CPSC 340:
Machine Learning and Data Mining

More PCA

Summer 2021

In This Lecture

1. Formal Details of PCA
2. Sequential Fitting and SVD
3. Alternative Optimization

Coming Up Next

PCA OBJECTIVE FUNCTION AND "VARIANCE EXPLAINED"

PCA Objective Function

- In PCA we minimize the squared error of the approximation:

$$f(W,Z) = \sum_{i=1}^{n} \| \underbrace{W^T z_i}_{\text{approximation}} - \underbrace{x_i}_{\text{example 'i'}} \|^2$$

- This is equivalent to the k-means objective:
  - In k-means z_i only has a single '1' value and other entries are zero.
- But in PCA, z_i can be any real number.
  - We approximate x_i as a linear combination of all factors.

PCA Objective Function

- In PCA we minimize the squared error of the approximation:

$$f(W,Z) = \sum_{i=1}^{n} \| \underbrace{W^T z_i}_{\text{approximation}} - \underbrace{x_i}_{\text{example 'i'}} \|^2 = \sum_{i=1}^{n} \sum_{j=1}^{d} (\underbrace{\langle w^j, z_i \rangle}_{\text{approximation}} - \underbrace{x_{ij}}_{\text{feature 'j' of example 'i'}})^2$$

- We can also view this as solving 'd' regression problems:
  - Each w^j is trying to predict column 'x^j' from the basis z_i.
    - The output "y_i" we try to predict here is actually the features "x_i".
  - And unlike in regression we are also learning the features z_i.

Principal Component Analysis (PCA)

- The 3 different ways to write the PCA objective function:

$$f(W,Z) = \sum_{i=1}^{n}\sum_{j=1}^{d}(\langle w^j, z_i\rangle - x_{ij})^2 \quad \text{(approximating } x_{ij} \text{ by } \langle w^j, z_i\rangle\text{)}$$

$$= \sum_{i=1}^{n}\|W^T z_i - x_i\|^2 \quad \text{(approximating } x_i \text{ by } W^T z_i\text{)}$$

$$= \|ZW - X\|_F^2 \quad \text{(approximating } X \text{ by } ZW\text{)}$$

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

Replace each x_{ij} with $(x_{ij} - \mu_j)$

- 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

Non-Uniqueness of PCA

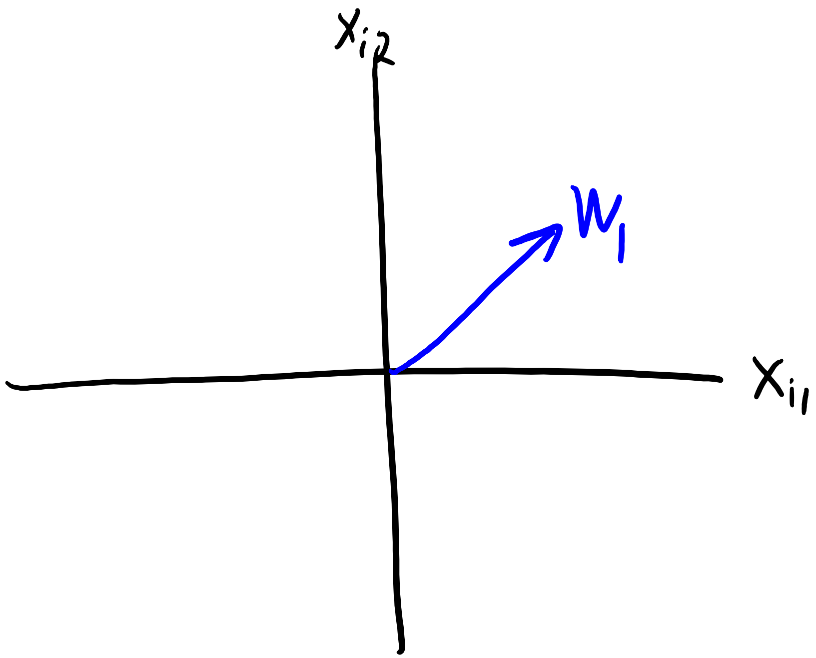
- Unlike k-means, we can efficiently find global optima of f(W,Z).
  - Algorithms coming later.

- Unfortunately, there never exists a unique global optimum.
  - There are actually several different sources of non-uniqueness.

- To understand these, we'll need idea of "span" from linear algebra.
  - This also helps explain the geometry of PCA.
  - We'll also see that some global optima may be better than others.

