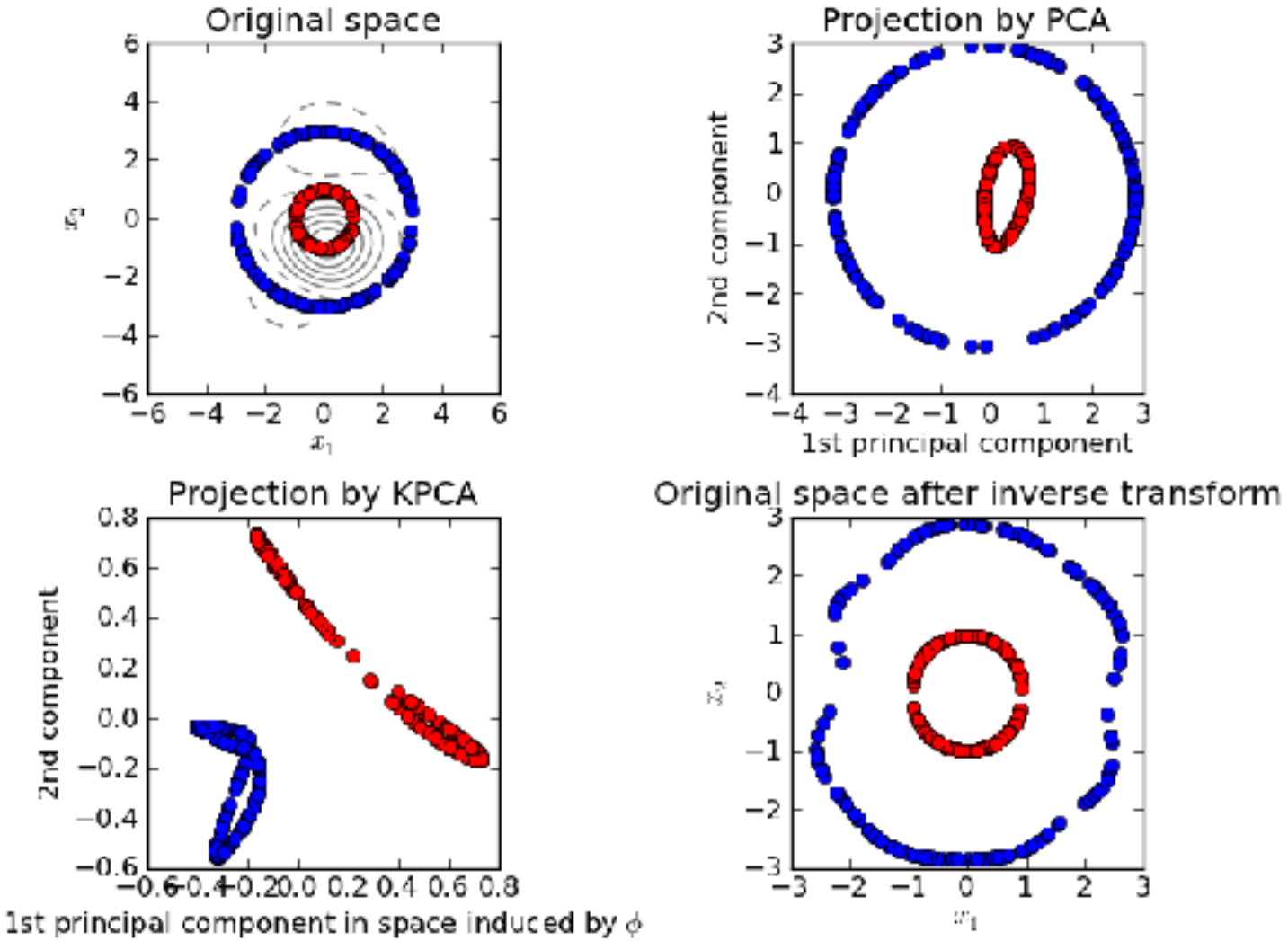
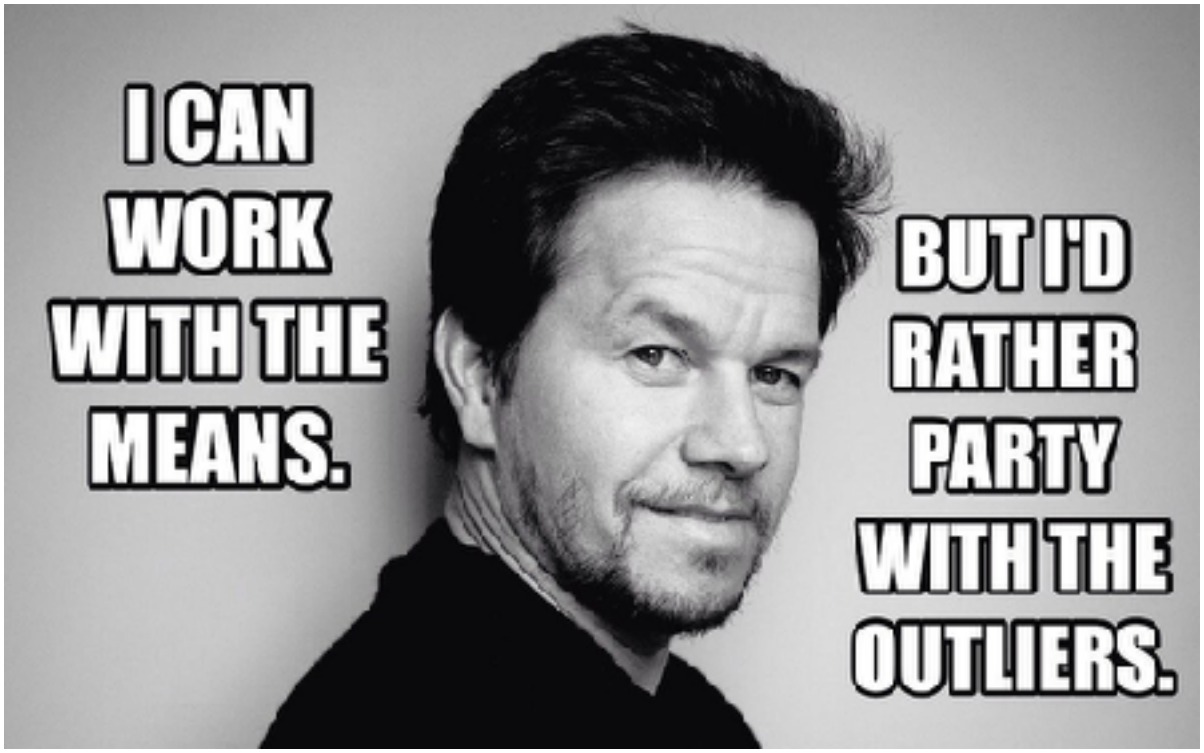

