

# Lecture 7: Dimensionality Reduction

**Pattern Recognition (in Computer Vision)** 

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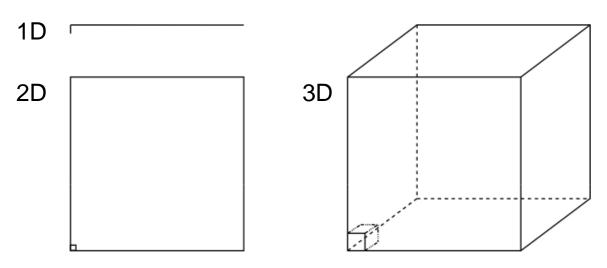
#### (Tentative) Schedule

- L1. Introduction to PR
- L2. Images and Transformations
- L3. Color and Filters
- L4. Features and Fitting
- L5. Feature Descriptors
- L6. Clustering and Segmentation
- L7. Dimensionality Reduction
- L8. Face identification
- L9. Bayesian Decision Theory
- L10. Image Classification
- L11. Regularization and Optimization
- L12. Image Classification with CNNs
- L13. CNN Architectures

- L14. Training Neural Networks
- L15. Object Detection and Image Segmentation
- L16. Recurrent Neural Networks
- L17. Attention and Transformers
- L18. Generative Models
- L19. Self-supervised Learning

#### Recap-Curse of dimensionality

- Assume 5000 points uniformly distributed in the unit hypercube and we want to apply 5-NN. Suppose our query point is at the origin.
  - In 1-dimension, we must go a distance of 5/5000 = 0.001 on the average to capture 5 nearest neighbors.
  - In 2 dimensions, we must go  $\sqrt{0.001}$  to get a square that contains 0.001 of the volume.
  - In d dimensions, we must go  $(0.001)^{1/d}$ .



#### What we will learn today

- Singular value decomposition
- Principal Component Analysis (PCA)
- Image compression

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- There are several computer algorithms that can "factorize" a matrix, representing it as the product of some other matrices.
- The most useful of these is the Singular Value Decomposition.
- Represents any matrix A as a product of three matrices:  $U\Sigma V^T$ .
- Python command:
  - [U,S,V]= numpy.linalg.svd(A)

$$U\Sigma V^T=A$$

 Where U and V are rotation matrices, and Σ is a scaling matrix. For example:

$$\begin{bmatrix} -.40 & .916 \\ .916 & .40 \end{bmatrix} \times \begin{bmatrix} 5.39 & 0 \\ 0 & 3.154 \end{bmatrix} \times \begin{bmatrix} -.05 & .999 \\ .999 & .05 \end{bmatrix} = \begin{bmatrix} 3 & -2 \\ 1 & 5 \end{bmatrix}$$

https://en.wikipedia.org/wiki/Rotation\_matrix

- Beyond 2 × 2 matrices:
  - In general, if A is  $m \times n$ , then U will be  $m \times m$ ,  $\Sigma$  will be  $m \times n$ , and  $V^T$  will be  $n \times n$ .
  - (Note the dimensions work out to produce  $m \times n$  after multiplication)

$$\begin{bmatrix} -.39 & -.92 \\ -.92 & .39 \end{bmatrix} \times \begin{bmatrix} 9.51 & 0 & 0 \\ 0 & .77 & 0 \end{bmatrix} \times \begin{bmatrix} -.42 & -.57 & -.70 \\ .81 & .11 & -.58 \\ .41 & -.82 & .41 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$

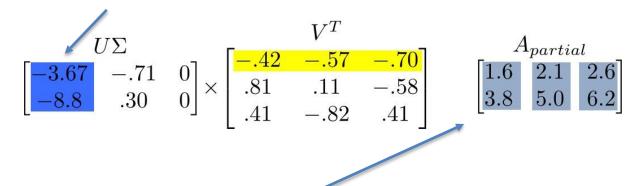
- U and V are always rotation matrices.
  - Geometric rotation may not be an applicable concept, depending on the matrix. So we call them "unitary" matrices – each column is a unit vector.
- Σ is a diagonal matrix
  - The number of nonzero entries = rank of A
  - The algorithm always sorts the entries high to low

$$\begin{bmatrix} -.39 & -.92 \\ -.92 & .39 \end{bmatrix} \times \begin{bmatrix} 9.51 & 0 & 0 \\ 0 & .77 & 0 \end{bmatrix} \times \begin{bmatrix} -.42 & -.57 & -.70 \\ .81 & .11 & -.58 \\ .41 & -.82 & .41 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$

