# CPSC 340: Machine Learning and Data Mining

More PCA Summer 2021

#### In This Lecture

#### 1. How to Learn PCA:

- Sequential Fitting and SVD
- Alternating Minimization

#### 2. Eigenfaces

Coming Up Next

#### PCA OBJECTIVE FUNCTION

#### PCA Objective Function

In PCA we minimize the squared error of the approximation:

$$f(W,Z) = \sum_{i=1}^{2} ||W|_{Z_{i}} - x_{i}||^{2}$$

$$||W|_{Z_{i}} - x_{i}||^{2}$$

- This is equivalent to the k-means objective:
  - Think of  $z_i$  as one-hot encoding of  $\hat{y_i}$
- But in PCA, z<sub>i</sub> can be any real number.
  - We approximate x<sub>i</sub> as a linear combination of all factors.

## PCA Objective Function

In PCA we minimize the squared error of the approximation:

$$f(W,z) = \sum_{j=1}^{n} ||W^{T}z_{j} - x_{j}||^{2} = \sum_{j=1}^{n} \int_{approximation}^{d} (\langle w_{j}z_{j} \rangle - x_{ij})^{2}$$

$$approximation feature's if example 'i' in the proximation of the example 'i' in the e$$

- We can also view this as solving 'd' regression problems:
  - Each wi is a model predicting column xi from the features of  $z_i$ . Moldin  $(7, x^i)$ 
    - The output " $y_i$ " = each feature of  $x_i$ .
  - Unlike in regression: learn the features of z<sub>i</sub>.

## Principal Component Analysis (PCA)

The 3 different ways to write the PCA objective function:

$$f(W,Z) = \sum_{i=1}^{n} \sum_{j=1}^{d} (\langle w_{i}, z_{i} \rangle - x_{ij})^{2} \qquad (approximating x_{ij} by \langle w_{i}, z_{i} \rangle)$$

$$= \sum_{i=1}^{n} ||W^{T}z_{i} - x_{i}||^{2} \qquad (approximating x_{i} by W_{Z_{i}}^{T})$$

$$= ||ZW - X||_{F}^{2} \qquad (approximating X_{ij} by Z_{W})$$

#### Digression: Data Centering (Important)

- In PCA, we assume that the data X is "centered".
  - Each column of X has a mean of zero.
- It's easy to center the data:

Set 
$$M_j = \frac{1}{n} \sum_{i=1}^{n} x_{ij}$$
 (mean of colum 'j')

Replace each  $x_{ij}$  with  $(x_{ij} - M_j)$ 

- There are PCA variations that estimate "bias in each coordinate".
  - In basic model this is equivalent to centering the data.

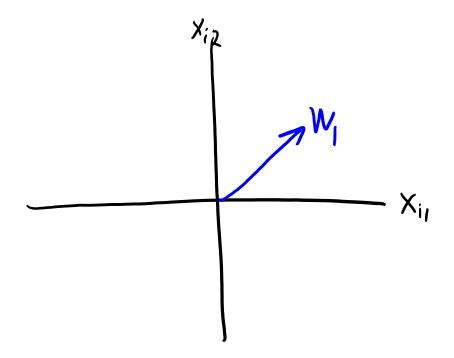
Coming Up Next

## NON-UNIQUENESS OF PCA AND SPANS OF FACTORS

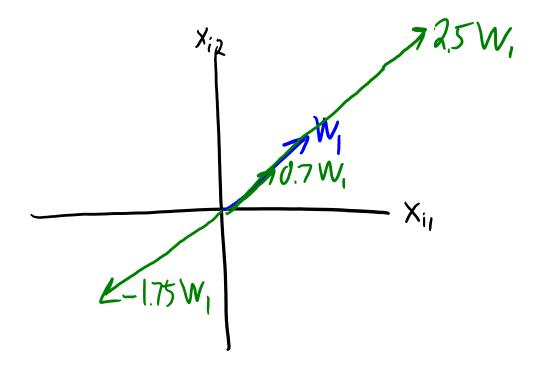
#### Non-Uniqueness of PCA

- Unlike k-means, we can efficiently find global optima of f(W,Z).
  - Algorithms coming later.
- Unfortunately, PCA never has a unique global optimum.
  - Several different sources of non-uniqueness (coming up soon)
- To understand these, we'll use "span" from linear algebra.
  - Helps explain the geometry of PCA.
  - Some global optima may be better than others. (coming up soon)

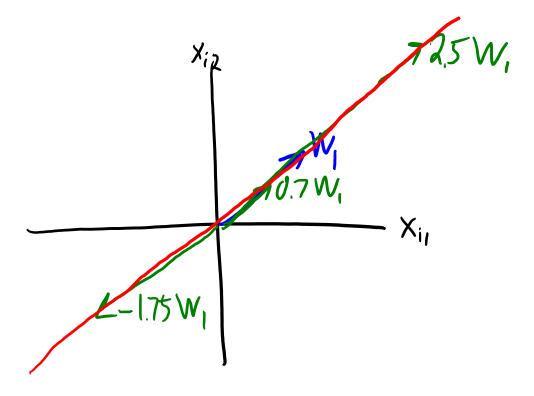
Consider a single vector w<sub>1</sub> (k=1).



- Consider a single vector w<sub>1</sub> (k=1).
- The span( $w_1$ ) is all vectors of the form  $z_i w_1$  for a scalar  $z_i$ .

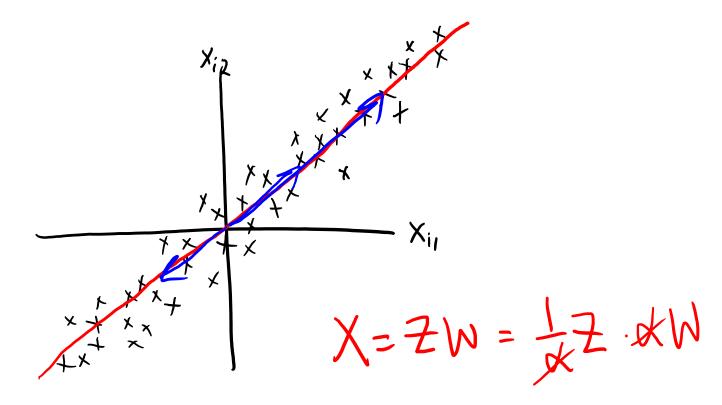


- Consider a single vector w<sub>1</sub> (k=1).
- The span( $w_1$ ) is all vectors of the form  $z_i w_1$  for a scalar  $z_i$ .



• If  $w_1 \neq 0$ , this forms a line.

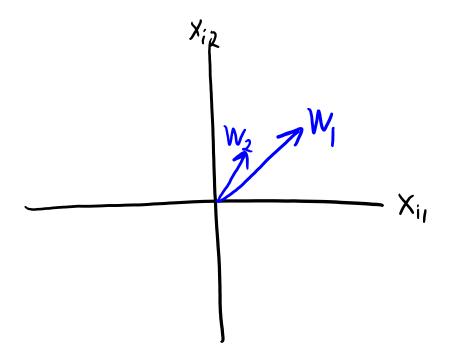
- Span of many different vectors gives same line.
  - Mathematically:  $\alpha w_1$  defines the same line as  $w_1$  for any scalar  $\alpha \neq 0$ .