Original space
Projection by PCA
2nd component
1st principal component
Projection by KPCA
2nd component
1st principal component in space induced by ϕ
Original space after inverse transform

Image Processing and Representation

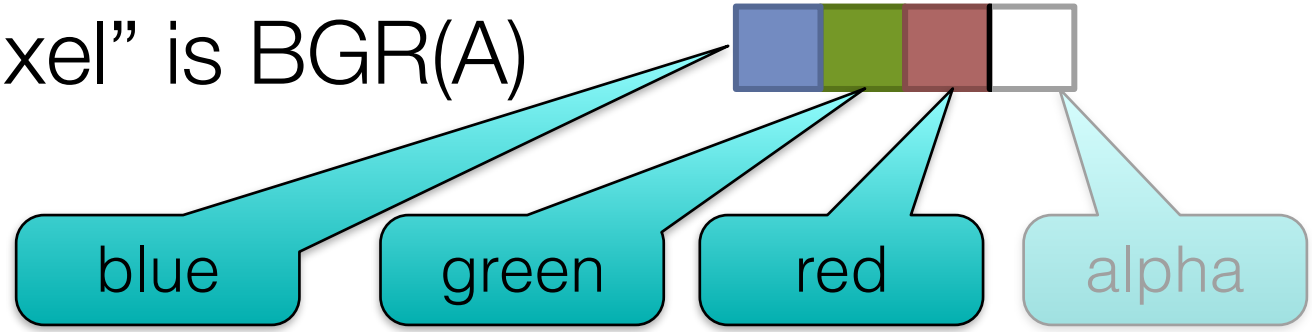


What is image processing

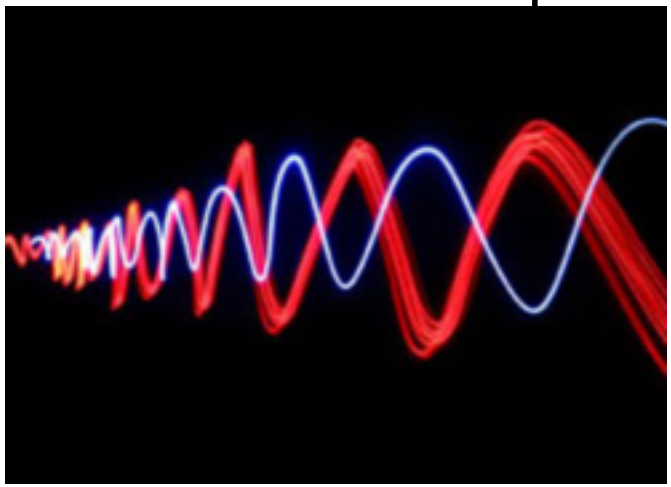
- the **art** and **science** of manipulating pixels
  - combining images (blending or compositing)
  - enhancing edges and lines
  - adjusting contrast, color
  - warping, transformation
  - filtering
  - features extraction