- We've discussed SVD in terms of geometric transformation matrices.
- But SVD of an image matrix can also be very useful.
- To understand this, we'll look at a less geometric interpretation of what SVD is doing.

$$\begin{bmatrix} -.39 & -.92 \\ -.92 & .39 \end{bmatrix} \times \begin{bmatrix} 9.51 & 0 & 0 \\ 0 & .77 & 0 \end{bmatrix} \times \begin{bmatrix} -.42 & -.57 & -.70 \\ .81 & .11 & -.58 \\ .41 & -.82 & .41 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$

- Look at how the multiplication works out, left to right:
- Column 1 of U gets scaled by the first value from Σ.



 The resulting vector gets scaled by row 1 of V<sup>T</sup> to produce a contribution to the columns of A.

• Each product of (column i of U)-(value i from  $\Sigma$ )-(row i of  $V^T$ ) produces a component of the final A.

- We're building A as a linear combination of the columns of U.
- Using all columns of U, we'll rebuild the original matrix perfectly.
- But, in real-world data, often we can just use the first few columns of *U* and we'll get something close (e.g. the first A<sub>partial</sub>, above).

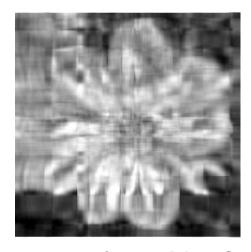
- We can call those first few columns of *U* the *Principal* Components of the data.
- They show the major patterns that can be added to produce the columns of the original matrix.
- The rows of  $V^T$  show how the *principal components* are mixed to produce the columns of the matrix.

$$\begin{bmatrix} -.39 & -.92 \\ -.92 & .39 \end{bmatrix} \times \begin{bmatrix} 9.51 & 0 & 0 \\ 0 & .77 & 0 \end{bmatrix} \times \begin{bmatrix} -.42 & -.57 & -.70 \\ .81 & .11 & -.58 \\ .41 & -.82 & .41 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$

We can look at  $\Sigma$  to see that the first column has a large effect

while the second column has a much smaller effect in this example





- For this image, using only the first 10 of 300 principal components produces a recognizable reconstruction.
- So, SVD can be used for image compression.

#### SVD for symmetric matrices

 If A is a symmetric matrix, it can be decomposed as the following:

$$A = \Phi \Sigma \Phi^T$$

• Compared to a traditional SVD decomposition,  $U = V^T$  and is an orthogonal matrix.

#### Principal Component Analysis

$$\begin{bmatrix} -3.67 & -.71 & 0 \\ -8.8 & .30 & 0 \end{bmatrix} \times \begin{bmatrix} -.42 & -.57 & -.70 \\ .81 & .11 & -.58 \\ .41 & -.82 & .41 \end{bmatrix} \qquad \begin{bmatrix} 1.6 & 2.1 & 2.6 \\ 3.8 & 5.0 & 6.2 \end{bmatrix}$$

- Remember, columns of *U* are the *Principal Components* of the data: the major patterns that can be added to produce the columns of the original matrix.
- One use of this is to construct a matrix where each column is a separate data sample.
- Run SVD on that matrix, and look at the first few columns of *U* to see patterns that are common among the columns.
- This is called Principal Component Analysis (or PCA) of the data samples.

#### Principal Component Analysis

$$\begin{bmatrix} -3.67 & -.71 & 0 \\ -8.8 & .30 & 0 \end{bmatrix} \times \begin{bmatrix} -.42 & -.57 & -.70 \\ .81 & .11 & -.58 \\ .41 & -.82 & .41 \end{bmatrix} \qquad \begin{bmatrix} 1.6 & 2.1 & 2.6 \\ 3.8 & 5.0 & 6.2 \end{bmatrix}$$

- Often, raw data samples have a lot of redundancy and patterns.
- PCA can allow you to represent data samples as weights on the principal components, rather than using the original raw form of the data.
- By representing each sample as just those weights, you can represent just the "meat" of what's different between samples.
- This minimal representation makes machine learning and other algorithms much more efficient.