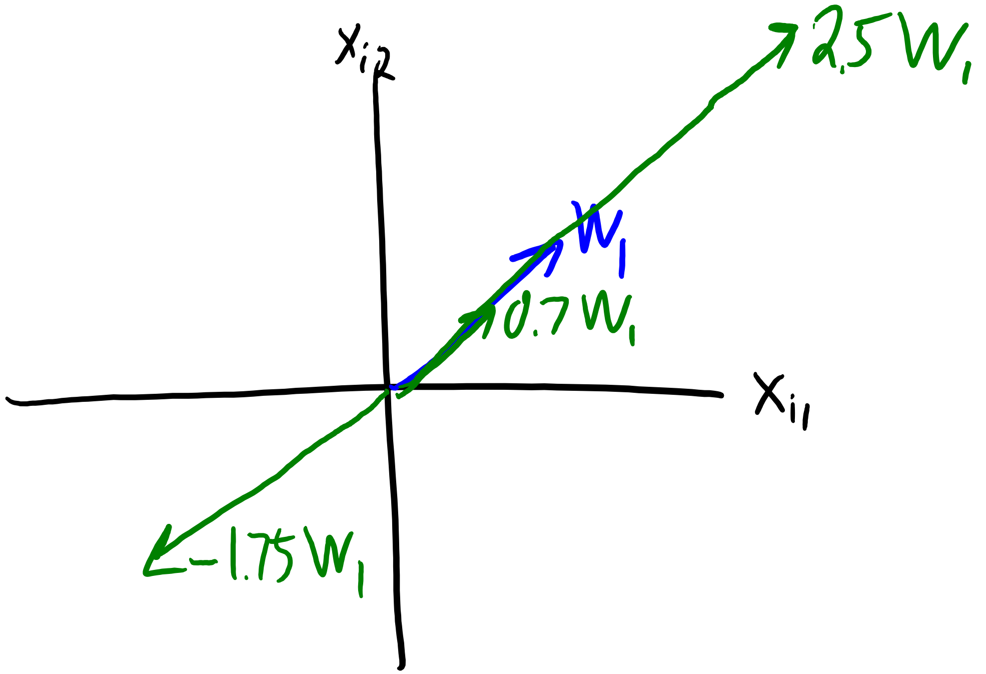
Span of 1 Vector

- Consider a single vector w_1 ($k=1$).



Span of 1 Vector

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



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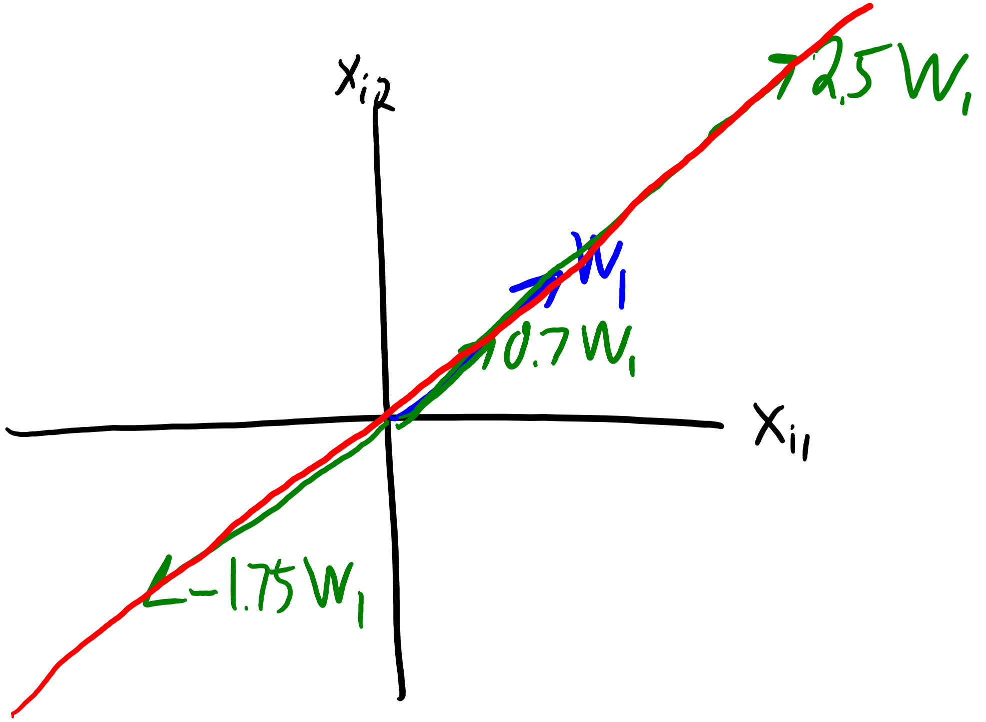
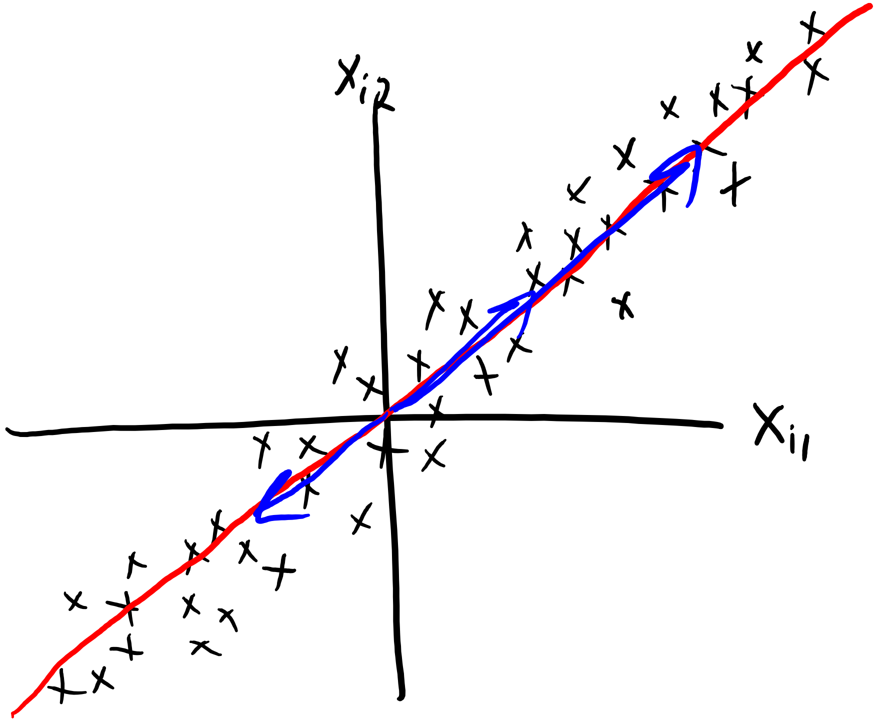


- If $w_1 \neq 0$, this forms a line.