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



sensor

sensor

sensor

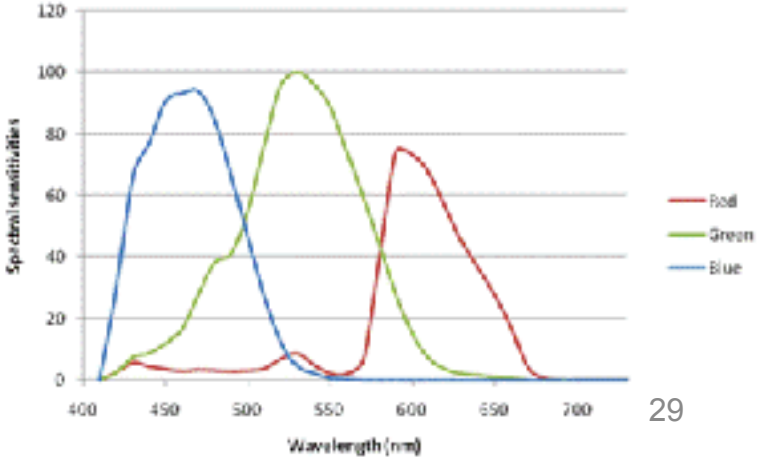


Image Representation

- need a compact representation

- **grayscale**

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

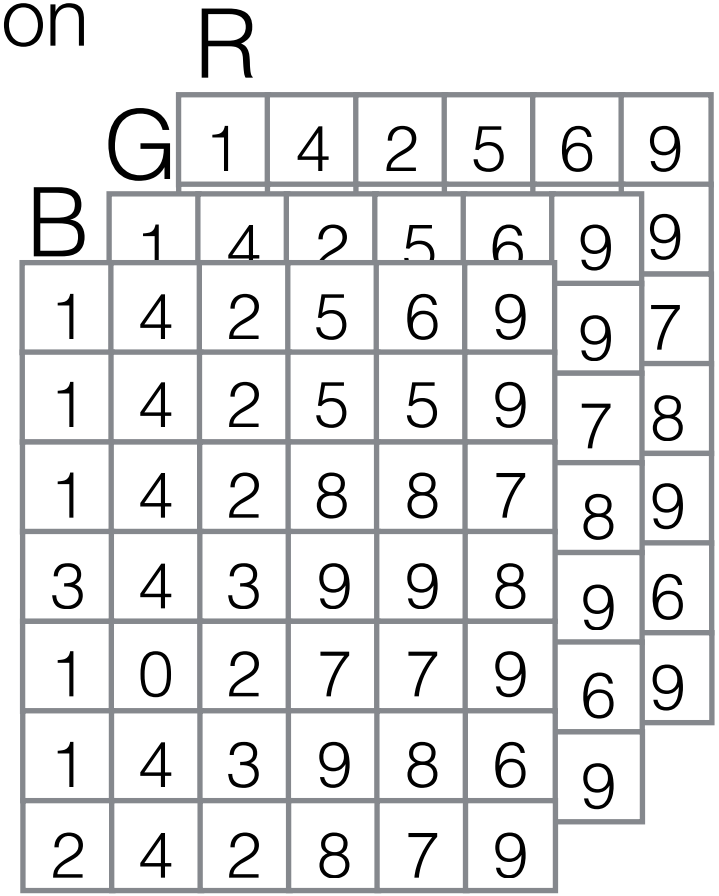
  "luminance"

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

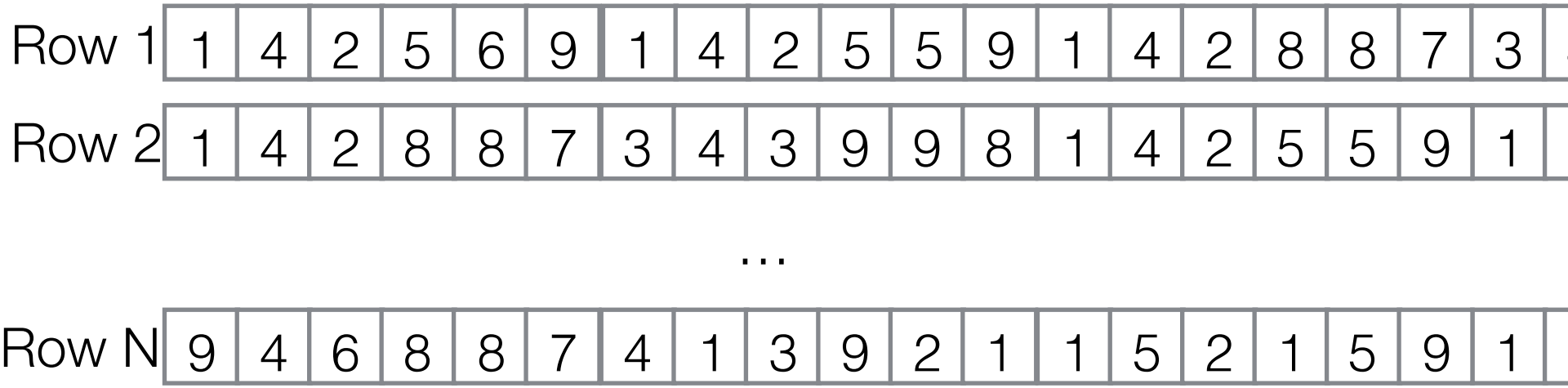
Problem: need to represent image as table data