#### How is SVD computed?

- For this class: tell PYTHON to do it. Use the result.
- But, if you're interested, one computer algorithm to do it makes use of Eigenvectors!

#### Eigenvector definition

- Suppose we have a square matrix A. We can solve for vector x and scalar  $\lambda$  such that  $Ax = \lambda x$ .
- In other words, find vectors where, if we transform them with A,
   the only effect is to scale them with no change in direction.
- These vectors are called eigenvectors, and the scaling factors λ
  are called eigenvalues.
- An  $m \times m$  matrix will have  $\leq m$  eigenvectors where  $\lambda$  is nonzero.

#### Finding eigenvectors

- Computers can find an x such that  $Ax = \lambda x$  using this iterative algorithm:
  - X = random unit vector
  - while(x hasn't converged)
    - $\bullet X = Ax$
    - normalize x
- x will quickly converge to an eigenvector.
- Some simple modifications will let this algorithm find all eigenvectors.

## Finding SVD

- Eigenvectors are for square matrices, but SVD is for all matrices
- To do svd(A), computers can do this:
  - Take eigenvectors of AA<sup>T</sup> (matrix is always square).
    - These eigenvectors are the columns of U.
    - Square root of eigenvalues are the singular values (the entries of  $\Sigma$ ).
  - Take eigenvectors of A<sup>T</sup>A (matrix is always square).
    - These eigenvectors are columns of V (or rows of V<sup>T</sup>)

#### Finding SVD

- Moral of the story: SVD is fast, even for large matrices
- It's useful for a lot of stuff.
- There are also other algorithms to compute SVD or part of the SVD.
  - Python's np.linalg.svd() command has options to efficiently compute only what you need, if performance becomes an issue.

A detailed geometric explanation of SVD is here: <a href="http://www.ams.org/samplings/feature-column/fcarc-svd">http://www.ams.org/samplings/feature-column/fcarc-svd</a>

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#### Covariance

- Variance and Covariance are a measure of the "spread" of a set of points around their center of mass (mean).
- Variance measure of the deviation from the mean for points in one dimension, e.g. heights.
- Covariance as a measure of how much each of the dimensions vary from the mean with respect to each other.
- Covariance is measured between 2 dimensions to see if there is a relationship between the 2 dimensions e.g. number of hours studied & marks obtained.
- The covariance between one dimension and itself is the variance.

covariance 
$$(X,Y) = \sum_{i=1}^{n} (\overline{X_i} - X) (\overline{Y_i} - Y)$$
  
 $(n-1)$ 

#### unbiased estimate

So, if you had a 3-dimensional data set (x, y, z), then you could measure the covariance between the x and y dimensions, the y and z dimensions, and the x and z dimensions. Measuring the covariance between x and x, or y and y, or z and z would give you the variance of the x, y and z dimensions respectively.

#### Covariance matrix

 Representing Covariance between dimensions as a matrix, e.g. for 3 dimensions.

$$C = cov(x,x) cov(x,y) cov(x,z)$$

$$cov(y,x) cov(y,y) cov(x,z)$$

$$cov(z,x) cov(z,y) cov(z,z)$$
Variances

- Diagonal is the variances of x, y and z.
- cov(x,y) = cov(y,x) hence matrix is symmetrical about the diagonal.
- N-dimensional data will result in  $N \times N$  covariance matrix.