Span of 1 Vector

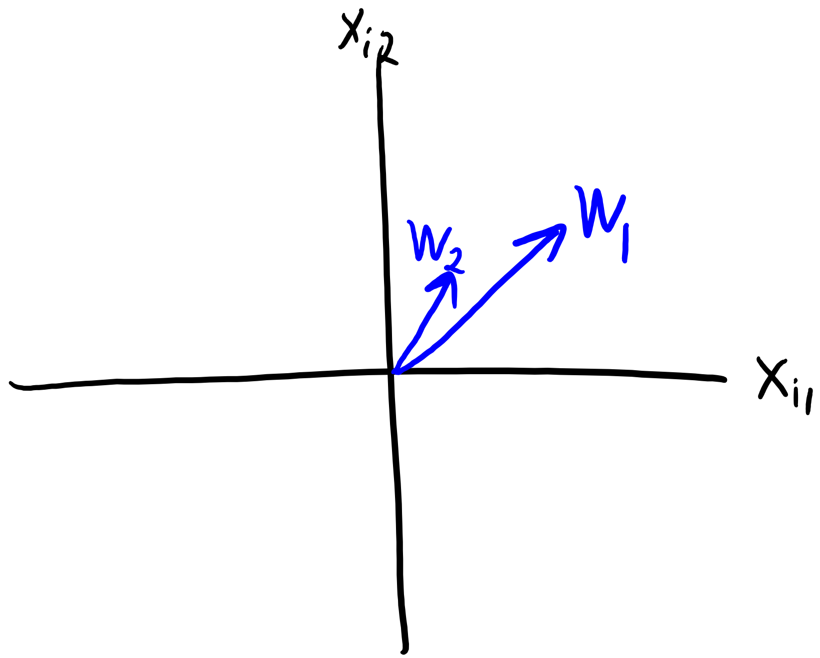
- Span of many different vectors gives same line.
  - Mathematically: αw_1 defines the same line as w_1 for any scalar $\alpha \neq 0$.



  - PCA solution can only be defined up to scalar multiplication.
    - If (W,Z) is a solution, then (αW,(1/α)Z) is also a solution. $\|(\alpha W)(\frac{1}{\alpha}Z) - X\|_F^2 = \|WZ - X\|_F^2$

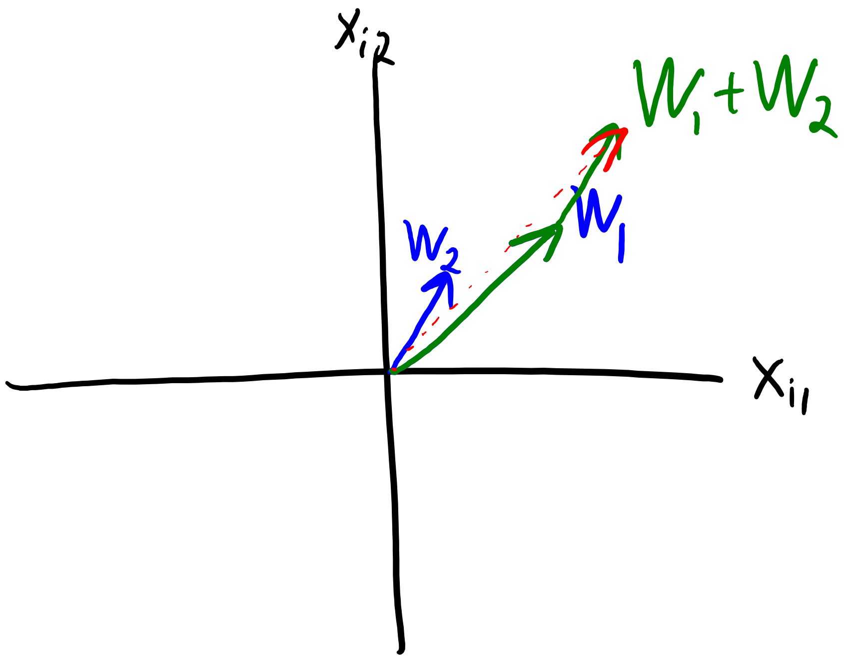
Span of 2 Vectors

- Consider two vector w_1 and w_2 (k=2).



Span of 2 Vectors

- Consider two vector w_1 and w_2 ($k=2$).
  - The span(w_1,w_2) is all vectors of form $z_{i1}w_1 + z_{i2}w_2$ for a scalars z_{i1} and z_{i2}.