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

Solution: row concatenation



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

- Images Representation
- Randomized PCA
- Kernel PCA

`04.Dimension Reduction and Images.ipynb`

Features of Images

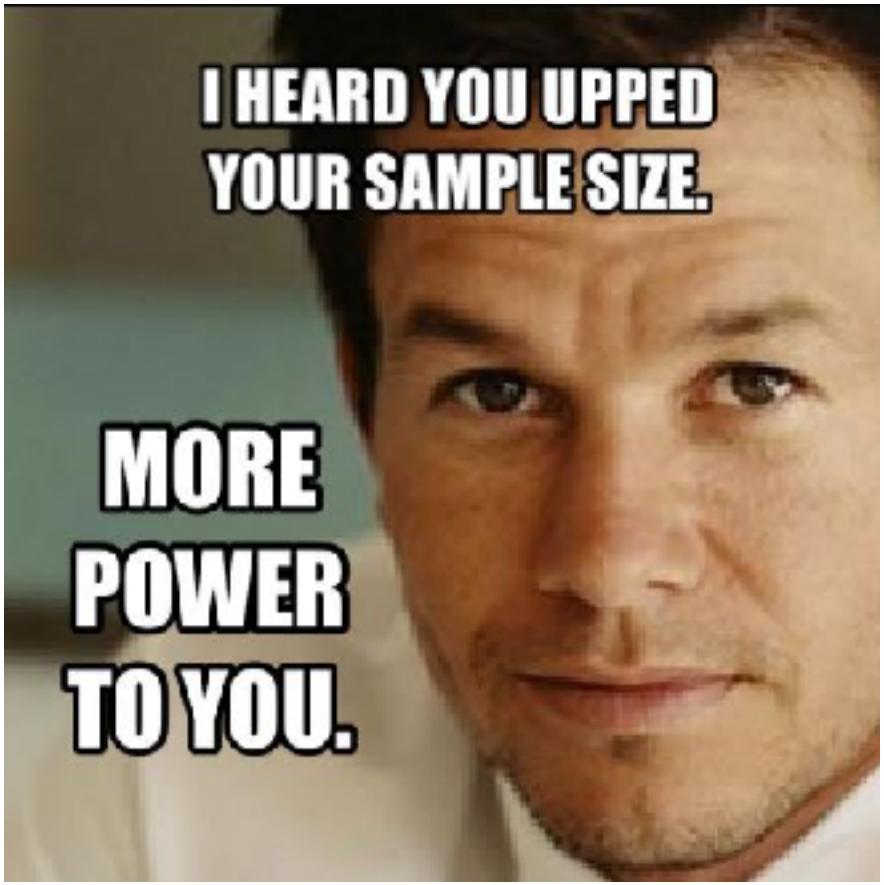
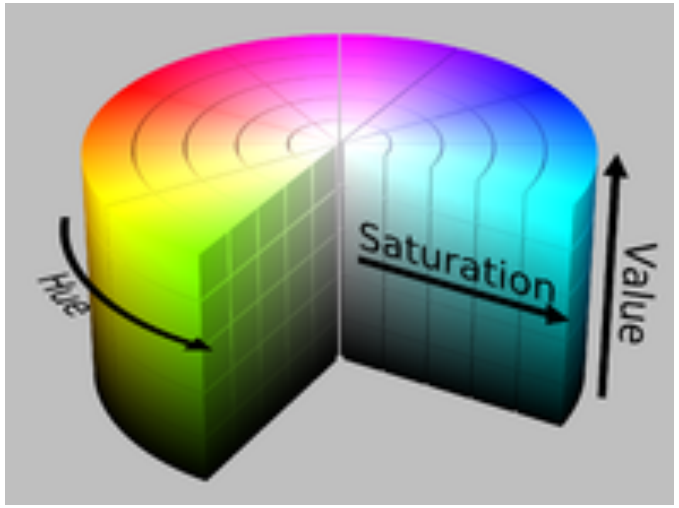
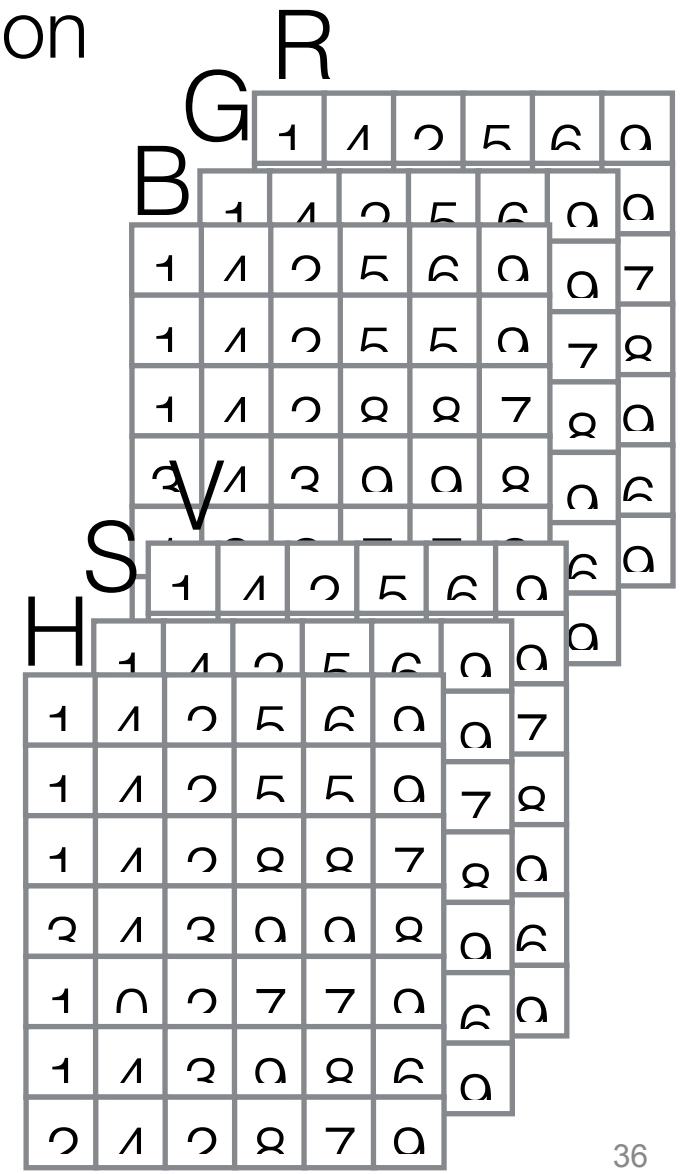


Image Representation

- need a compact representation

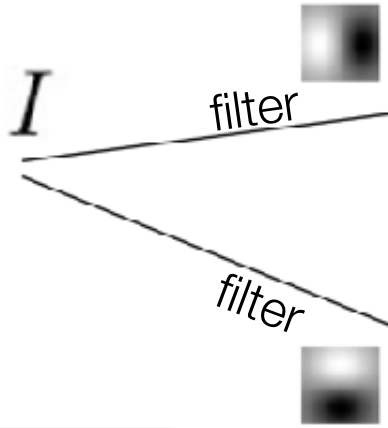
- **hsv**
  - what we perceive as color (ish)
    - hue: the color value
    - saturation: the richness of the color relative to brightness
    - value: the gray level intensity

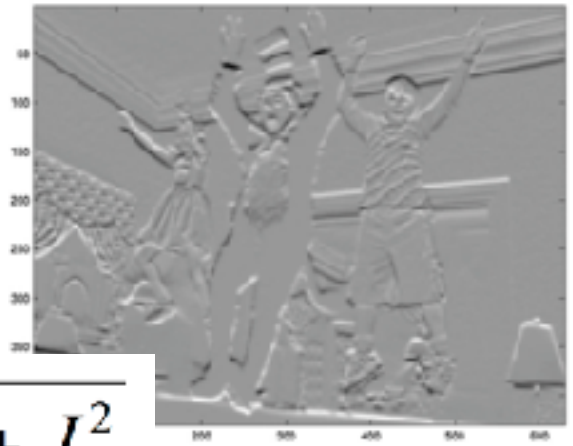




Common operations

- the gradient (2D derivative)