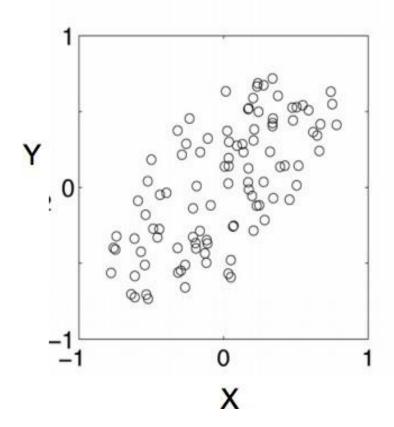
#### Covariance

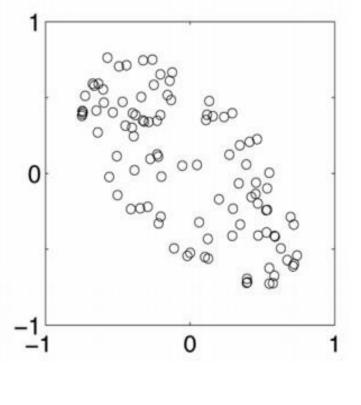
- What is the interpretation of covariance calculations?
  - e.g.: 2 dimensional data set
  - x: number of hours studied for a subject
  - y: marks obtained in that subject
  - covariance value is say: 104.53
  - what does this value mean?

#### Covariance interpretation

# positive covariance

# negative covariance



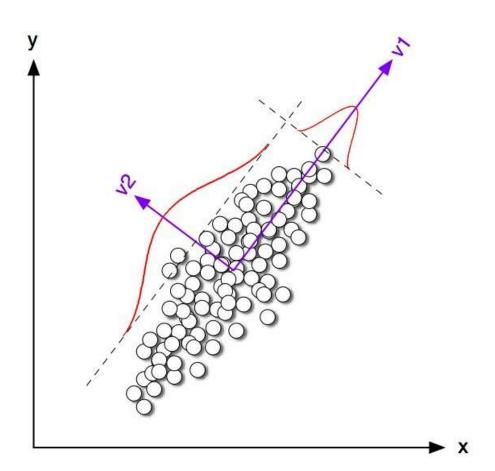


#### Covariance interpretation

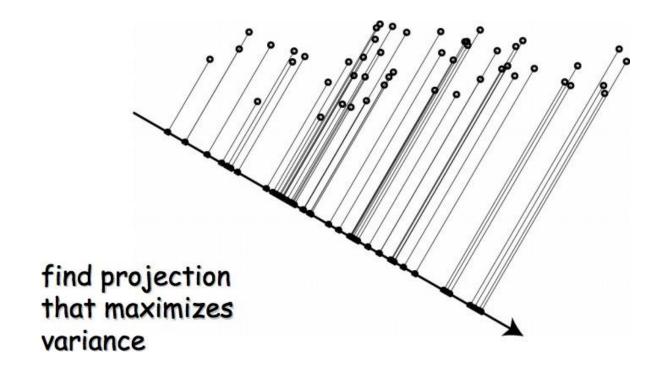
- Exact value is not as important as it's sign.
- A positive value of covariance indicates both dimensions increase or decrease together e.g. as the number of hours studied increases, the marks in that subject increase.
- A negative value indicates while one increases the other decreases, or vice-versa, e.g. active social life vs performance in CS dept.
- If covariance is zero: the two dimensions are independent of each other e.g. heights of students vs the marks obtained in a subject

#### Example data

Covariance between the two axis is high. Can we reduce the number of dimensions to just 1?

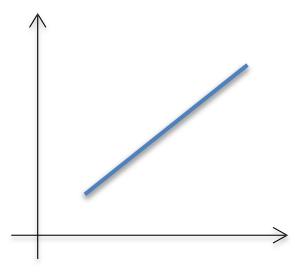


#### Geometric interpretation of PCA



#### Geometric interpretation of PCA

- Let's say we have a set of 2D data points x. But we see that all the points lie on a line in 2D.
- So, 2 dimensions are redundant to express the data. We can express all the points with just one dimension.

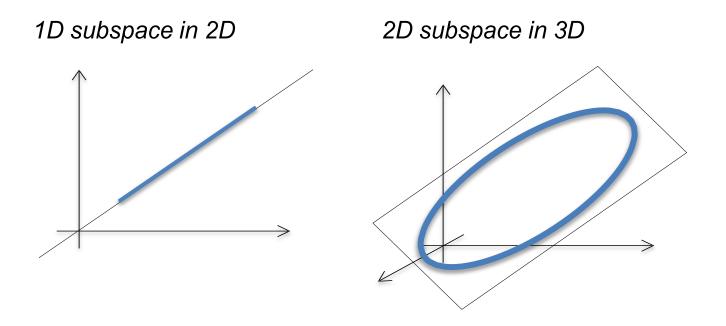


#### PCA: Principle Component Analysis

- Given a set of points, how do we know if they can be compressed like in the previous example?
  - The answer is to look into the correlation between the points.
  - The tool for doing this is called PCA.