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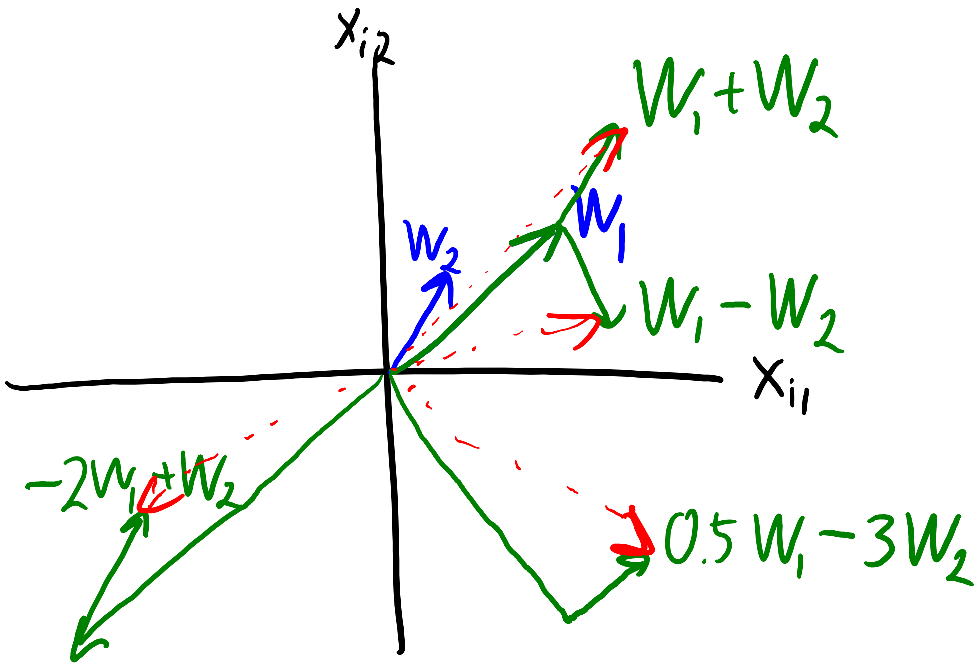

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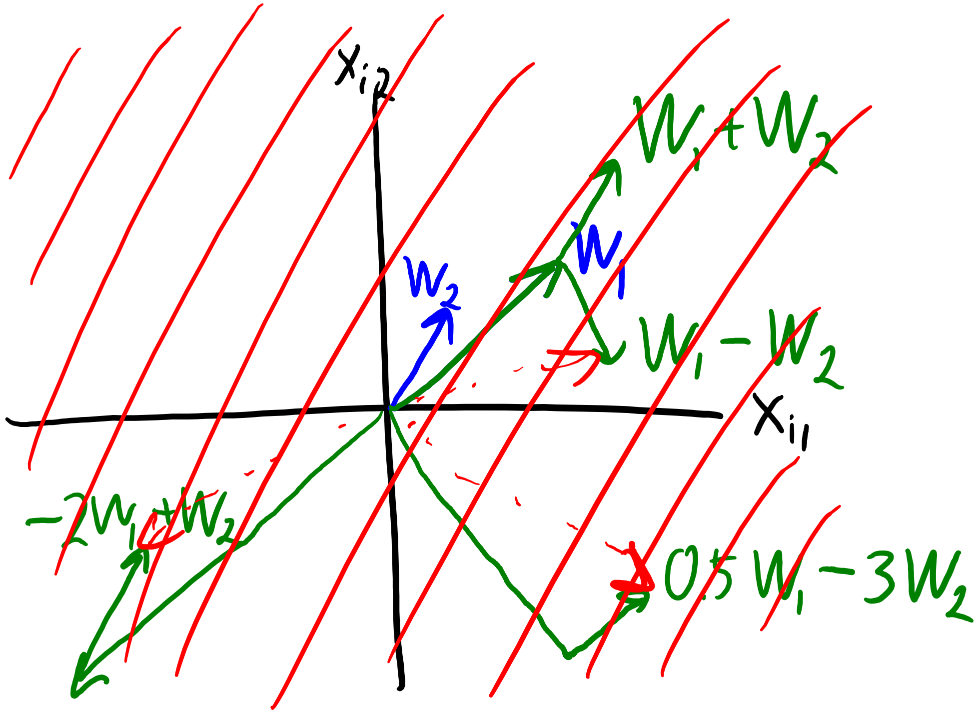

  - For most non-zero 2d vectors, span(w_1,w_2) is a plane.
    - In the case of two vectors in R^2, the plane will be *all* of R^2.