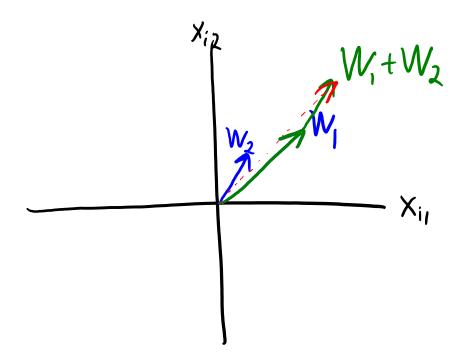
- PCA solution is non-unique: (solution \* scalar) is still PCA solution.
  - If (W,Z) is a solution, then  $(\alpha W,(1/\alpha)Z)$  is also a solution.

$$\|(x W)(\frac{1}{4}Z) - X\|_{F}^{2} = \|W2x\|_{F}^{2}$$

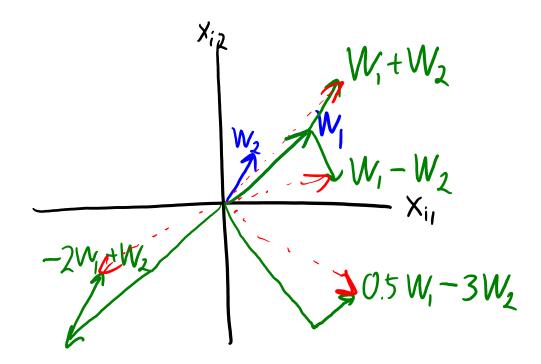
• Consider two vectors  $w_1$  and  $w_2$  (k=2).



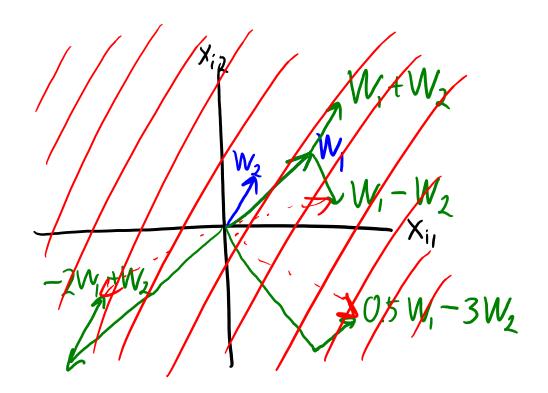
- Consider two vectors w<sub>1</sub> and w<sub>2</sub> (k=2).
  - The span( $w_1, w_2$ ) is all vectors of form  $z_{i1}w_1 + z_{i2}w_2$  for any scalars  $z_{i1}$  and  $z_{i2}$ .



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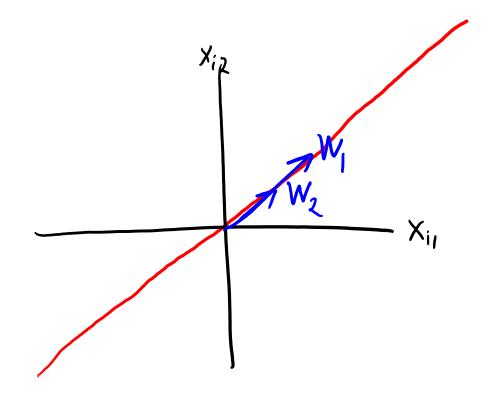


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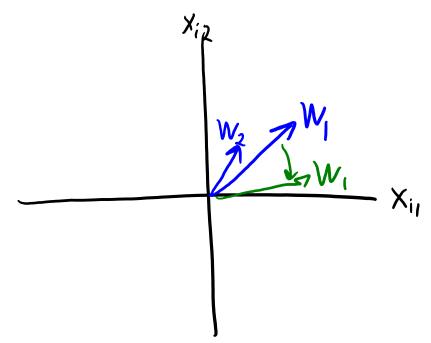
- For most non-zero 2d vectors, span( $w_1, w_2$ ) is a plane.
  - In the case of two vectors in R<sup>2</sup>, the plane will be \*all\* of R<sup>2</sup>.

- Consider two vectors w<sub>1</sub> and w<sub>2</sub> (k=2).
  - The span( $w_1, w_2$ ) is all vectors of form  $z_{i1}w_1 + z_{i2}w_2$  for any scalars  $z_{i1}$  and  $z_{i2}$ .



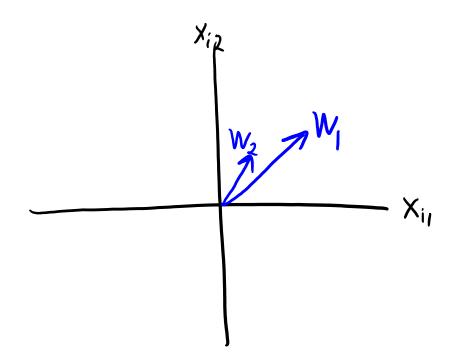
- For most non-zero 2d vectors, span( $w_1, w_2$ ) is plane.
  - Exception is if  $w_2$  is in span of  $w_1$  ("collinear"), then span( $w_1, w_2$ ) is just a line.

- Consider two vectors w<sub>1</sub> and w<sub>2</sub> (k=2).
  - The span( $w_1, w_2$ ) is all vectors of form  $z_{i1}w_1 + z_{i2}w_2$  for any scalars  $z_{i1}$  and  $z_{i2}$ .

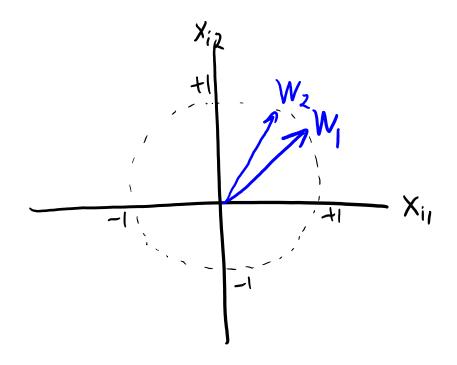


- New issues for PCA ( $k \ge 2$ ):
  - We have label switching:  $span(w_1, w_2) = span(w_2, w_1)$ .
  - We can rotate factors within the plane (if not rotated to be collinear).

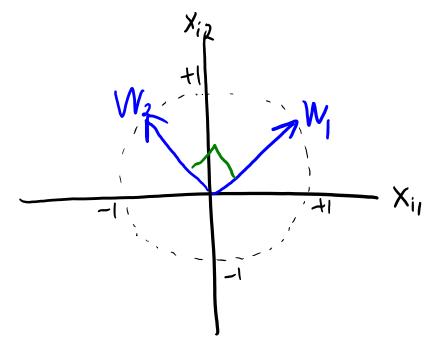
- 2 tricks to make vectors defining a plane "more unique":
  - Normalization: enforce that  $||w_1|| = 1$  and  $||w_2|| = 1$ .