#### **PCA** Formulation

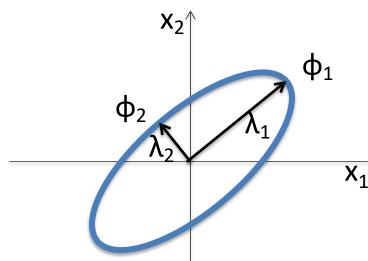
- Basic idea:
  - If the data lives in a subspace, it is going to look very flat when viewed from the full space, e.g.



#### **PCA** Formulation

- Assume x is Gaussian with covariance Σ.
- Recall that a gaussian is defined with it's mean and variance:

$$\mathbf{X} \, \sim \, \mathcal{N}(oldsymbol{\mu}, \, oldsymbol{\Sigma})$$



• Recall that  $\mu$  and  $\Sigma$  of a gaussian are defined as:

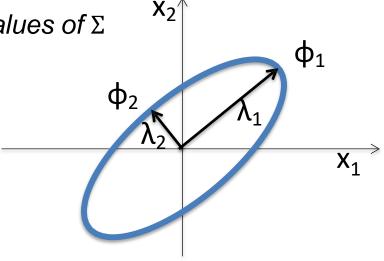
$$oldsymbol{\mu} = \mathrm{E}[\mathbf{X}] = [\mathrm{E}[X_1], \mathrm{E}[X_2], \ldots, \mathrm{E}[X_k]]^{\mathrm{T}}$$

$$\mathbf{\Sigma} =: \mathrm{E}[(\mathbf{X} - oldsymbol{\mu})(\mathbf{X} - oldsymbol{\mu})^{\mathrm{T}}] = [\mathrm{Cov}[X_i, X_j]; 1 \leq i, j \leq k]$$

#### **PCA** Formulation

- If x is Gaussian with covariance Σ,
  - Principal components φ<sub>i</sub> are the eigenvectors of Σ

• Principal lengths  $\lambda_i$  are the eigenvalues of  $\Sigma$ 



- by computing the eigenvalues we know the data is
  - Not flat if  $\lambda_1 \approx \lambda_2$
  - Flat if  $\lambda_1 >> \lambda_2$

# PCA Algorithm (training)

- Given sample  $\mathcal{D} = \{x_1, ..., x_n\}, x_i \in \mathcal{R}^d$ 
  - Compute sample mean:  $\hat{\mu} = \frac{1}{n} \sum_{i} x_{i}$ .
  - Compute sample covariance:  $\hat{\Sigma} = \frac{1}{n} \sum_{i} (x_i \hat{\mu}) (x_i \hat{\mu})^T$ .
  - Compute eigenvalues and eigenvectors of  $\hat{\Sigma}$ .

$$\hat{\Sigma} = \Phi \Lambda \Phi^T, \Lambda = diag(\sigma_1^2, ..., \sigma_n^2), \Phi^T \Phi = I$$

- Order eigenvalues  $\sigma_1^2 > \cdots > \sigma_n^2$ .
- If, for a certain k,  $\sigma_k \ll \sigma_1$ , eliminate the eigenvalues and eigenvectors above k.

# PCA Algorithm (testing)

- Given principal compoents  $\Phi_i$ ,  $i \in 1, ..., k$  and a test sample  $\mathcal{T} = \{t_1, ..., t_n\}$ ,  $t_i \in \mathcal{R}^d$ 
  - Subtract mean to each point  $t'_i = t_i \hat{\mu}$
  - Project onto eigenvector space  $y_i = At'_i$ , where

$$\mathbf{A} = \begin{bmatrix} \phi_1^T \\ \vdots \\ \phi_k^T \end{bmatrix}$$

• Use  $T' = \{y_1, ..., y_n\}$  to estimate class conditional densities and do all further processing on y.