Span of 2 Vectors

- Consider two vector w_1 and w_2 ($k=2$).
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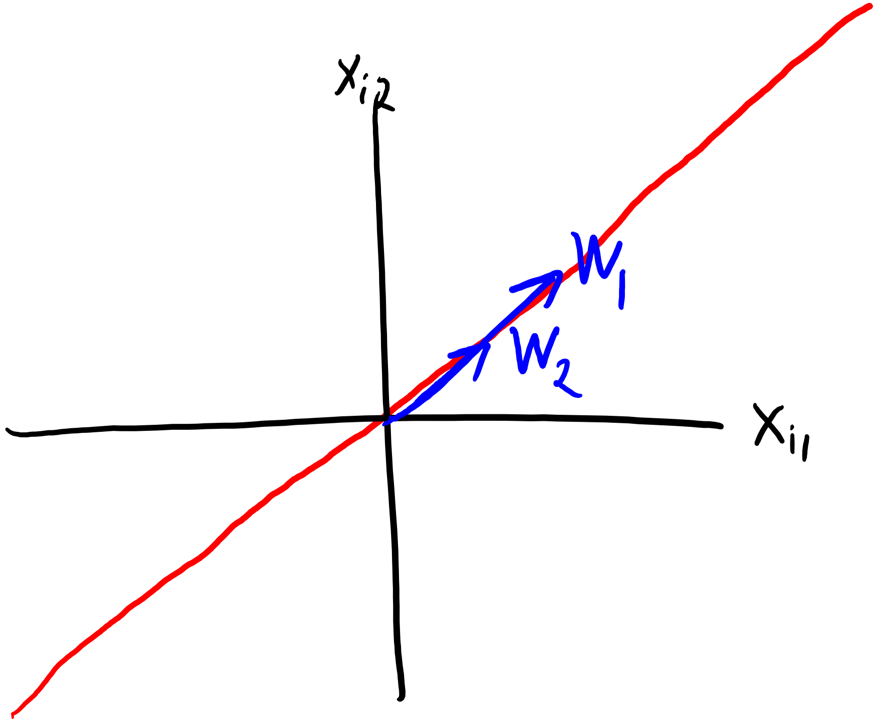
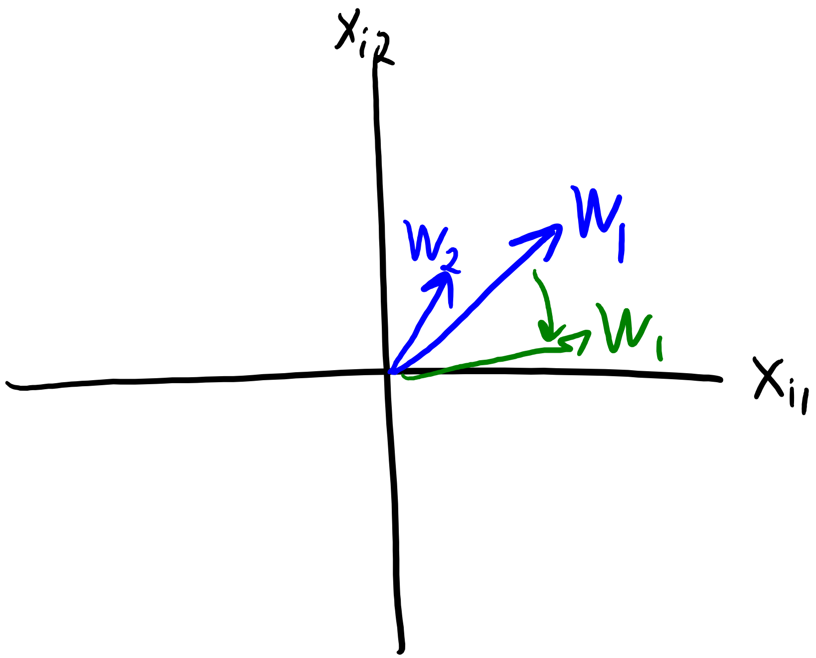


  - For most non-zero 2d vectors, span(w_1,w_2) is plane.
    - Exception is if w_2 is in span of w_1 ("collinear"), then span(w_1,w_2) is just a line.

Span of 2 Vectors

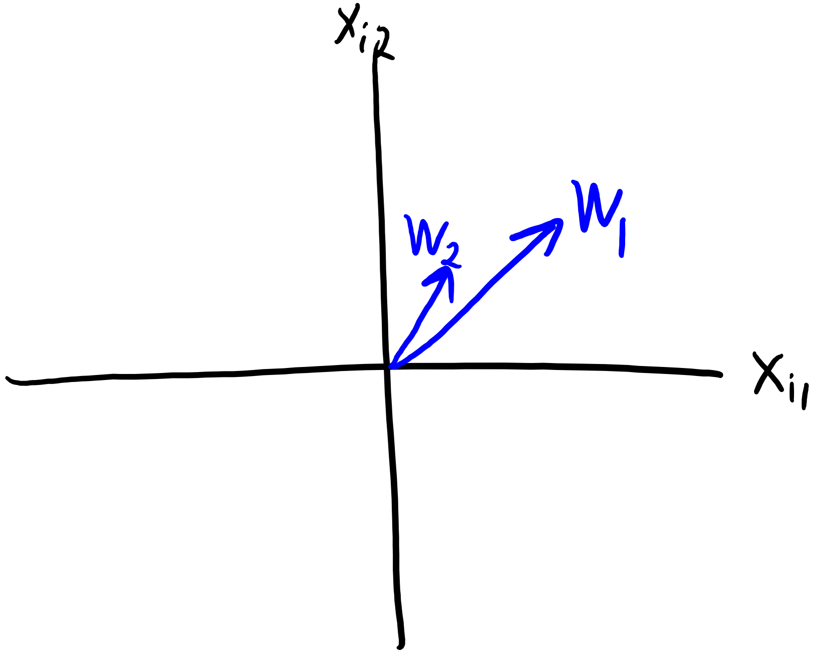
- Consider two vector w_1 and w_2 ($k=2$).
  - The span(w_1,w_2) is all vectors of form $z_{i1}w_1 + z_{i2}w_2$ for a scalars z_{i1} and z_{i2}.



  - New issues for PCA ($k >= 2$):
    - 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).