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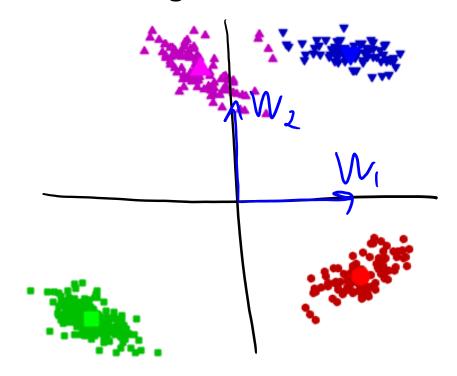
- 2 tricks to make vectors defining a plane "more unique":
  - Normalization: enforce that  $||w_1|| = 1$  and  $||w_2|| = 1$ .
  - Orthogonality: enforce that  $w_1^T w_2 = 0$  ("perpendicular").



- Can't grow/shrink vectors (though I can still reflect).
- Can't rotate one vector (but I can still rotate \*both\*).

#### Digression: PCA only makes sense for $k \le d$

• Remember our clustering dataset with 4 clusters:



- It doesn't make sense to use PCA with k=4 on this dataset.
  - Only need two vectors [1 0] and [0 1] to exactly represent all 2d points.
    - With k=2, set Z=X and W=I to get X=ZW exactly.

## Span in Higher Dimensions

- In higher-dimensional spaces:
  - Span of 1 non-zero vector  $\mathbf{w}_1$  is a line.
  - Span of 2 non-zero vectors  $w_1$  and  $w_2$  is a plane (if not collinear).
    - Can be visualized as a 2D plot.
  - Span of 3 non-zeros vectors  $\{w_1, w_2, w_3\}$  is a 3d space (if not "coplanar").



- This is how the W matrix in PCA defines lines, planes, spaces, etc.
  - Each time we increase 'k', we add an extra "dimension" to the "subspace".

## Making PCA Unique

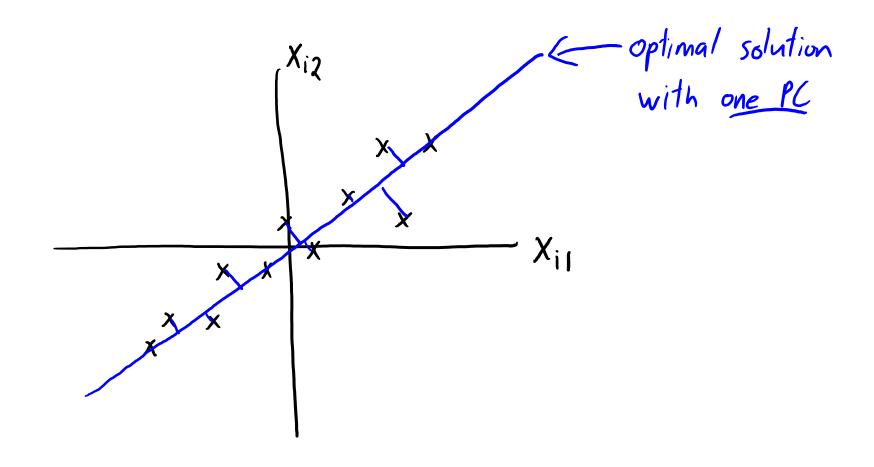
- We've identified several reasons that optimal W is non-unique:
  - Multiply any w<sub>c</sub> by any non-zero scalar.
  - Rotate any w<sub>c</sub> almost arbitrarily within the span.
  - Switch any  $w_c$  with any other  $w_{c'}$ .

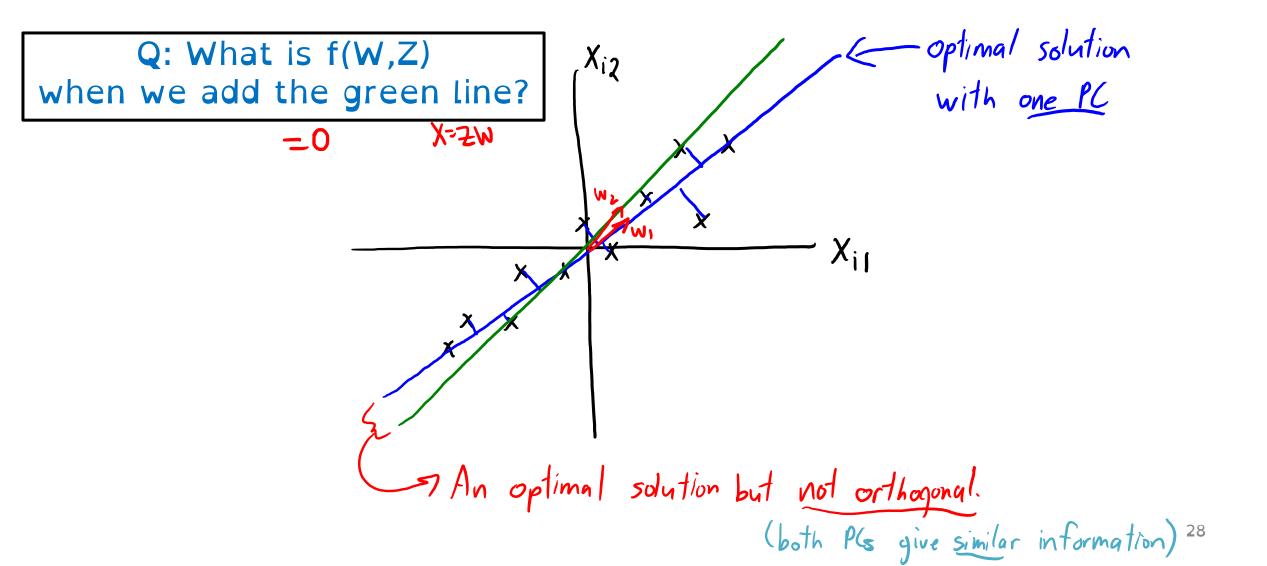
- PCA implementations add constraints to make solution unique:

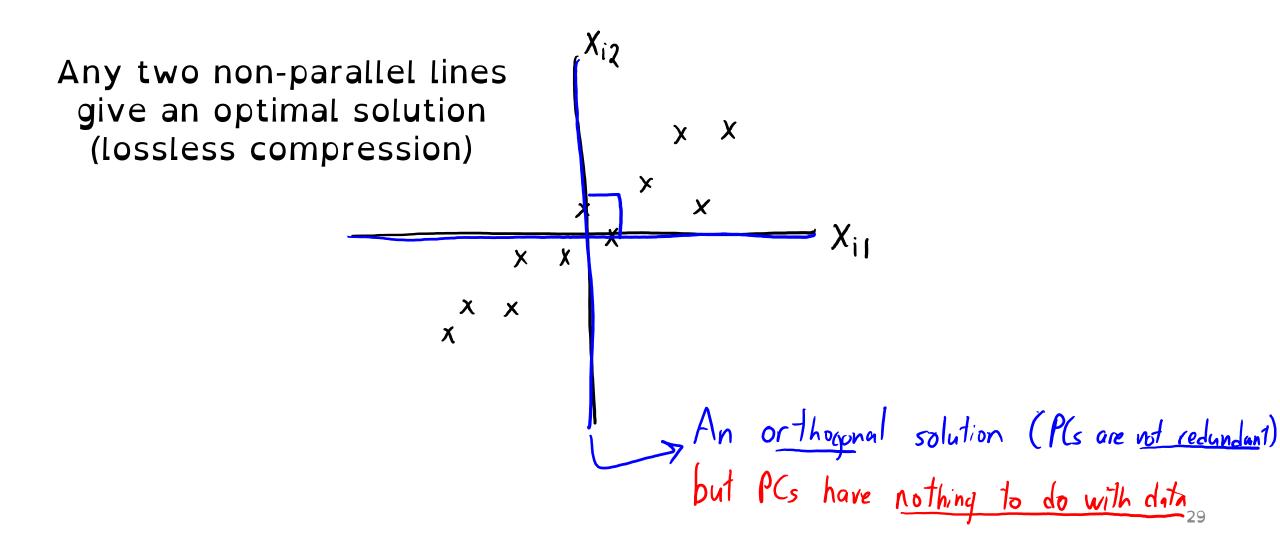
  - Normalization: enforce that  $||w_c|| = 1$ . Orthogonality: enforce that  $w_c^T w_{c'} = 0$  for all  $c \neq c'$ .
  - Sequential fitting: First fit w<sub>1</sub> ("first principal component") giving a line.
    - Then fit  $w_2$  given  $w_1$  ("second principal component") giving a plane.
    - Then we fit w<sub>3</sub> given w<sub>1</sub> and w<sub>2</sub> ("third principal component") giving a water. \*\*