- An alternative manner to compute the principal components, based on singular value decomposition.
- Quick reminder: SVD
  - Any real  $n \times m$  matrix (n > m) can be decomposed as

$$A = M\Pi N^T$$

- Where M is an  $(n \times m)$  column orthonormal matrix of left singular vectors (columns of M)
- $\Pi$  is an  $(m \times m)$  diagonal matrix of singular values
- $N^T$  is an  $(m \times m)$  row orthonormal matrix of right singular vectors (columns of N)

$$M^T M = I \qquad N^T N = I$$

To relate this to PCA, we consider the data matrix

$$X = \begin{bmatrix} 1 & & 1 \\ x_1 & \dots & x_n \\ 1 & & 1 \end{bmatrix}$$

The sample mean is

$$\mu = \frac{1}{n} \sum_{i} X_{i} = \frac{1}{n} \begin{bmatrix} 1 & & & | \\ X_{1} & \dots & X_{n} \\ | & & | \end{bmatrix} \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} = \frac{1}{n} X 1$$

- Center the data by subtracting the mean to each column of X
- The centered data matrix is

$$X_{c} = \begin{bmatrix} 1 & 1 & 1 \\ X_{1} & \dots & X_{n} \\ 1 & 1 \end{bmatrix} - \begin{bmatrix} 1 & 1 \\ \mu & \dots & \mu \\ 1 & 1 \end{bmatrix}$$
$$= X - \mu \mathbf{1}^{T} = X - \frac{1}{n} X \mathbf{1} \mathbf{1}^{T} = X \left( I - \frac{1}{n} \mathbf{1} \mathbf{1}^{T} \right)$$

The sample covariance matrix is

$$\Sigma = \frac{1}{n} \sum_{i} (x_i - \mu)(x_i - \mu)^T = \frac{1}{n} \sum_{i} x_i^c (x_i^c)^T$$

where  $x_i^c$  is the *i*th column of  $X_c$ 

This can be written as

$$\Sigma = \frac{1}{n} \begin{bmatrix} 1 & & 1 \\ x_1^c & \dots & x_n^c \\ 1 & & 1 \end{bmatrix} \begin{bmatrix} - & x_1^c & - \\ & \vdots & \\ - & x_n^c & - \end{bmatrix} = \frac{1}{n} X_c X_c^T$$

The matrix

$$\boldsymbol{X}_{c}^{T} = \begin{bmatrix} - & \boldsymbol{X}_{1}^{c} & - \\ & \vdots & \\ - & \boldsymbol{X}_{n}^{c} & - \end{bmatrix}$$

is real  $(n \times d)$ . Assuming n > d it has SVD decomposition

$$X_c^T = M\Pi N^T$$

$$\mathbf{M}^T \mathbf{M} = \mathbf{I} \qquad \mathbf{N}^T \mathbf{N} = \mathbf{I}$$

and

$$\Sigma = \frac{1}{n} X_c X_c^T = \frac{1}{n} N \Pi M^T M \Pi N^T = \frac{1}{n} N \Pi^2 N^T$$

$$\Sigma = N \left( \frac{1}{n} \Pi^2 \right) N^T$$

- Note that N is  $(d \times d)$  and orthonormal, and  $\Pi^2$  is diagonal. This is just the eigenvalue decomposition of  $\Sigma$
- It follows that
  - The eigenvectors of Σ are the columns of N
  - The eigenvalues of Σ are

$$\lambda_i = \frac{1}{n} \pi_i^2$$

This gives an alternative algorithm for PCA.

- In summary, computation of PCA by SVD
- Given X with one example per column
  - Create the centered data matrix

$$\boldsymbol{X}_{c}^{T} = \left(\boldsymbol{I} - \frac{1}{n} \boldsymbol{1} \boldsymbol{1}^{T}\right) \boldsymbol{X}^{T}$$