Span of 2 Vectors

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



Span of 2 Vectors

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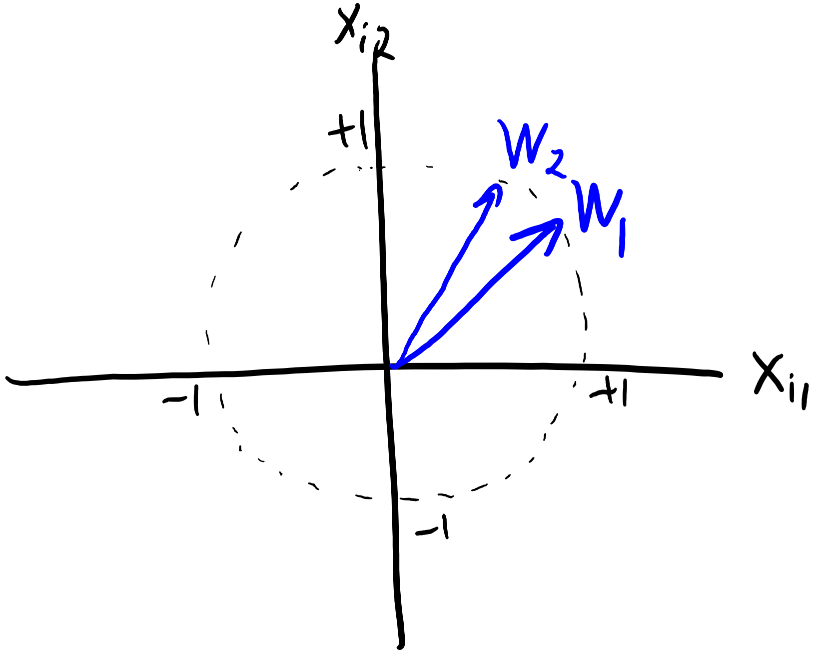
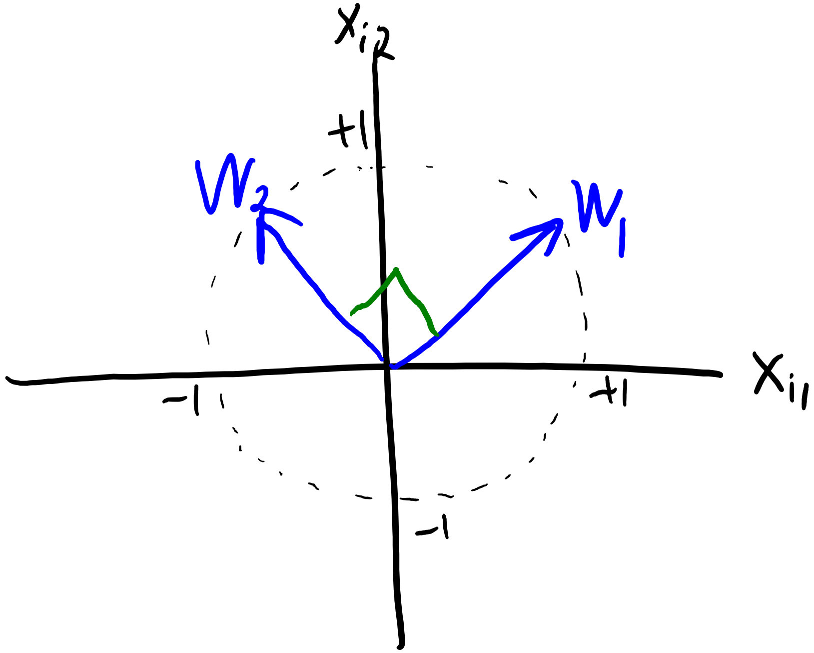


Span of 2 Vectors

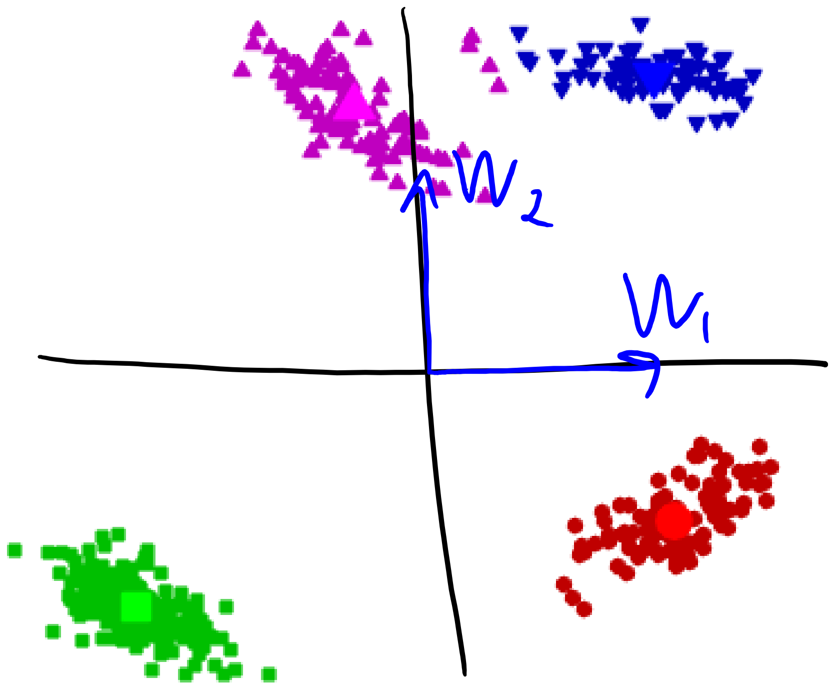
- 2 tricks to make vectors defining a plane "more unique":
  - Normalization: enforce that $||w_1|| = 1$ and $||w_2|| = 1$.
  - Orthogonality: enforce that $w_1^T w_2 = 0$ ("perpendicular").