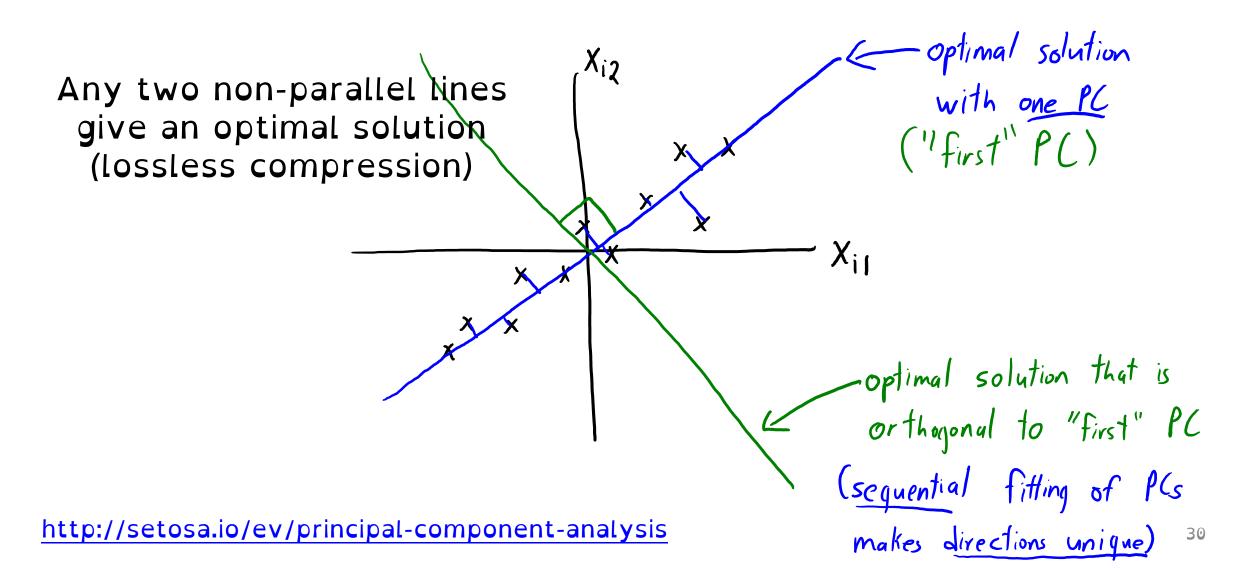
Coming Up Next

#### SEQUENTIAL FITTING AND SVD









#### PCA Computation: SVD

- How do we fit with normalization/orthogonality/sequential-fitting?
  - It can be done with the "singular value decomposition" (SVD).
  - Take CPSC 302 or MATH 307
- 4 lines of Python code:
  - mu = np.mean(X,axis=0)
  - X -= mu
  - U, s, Vh = np.linalg.svd(X)
  - W = Vh[:k, :]

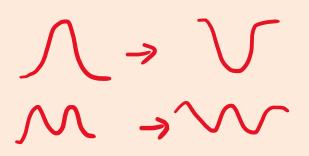
Computing Z is cheaper now:

$$Z = XW^{T}(WW^{T})^{-1} = XW^{T}$$

$$WW^{T} = \begin{bmatrix} -W_{1} - W_{2} - W_{3} - W_{4} \\ -W_{2} - W_{4} - W_{5} \end{bmatrix}$$

$$= \begin{bmatrix} 1000 - 0 \\ 6100 & 0 \\ 0 & -01 \end{bmatrix} = I$$

$$= I$$
31



Coming Up Next

#### ALTERNATING MINIMIZATION

#### PCA Computation

- With linear regression, we had the normal equations
  - But we also could do it with gradient descent, SGD, etc.
- With PCA we have the SVD
  - But we can also do it with gradient descent, SGD, etc.
- Gradient-based methods don't enforce uniqueness
  - Sensitive to initialization, don't enforce normalization, orthogonality, ordered PCs.
  - But you can do this in post-processing if you want.
- Why would we want this? We can use our tricks from Part 3 of the course:
  - We can do things like "robust" PCA (A6), "regularized" PCA, "sparse" PCA, "binary" PCA.
  - We can fit huge datasets where SVD is too expensive.

#### PCA Computation: Alternating Minimization

With centered data, the PCA objective is:

$$f(W,z) = \sum_{i=1}^{n} \sum_{j=1}^{d} (\langle w_{j}^{i} z_{i} \rangle - \chi_{ij})^{2}$$

- In k-means we optimized this with alternating minimization:
  - Fix "cluster assignments" Z and find the optimal "means" W.
  - Fix "means" W and find the optimal "cluster assignments" Z.
- Converges to a local optimum.
  - But may not find a global optimum (sensitive to initialization).

#### PCA Computation: Alternating Minimization

With centered data, the PCA objective is:

$$f(W, Z) = \sum_{i=1}^{n} \sum_{j=1}^{d} (\langle w_{j}^{i} z_{i} \rangle - \chi_{ij})^{2}$$

- In PCA we can also use alternating minimization:
  - Fix "scores" Z, find optimal "factors" W.
  - Fix "factors" W, find optimal "scores" Z.
- Converges to a local optimum.
  - Which will be a global optimum (if we randomly initialize W and Z).