Compute its SVD

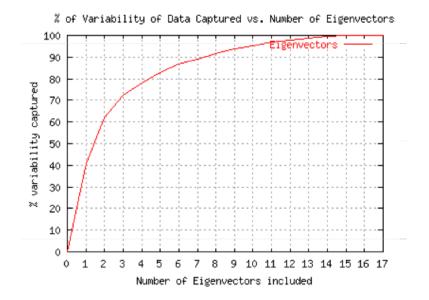
$$X_c^T = M\Pi N^T$$

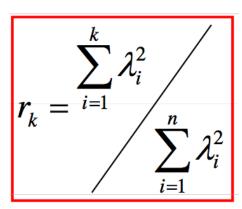
Principal components are columns of N, eigenvalues are

$$\lambda_i = \frac{1}{n} \pi_i^2$$

# Rule of thumb for finding the number of PCA components

- A natural measure is to pick the eigenvectors that explain p% of the data variability.
  - Can be done by plotting the ratio  $r_k$  as a function of k





E.g. we need 3 eigenvectors to cover 70% of the variability of this dataset.

## What we will learn today

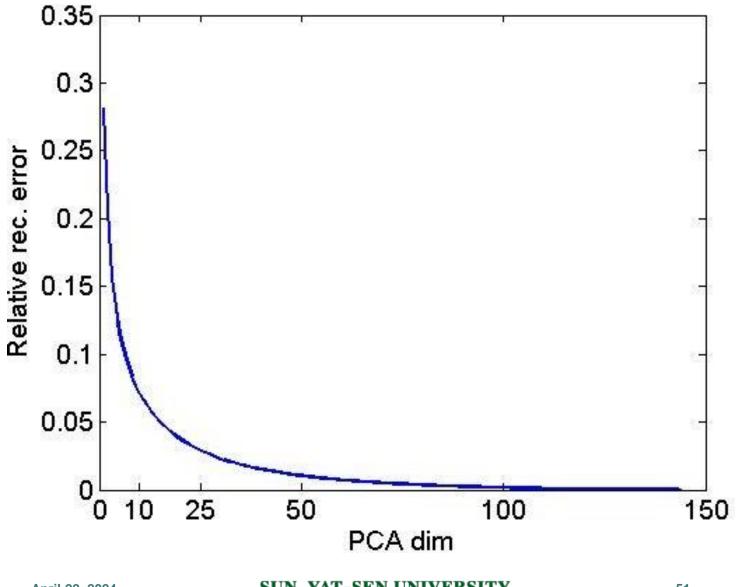
- Singular value decomposition
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- Image compression

## Original Image



- Divide the original 372x492 image into patches:
  - Each patch is an instance that contains 12x12 pixels on a grid
- View each as a 144-D vector