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

Digression: PCA only makes sense for k ≤ d

- Remember our clustering dataset with 4 clusters:



- It doesn't make sense to use PCA with k=4 on this dataset.
  - We only need two vectors [1 0] and [0 1] to exactly represent all 2d points.
    - With k=2, I could 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 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

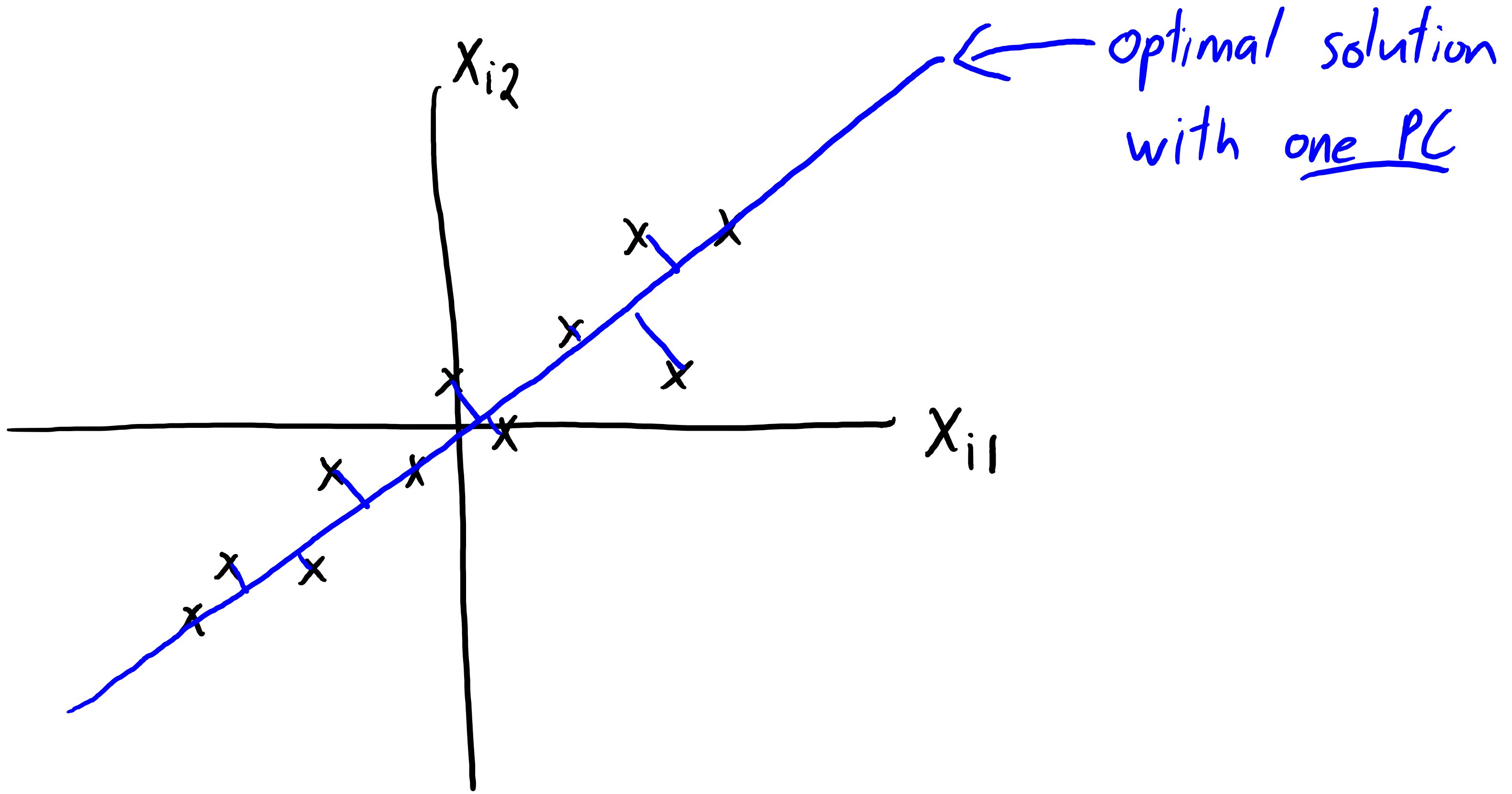
- We've identified several reasons that optimal W is non-unique:
  - Multiply any w_c by any non-zero scalar.
  - Rotate any w_c almost arbitrarily within the span.
  - Switch any w_c with any other $w_{c'}$.

- PCA implementations add constraints to make solution unique:
  - Normalization: we enforce that $||w_c|| = 1$.
  - 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.