#### PCA Computation: Alternating Minimization

With centered data, the PCA objective is:

$$f(W,z) = \sum_{i=1}^{n} \sum_{j=1}^{d} (\langle w_{j}^{i} z_{i} \rangle - \chi_{ij})^{2}$$

- Alternating minimization steps:
  - If we fix Z, this is a quadratic function of W (least squares column-wise):

$$\nabla_{W} f(W,Z) = Z^{T}ZW - Z^{T}X \qquad 50 \qquad W = (Z^{T}Z)^{T}(Z^{T}X)$$
(writing gradient as a matrix)

- If we fix W, this is a quadratic function of Z (transpose due to dimensions):

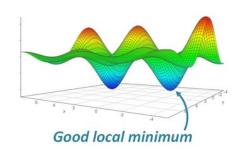
$$\nabla_z f(w,z) = ZWW^T - XW^T$$
 so  $Z = XW^T(\underline{w}\underline{w}^T)^{-1}$ 

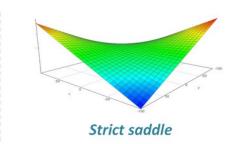
Those are usually wertible since keep and keep

#### PCA Computation: Alternating Minimization

With centered data, the PCA objective is:

$$f(W, 2) = \sum_{i=1}^{n} \sum_{j=1}^{d} (\langle w_{j}^{i} z_{i} \rangle - \chi_{ij})^{2}$$





- This objective is not jointly convex in W and Z.
  - You will find different W and Z depending on the initialization.
    - For example, if you initialize with all  $w_c = 0$ , then they will stay at zero.
  - But it's possible to show that all "stable" local optima are global optima.
    - You will converge to a global optimum in practice if you initialize randomly.
      - Randomization means you don't start on one of the unstable non-global critical points.
    - E.g., sample each initial  $z_{ij}$  from a normal distribution.

### PCA Computation: Stochastic Gradient

For big X matrices, you can also use stochastic gradient:

$$f(W,z) = \sum_{i=1}^{n} \sum_{j=1}^{d} (\langle w_{j}^{i} z_{i} \rangle - \chi_{ij})^{2} = \sum_{(i,j)} (\langle w_{j}^{i} z_{i} \rangle - \chi_{ij})^{2}$$

• Other variables stay the same, cost per iteration is only O(k). 38

## PCA Computation: Prediction

- At the end of training, the "model" is the  $\mu_i$  and the W matrix.
  - PCA is parametric.
- PCA prediction phase:
  - Given new data  $\tilde{X}$ , we can use  $\mu_j$  and W this to form  $\tilde{Z}$ :

1. (enter: replace each 
$$\tilde{x}_{ij}$$
 with  $(\tilde{x}_{ij} - u_j)$ 

2. Find  $\tilde{Z}$  minimizing squared error:

$$\tilde{Z} = \tilde{X} W^T (WW^T)$$

txx txd  $\tilde{x}_{ik}$   $\tilde{x}_{ik}$ 

## PCA Computation: Prediction

- At the end of training, the "model" is the  $\mu_i$  and the W matrix.
  - PCA is parametric.
- PCA prediction phase:
  - Given new data  $\tilde{X}$ , we can use  $\mu_j$  and W this to form  $\tilde{Z}$ :
  - The "reconstruction error" is how close approximation is to  $\tilde{X}$ :

$$\frac{1}{2} \frac{2}{2} W - \frac{2}{2} |_{F}^{2}$$
Centered version

- Our "error" from replacing the  $x_i$  with the  $z_i$  and W.

### Choosing 'k' by "Variance Explained"

Common to choose 'k' based on variance of the x<sub>ii</sub>.

$$Var(x_{ij}) = E[(x_{ij} - u_{ij})^2] = E[(x_{ij})^2] = Ad \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} x_{ij}^2 = \frac{1}{nd} ||x||_F^2$$

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$$Var(x_{ij}) = E[(x_{ij}$$

- For a given 'k' we compute (variance of errors)/(variance of  $x_{ii}$ ):

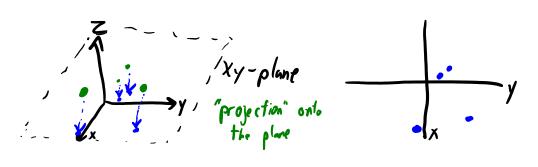
- Gives a number between 0 (k=d) and 1 (k=0), giving "variance remaining".
  - If you want to "explain 90% of variance", choose smallest 'k' where ratio is < 0.10.

#### "Variance Explained" in the Goat Situation

Recall: Crazy goats:







Interpretation of "variance remaining" formula:

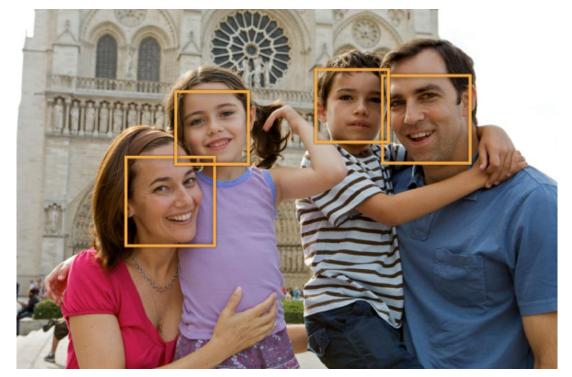
• If we had a 3D map the "variance remaining" would be 0.

Coming Up Next

#### **EIGENFACES**

### Application: Face Detection

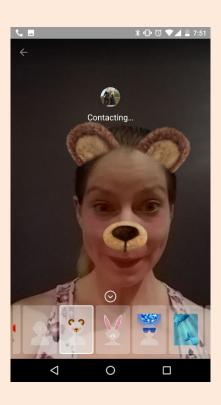
Consider problem of face detection:

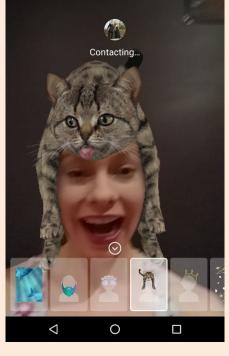


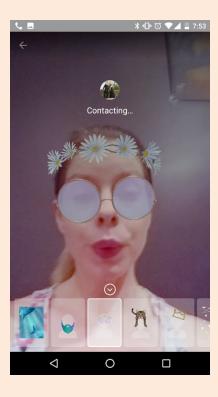
- Classic methods use "eigenfaces" as basis:
  - PCA applied to images of faces.