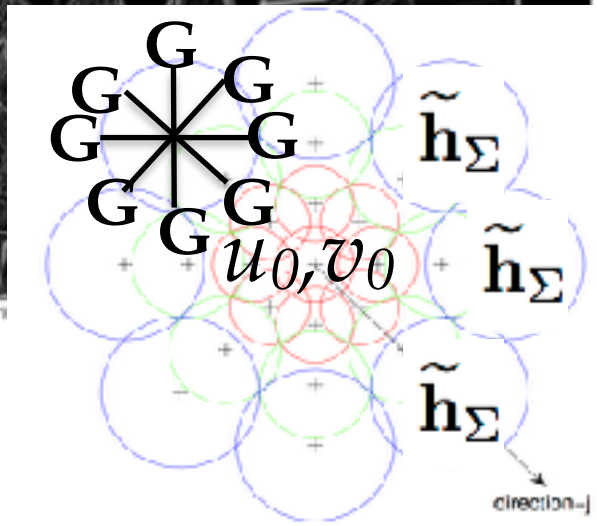


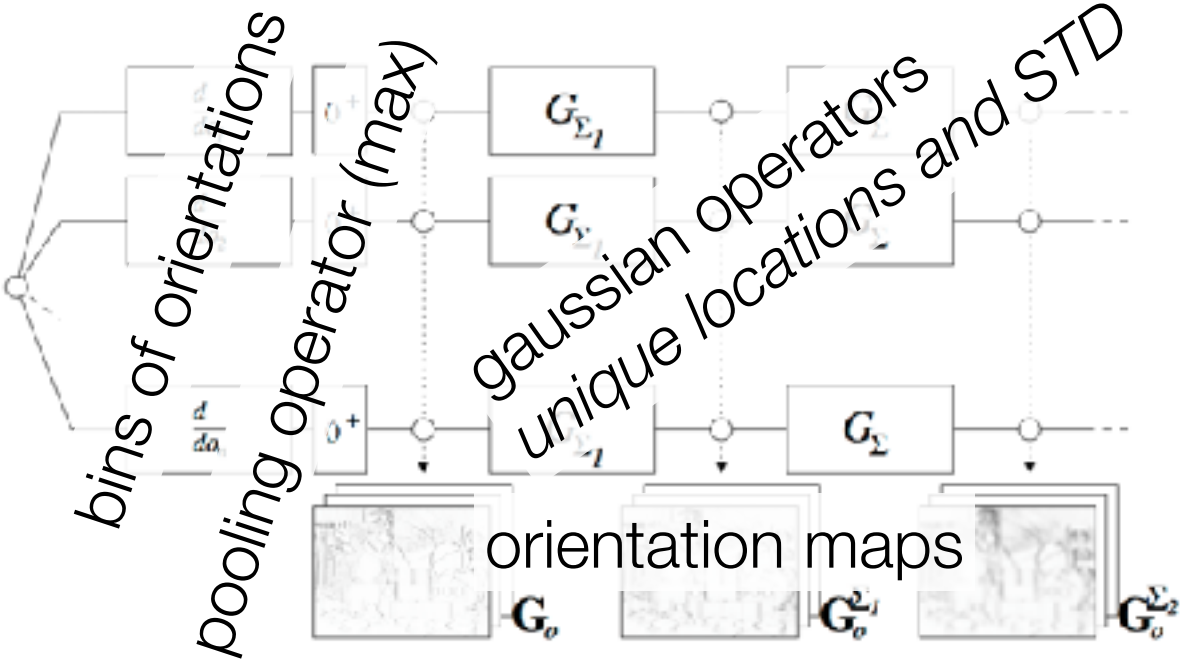
$$\|\nabla J\| = \sqrt{J_x^2 + J_y^2}$$

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

images: Jianbo Shi, Upenn

Common operations: DAISY



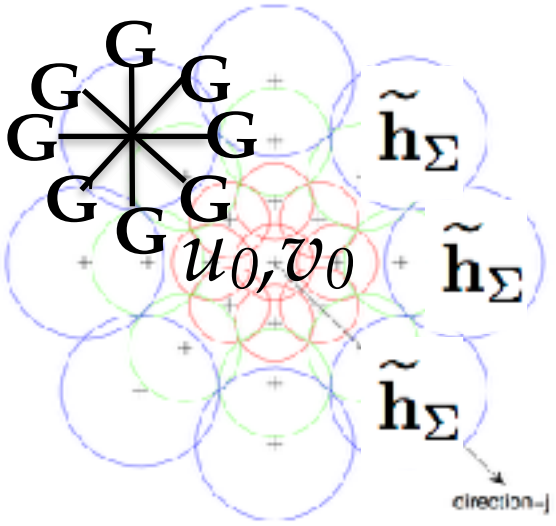


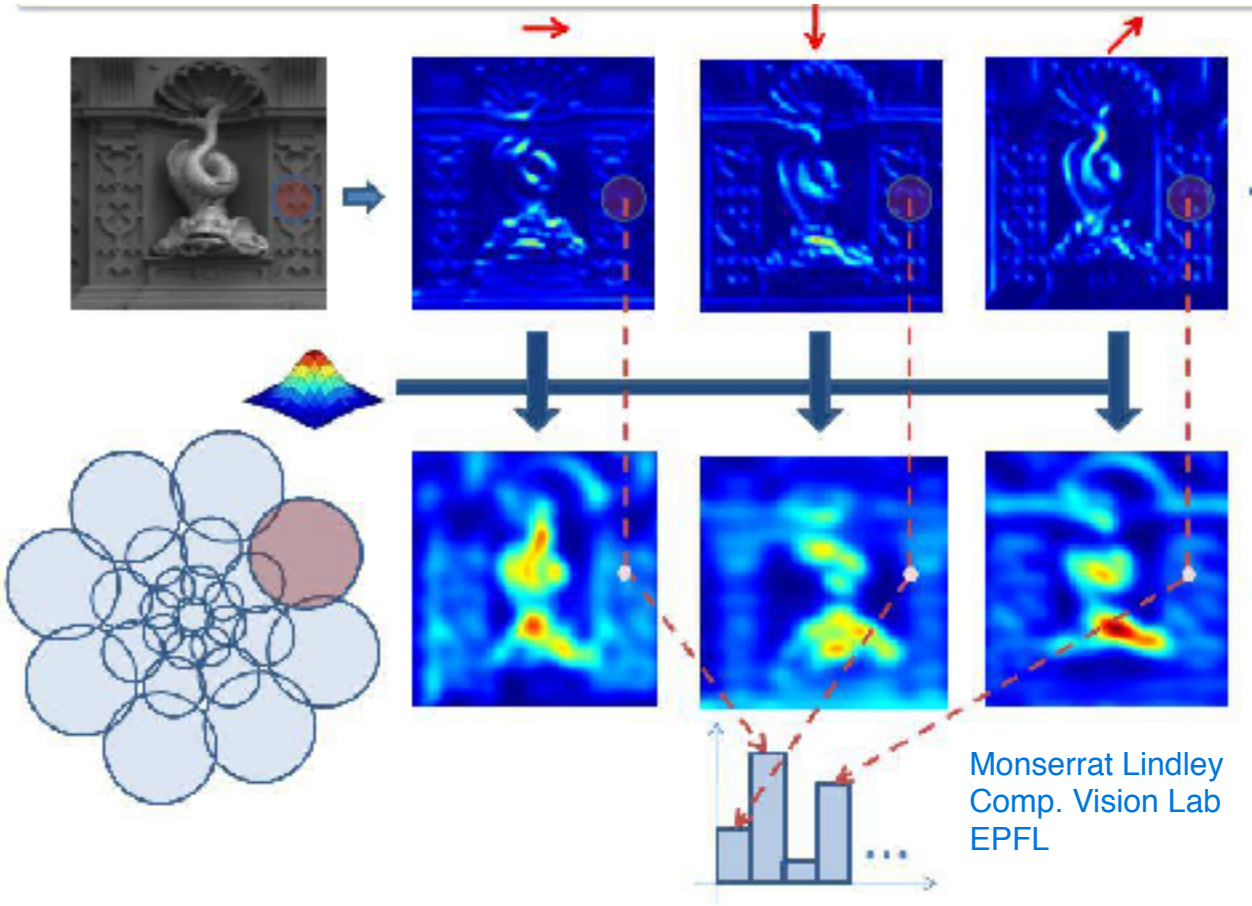
take normalized histogram at point u,v

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

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

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





take normalized histogram at point u,v

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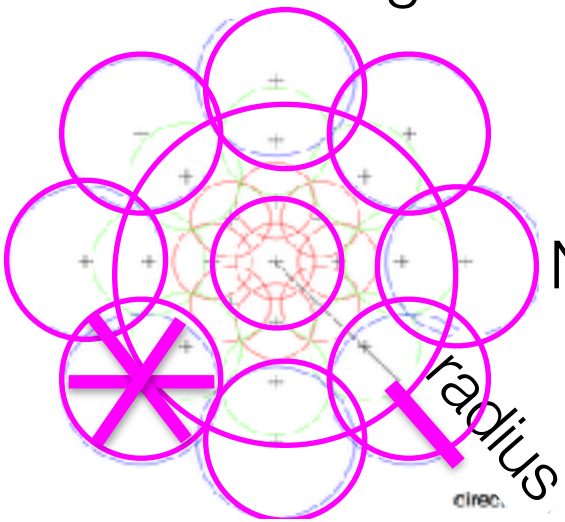
Tola et al. "Daisy: An efficient dense descriptor applied to wide-baseline stereo." Pattern Analysis and Machine Intelligence, IEEE Transactions