# L<sub>2</sub> error and PCA dim



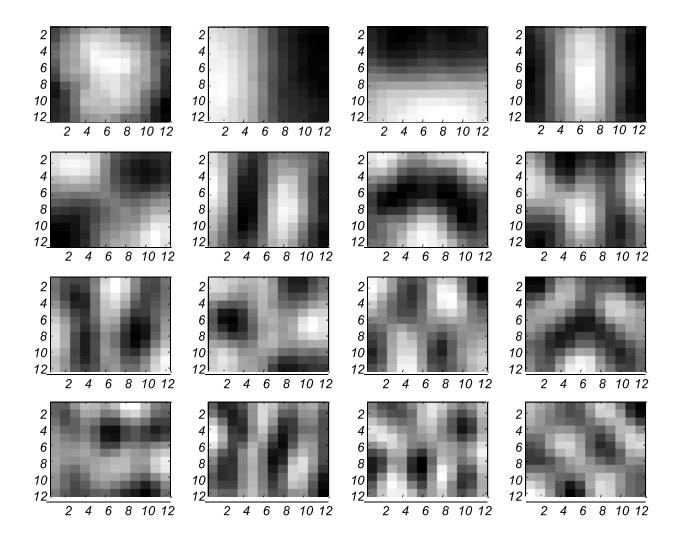
# PCA compression: 144D → 60D



# PCA compression: 144D → 16D



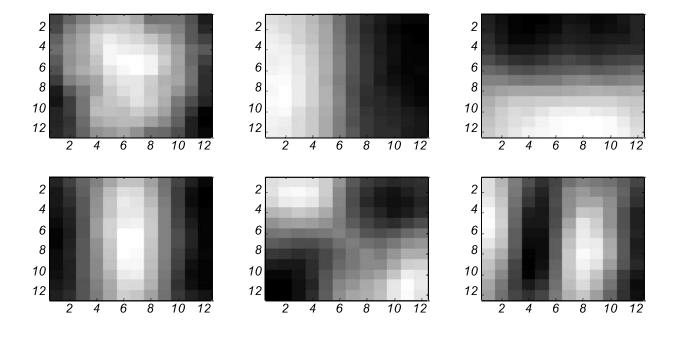
# 16 most important eigenvectors



# PCA compression: 144D → 6D



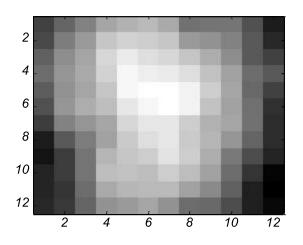
# 6 most important eigenvectors

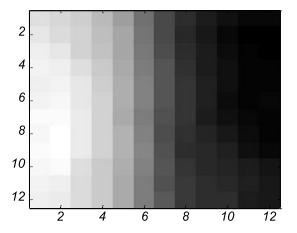


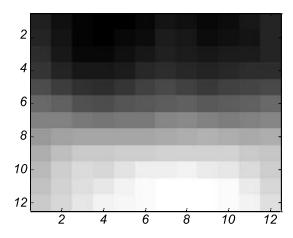
# PCA compression: 144D → 3D



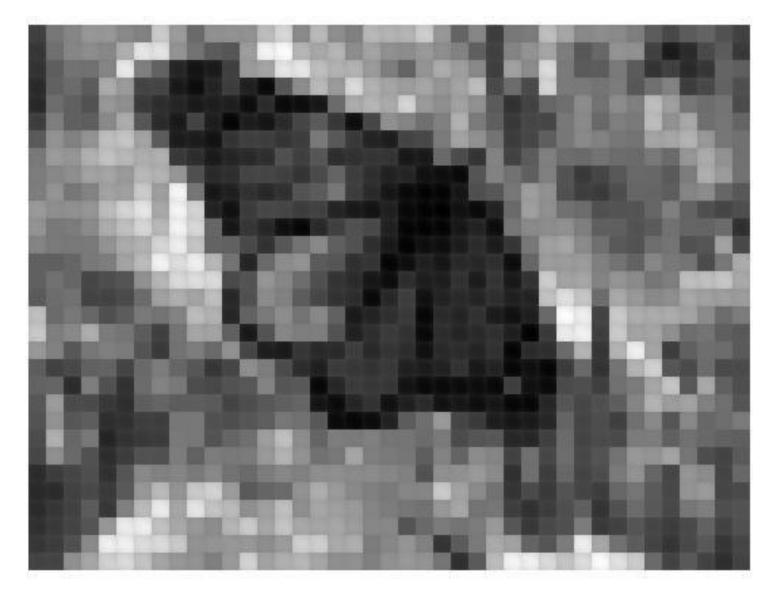
# 3 most important eigenvectors



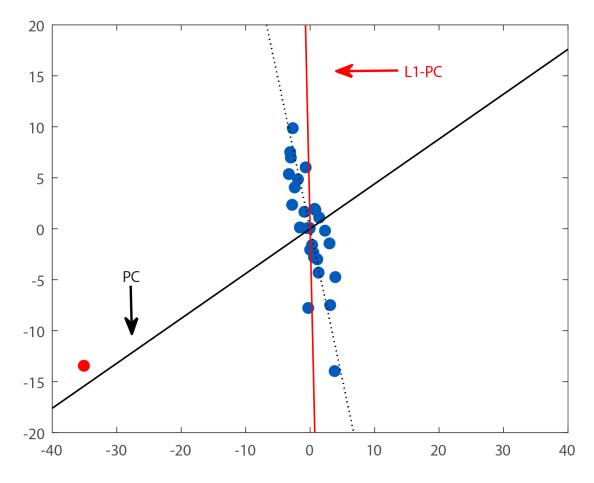




# PCA compression: 144D → 1D



#### PCA vs L1 PCA



https://en.wikipedia.org/wiki/L1-norm principal component analysis

## What we have learned today

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- Principal Component Analysis (PCA)
- Image compression



# Next time:

# Face Identification

**Pattern Recognition (in Computer Vision)** 

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