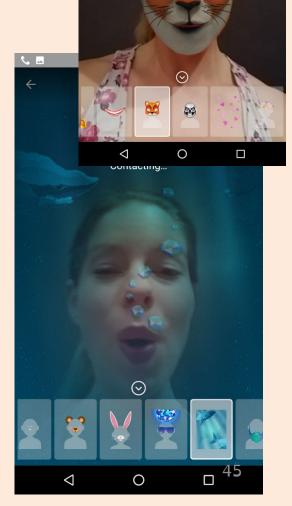


### Application: Face Detection

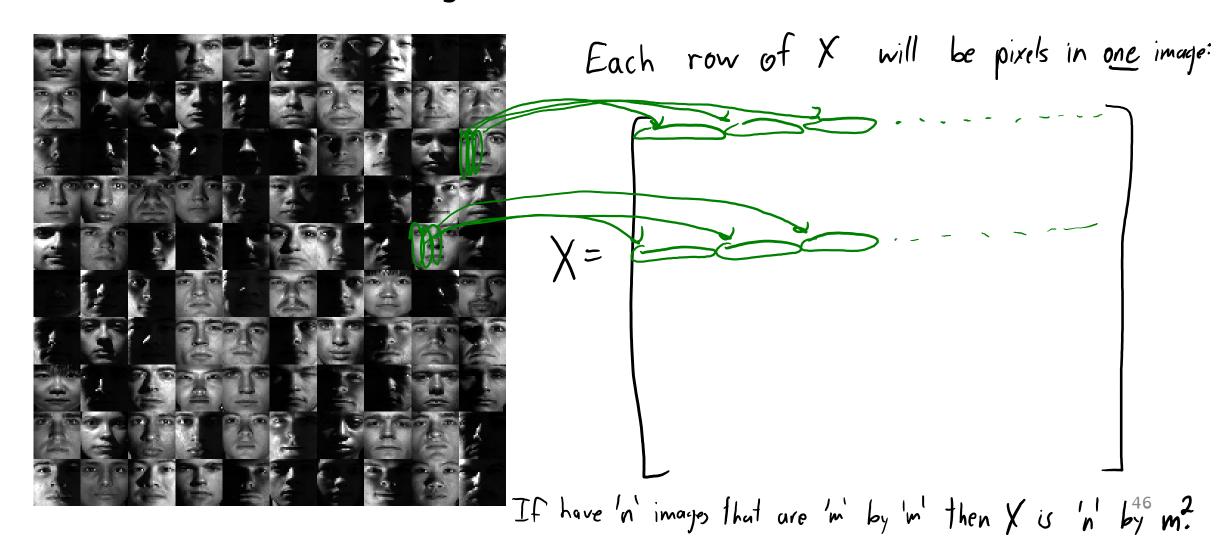








Collect a bunch of images of faces under different conditions:



Compute mean us of each column,



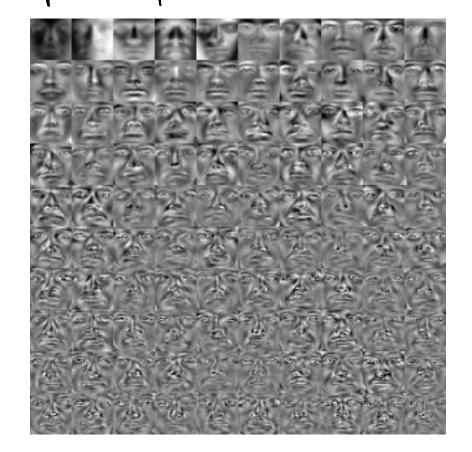
"canonical face" according to data

Replace each Xij by Xij - Mj

Each row of X will be pixels in one image:

$$X = \begin{bmatrix} x_1 - \mu \\ x_2 - \mu \end{bmatrix}$$

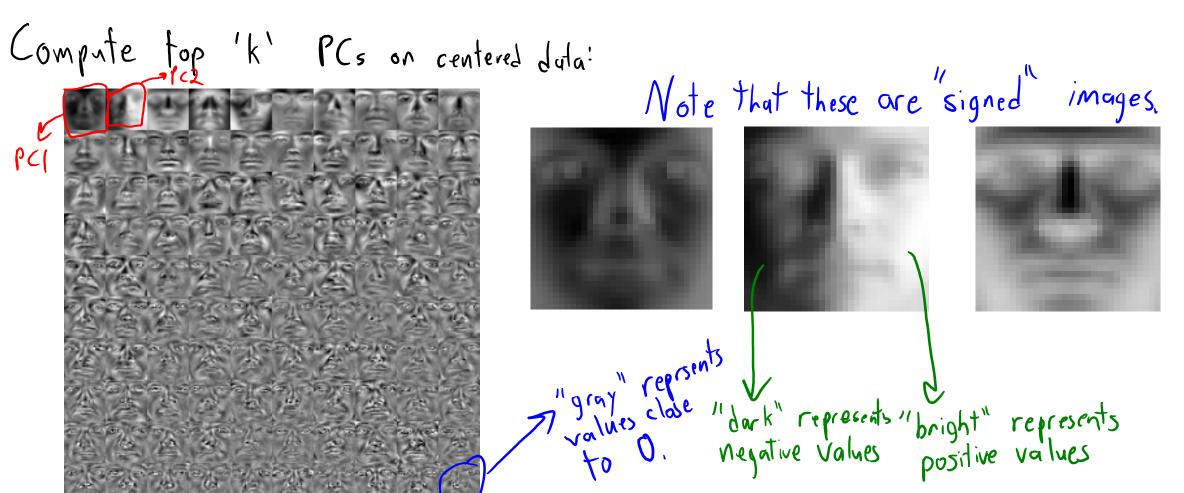
Compute top 'k' PCs on centered duta: Each row of X will be pixels in one image:



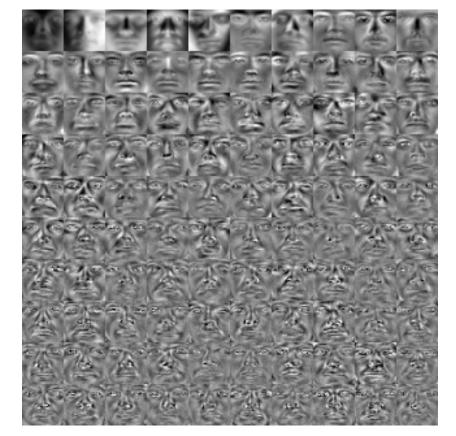
$$X_1 - M$$

$$X_2 - M$$

$$X_3 - M$$



Compute top 'k' PCs on centered dula:



$$\hat{x}_{i} = \frac{1}{2} + \frac{1$$

100 of the original faces:

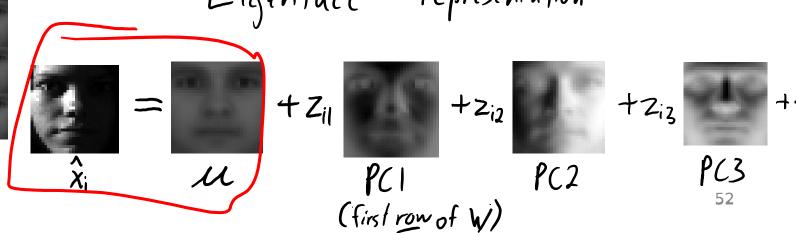


$$\hat{x}_{i} = \frac{1}{x_{i1}} + \frac{1}{x_{i2}} + \frac{1}{x_{i2}} + \frac{1}{x_{i3}} + \frac{1}{x_{i3}} + \frac{1}{x_{i4}} + \frac{1}{x_{$$

Reconstruction with K= 0

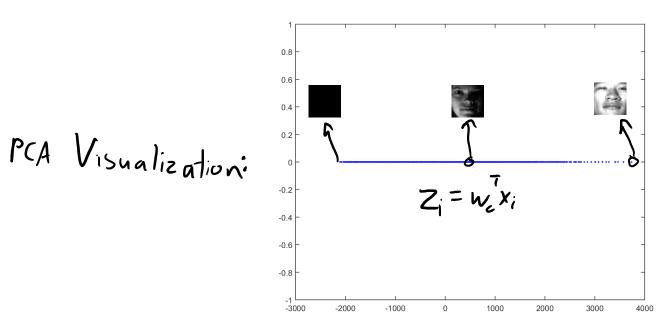


Variance explained: 0%



Reconstruction with K=1

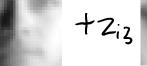




"Eigenface" representation:

+ Z11







Variance explained: 36%

M

PC2

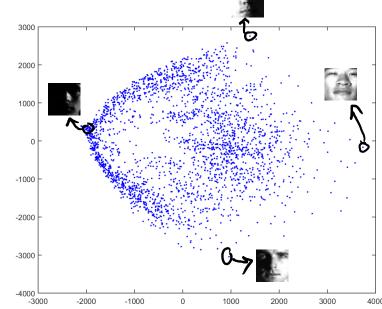
PC3

Reconstruction with K=2



Variance explained: 71%

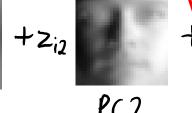
PCA Visualization



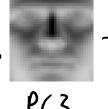
"Eigenface" representation:

$$\frac{1}{\hat{x}_{i}} = \frac{1}{\mathcal{L}} + Z_{il}$$









PC3

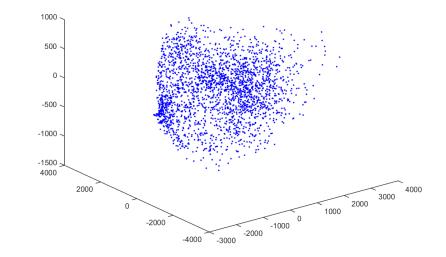
(first row of W.