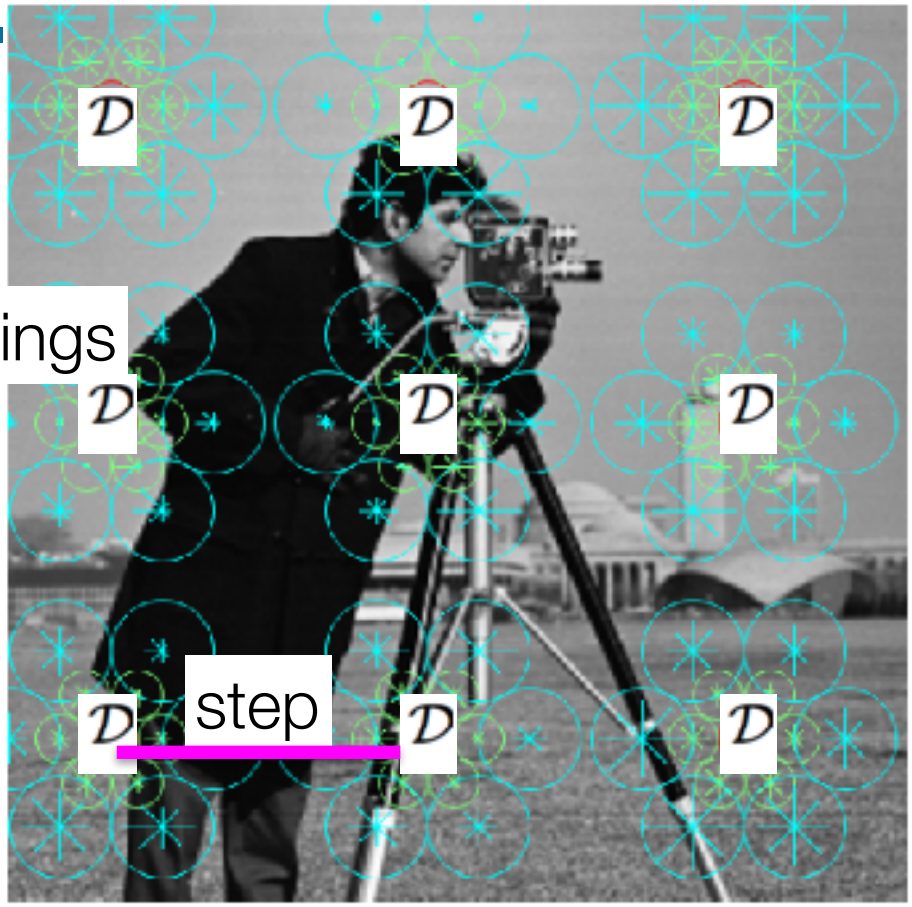
Common operations: DAISY

Num histograms



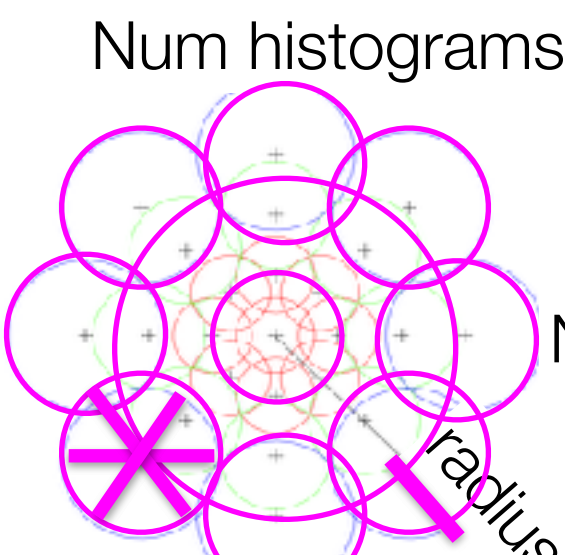
Num rings

num orientations (bins)

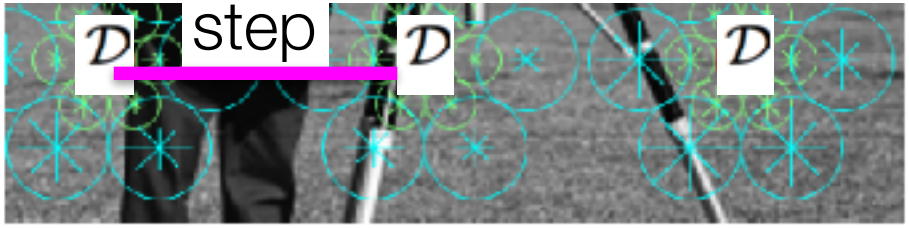


Params:
step, radius, num rings,
num histograms per ring,
orientations per histogram

Common operations: DAISY



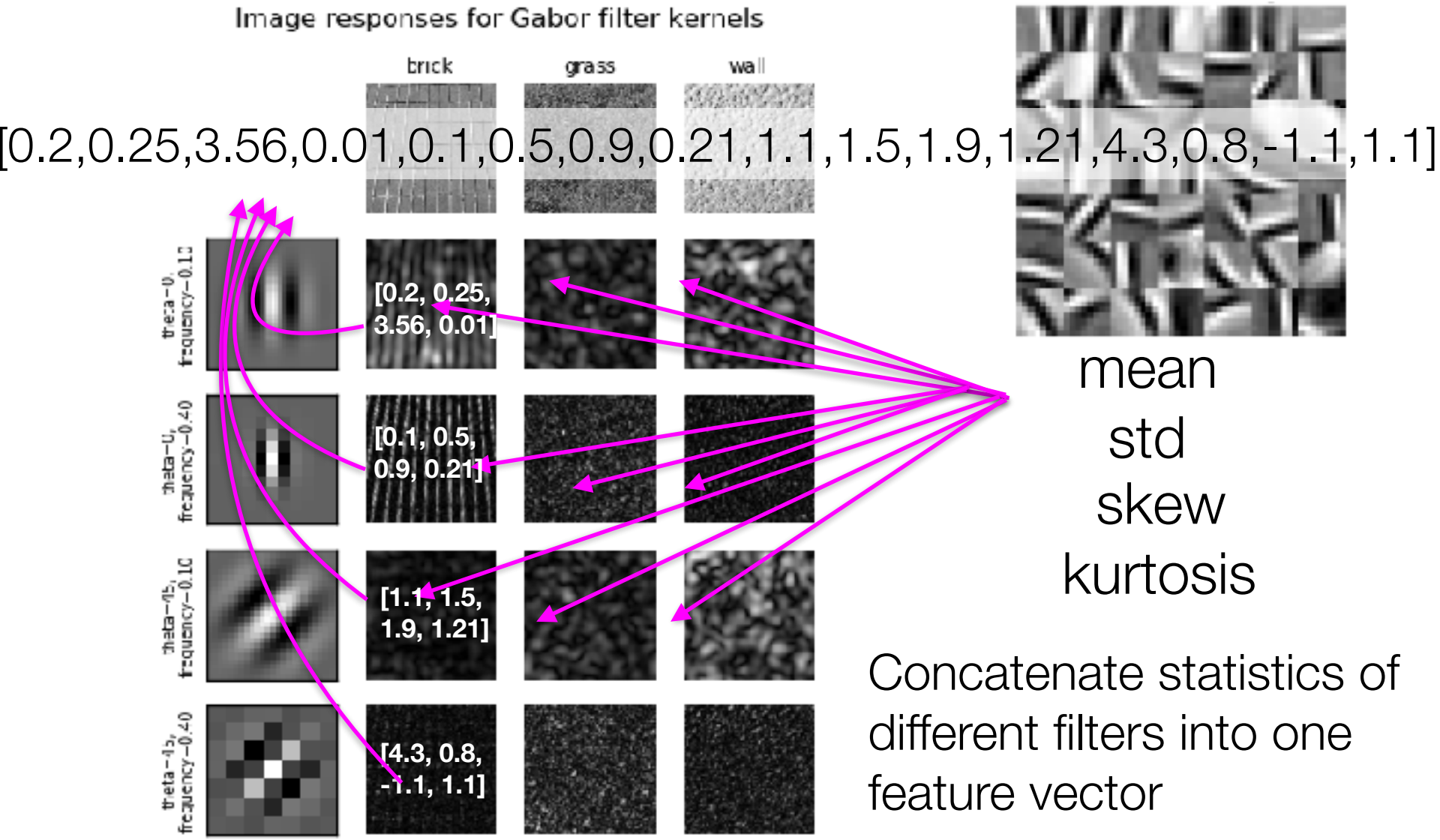
num Bag of Features Image Representation



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

Common operations: Gabor filter Banks (if time)

- common used for texture classification



Concatenate statistics of different filters into one feature vector

Demo

More Image Processing

- Gradients
- DAISY
- Gabor Filter Banks

Other Tutorials:

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

For Next Lecture

- Work on your text datasets!
- **Next Time**: In-Class Assignment One!!!
- **Next Week**: Project Questions Lecture

Supplemental Slides

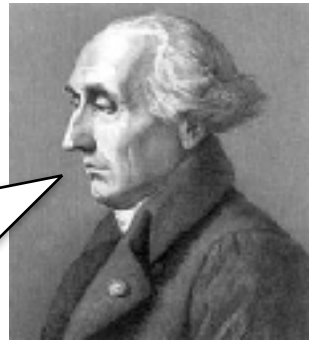
- Peruse these at your own leisure!
- These slides might assist you as additional visual aides
- **Slides courtesy of Tan, Steinbach, Kumar**
    - **Introduction to Data Mining**

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

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

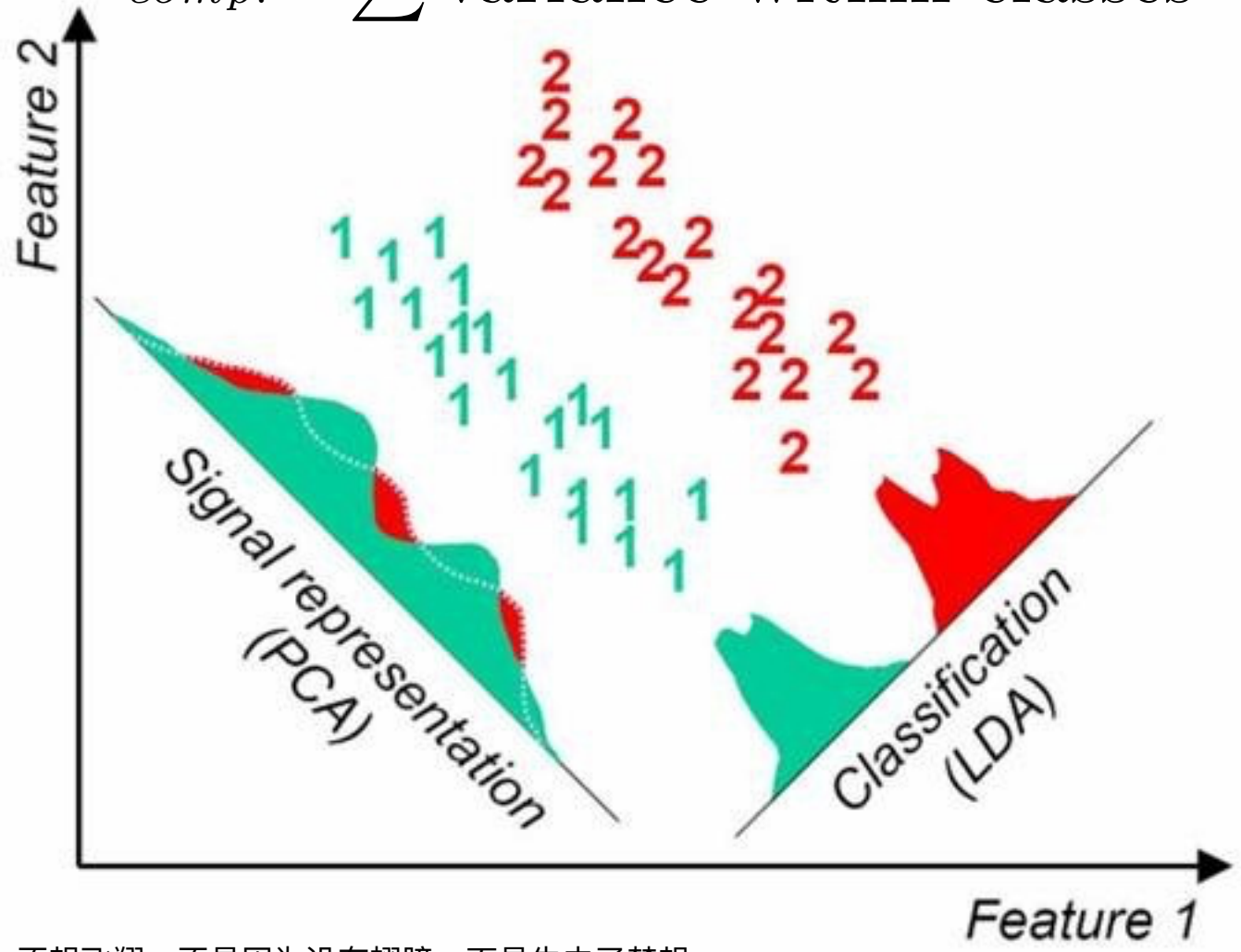
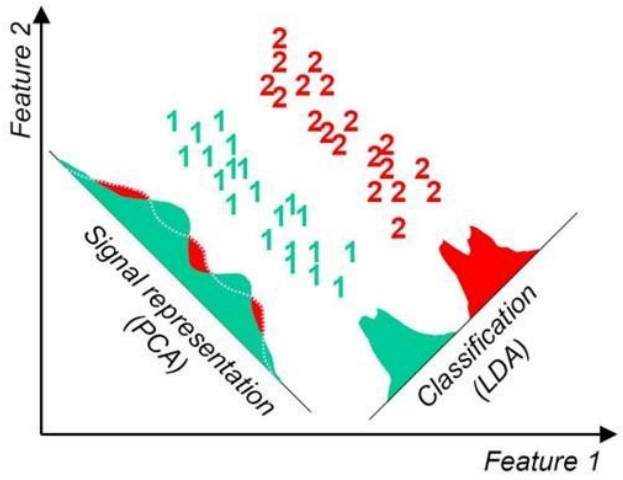


image source: 不想飞翔，不是因为没有翅膀，而是失去了梦想

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