Reconstruction with K= 3



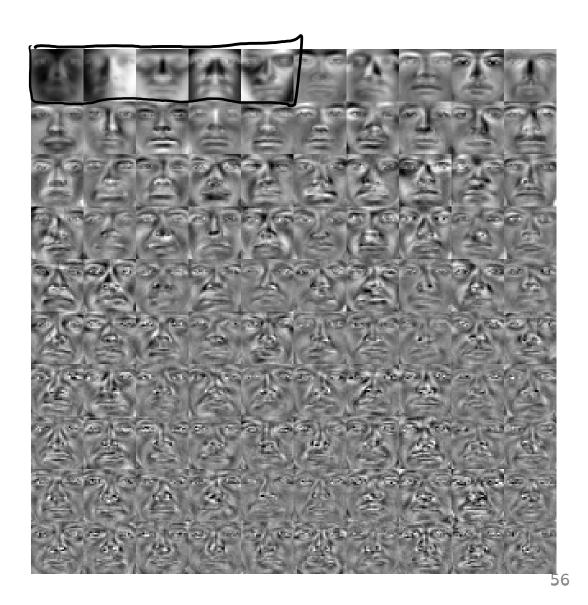
Variance explained: 76%

PCA Visualization



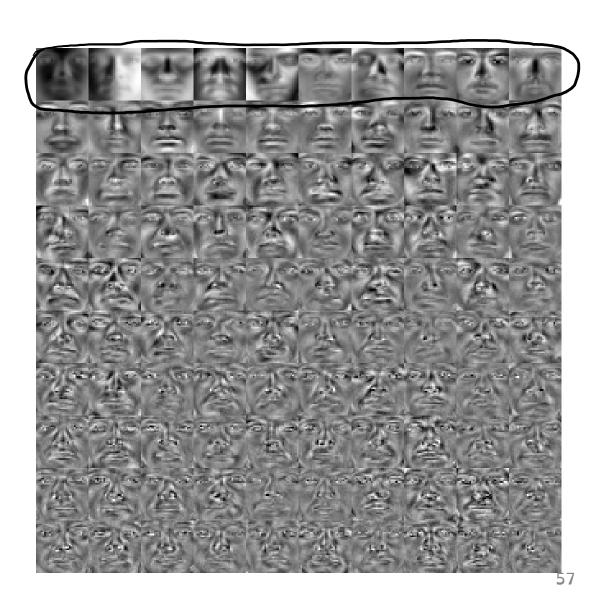


Variance explained: 86%



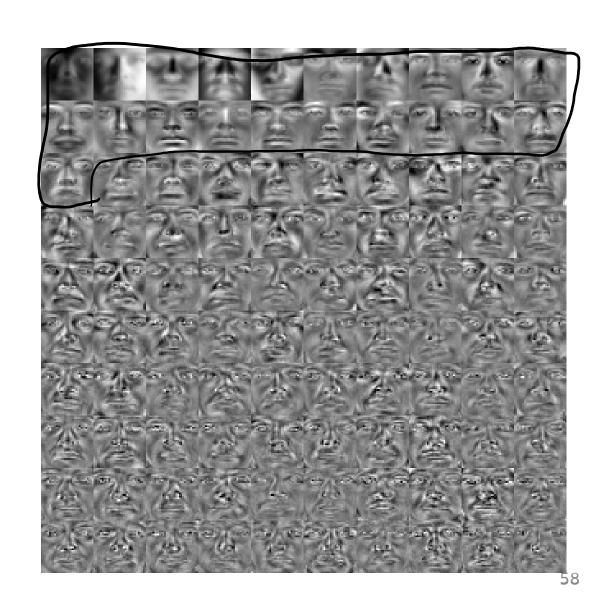


Variance explained: 85%



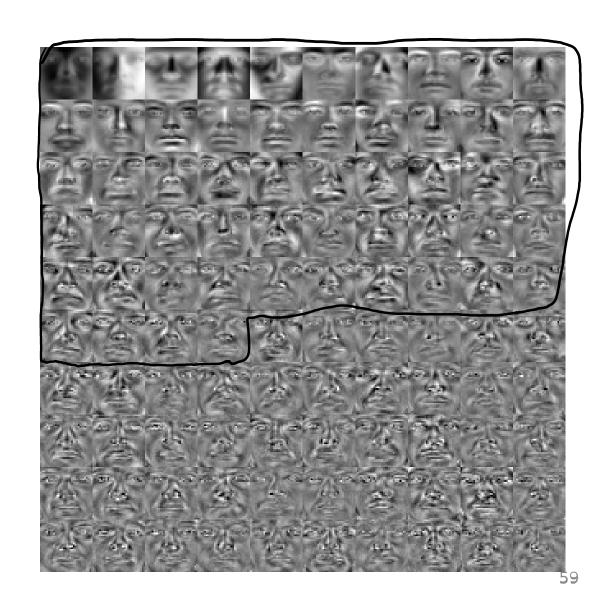


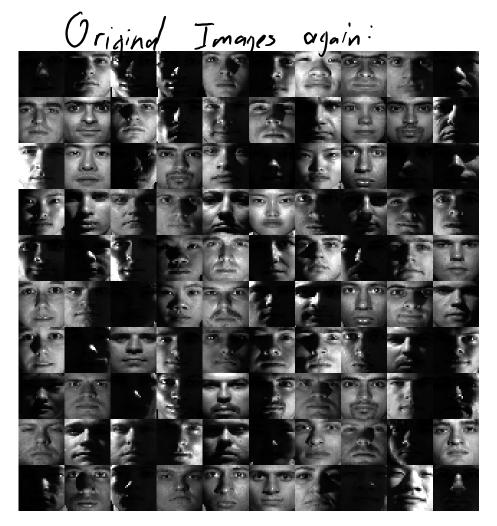
Variance explained: 90%



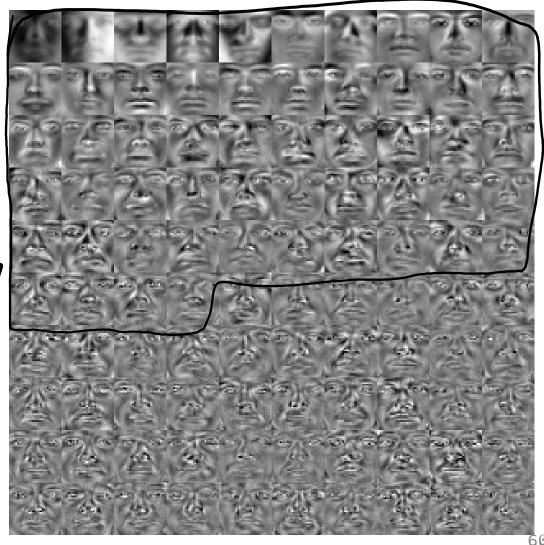


Variance explained: 95%





Plus these "eigenfaces" & and the mean



We con replace 1024 x; values by 54 z; values

### Summary

- PCA objective:
  - Minimizes squared error between elements of X and elements of ZW.
- Choosing 'k':
  - We can choose 'k' to explain "percentage of variance" in the data.
- PCA non-uniqueness:
  - Due to scaling, rotation, and label switching.
- Orthogonal basis and sequential fitting of PCs (via SVD):
  - Leads to non-redundant PCs with unique directions.
- Alternating minimization and stochastic gradient:
  - Iterative algorithms for minimizing PCA objective.
- · Next time: cancer signatures and NBA shot charts.

### Review Questions

• Q1: How is PCA's objective function similar to k-means clustering's objective function?

Q2: What makes PCA solutions non-unique?

• Q3: Why don't normalization and orthogonality guarantee the uniqueness of PCA solutions?

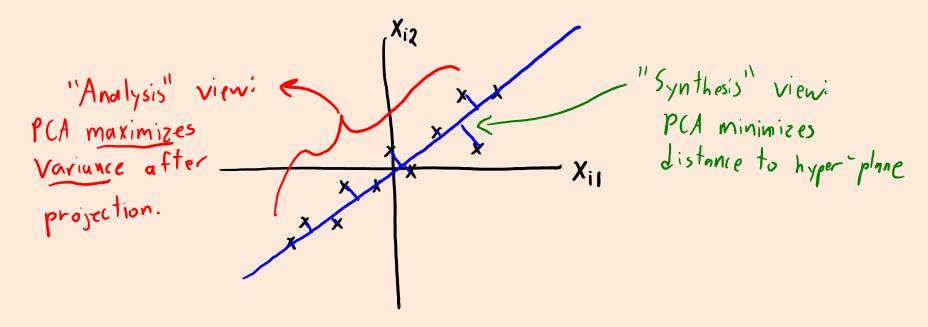
• Q4: How are "variance remaining" and "variance explained" related?

## Making PCA Unique

- PCA implementations add constraints to make solution unique:
  - Normalization: we enforce that  $||\mathbf{w}_c|| = 1$ .
  - Orthogonality: we enforce that  $w_c^T w_{c'} = 0$  for all  $c \neq c'$ .
  - Sequential fitting: We first fit  $w_1$  ("first principal component") giving a line.
    - Then fit  $w_2$  given  $w_1$  ("second principal component") giving a plane.
    - Then we fit  $w_3$  given  $w_1$  and  $w_2$  ("third principal component") giving a space.
    - ...
- Even with all this, the solution is only unique up to sign changes:
  - I can still replace any  $w_c$  by  $-w_c$ :
    - $-w_c$  is normalized, is orthogonal to the other  $w_{c'}$ , and spans the same space.
  - Possible fix: require that first non-zero element of each  $w_c$  is positive.
  - And this is assuming you don't have repeated singular values.
    - In that case you can rotate the repeated ones within the same plane.

### "Synthesis" View vs. "Analysis" View

- We said that PCA finds hyper-plane minimizing distance to data x<sub>i</sub>.
  - This is the "synthesis" view of PCA (connects to k-means and least squares).

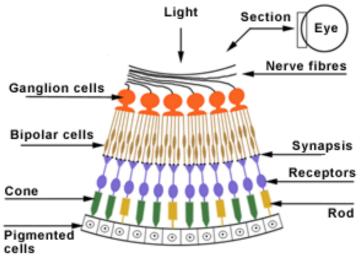


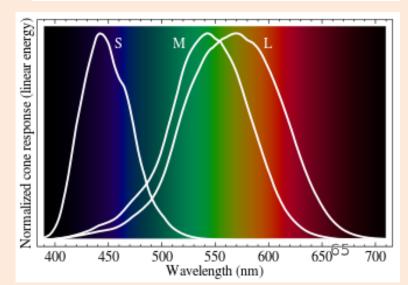
- "Analysis" view when we have orthogonality constraints:
  - PCA finds hyper-plane maximizing variance in z<sub>i</sub> space.
  - You pick W to "explain as much variance in the data" as possible.

### Colour Opponency in the Human Eye

Classic model of the eye is with 4 photoreceptors:

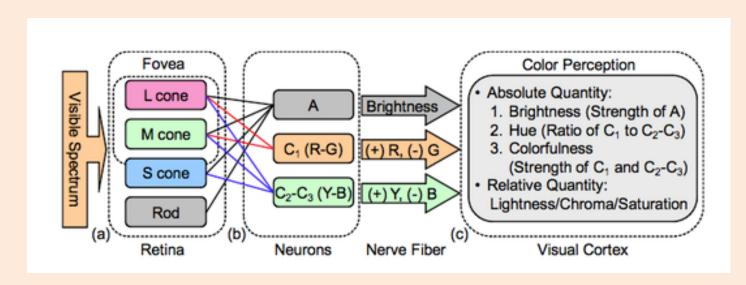
- Rods (more sensitive to brightness).
- L-Cones (most sensitive to red).
- M-Cones (most sensitive to green).
- S-Cones (most sensitive to blue).
- Two problems with this system:
  - Not orthogonal.
    - High correlation in particular between red/green.
  - We have 4 receptors for 3 colours.



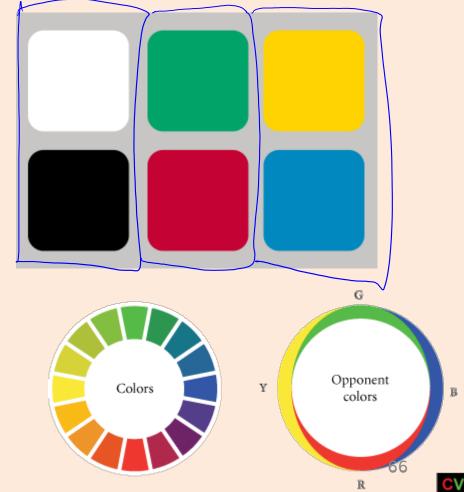


### Colour Opponency in the Human Eye

- Bipolar and ganglion cells seem to code using "opponent colors":
  - 3-variable orthogonal basis:



• This is similar to PCA (d = 4, k = 3).



## Colour Opponency Representation