Coming Up Next

SEQUENTIAL FITTING AND SVD

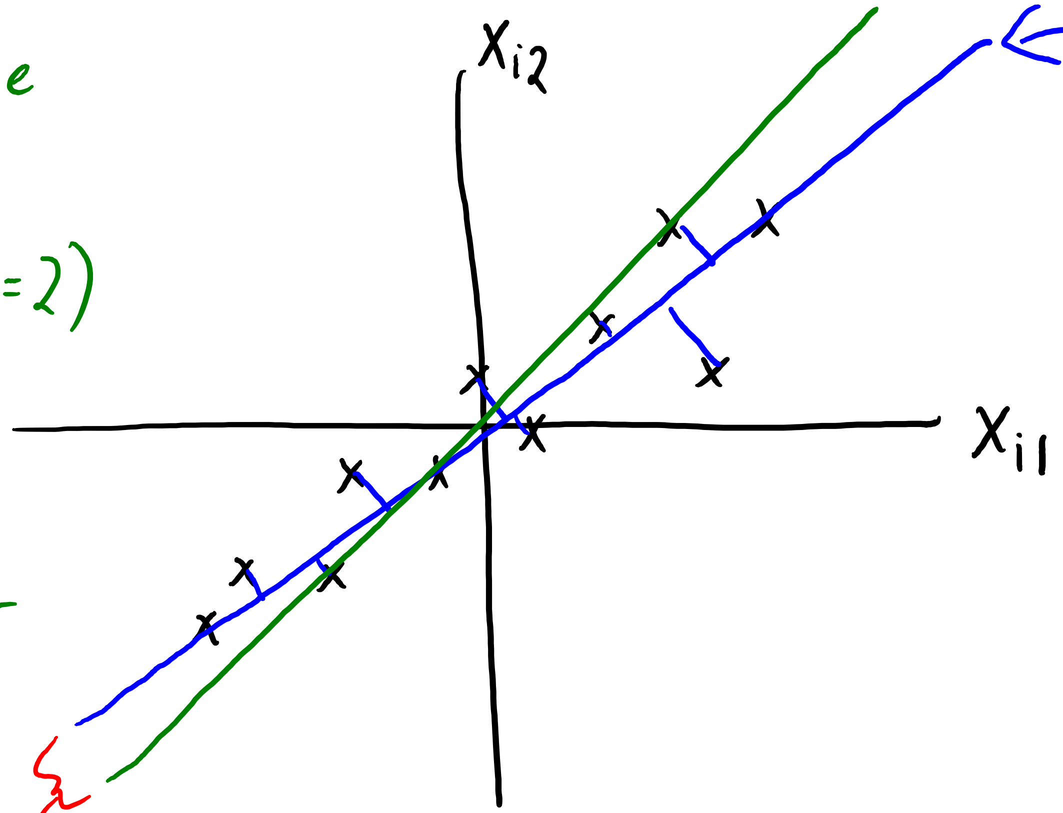
Basis, Orthogonality, Sequential Fitting



Basis, Orthogonality, Sequential Fitting

Any non-parrallel line gives optimal solution to second PC (when $d=2$)

I can get 0 error on every data point.



optimal solution with one PC

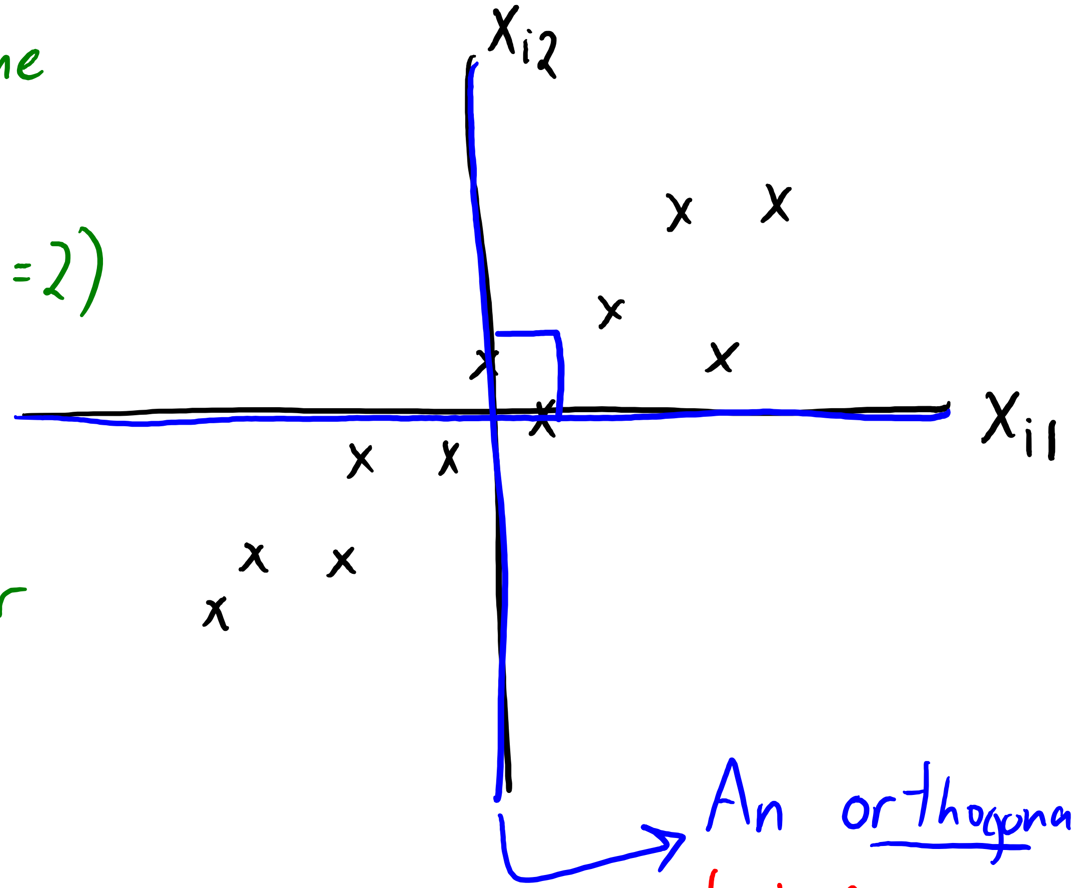
An optimal solution but not orthogonal.

(both PCs give similar information)

Basis, Orthogonality, Sequential Fitting

Any non-parralel line gives optimal solution to second PC (when d=2)

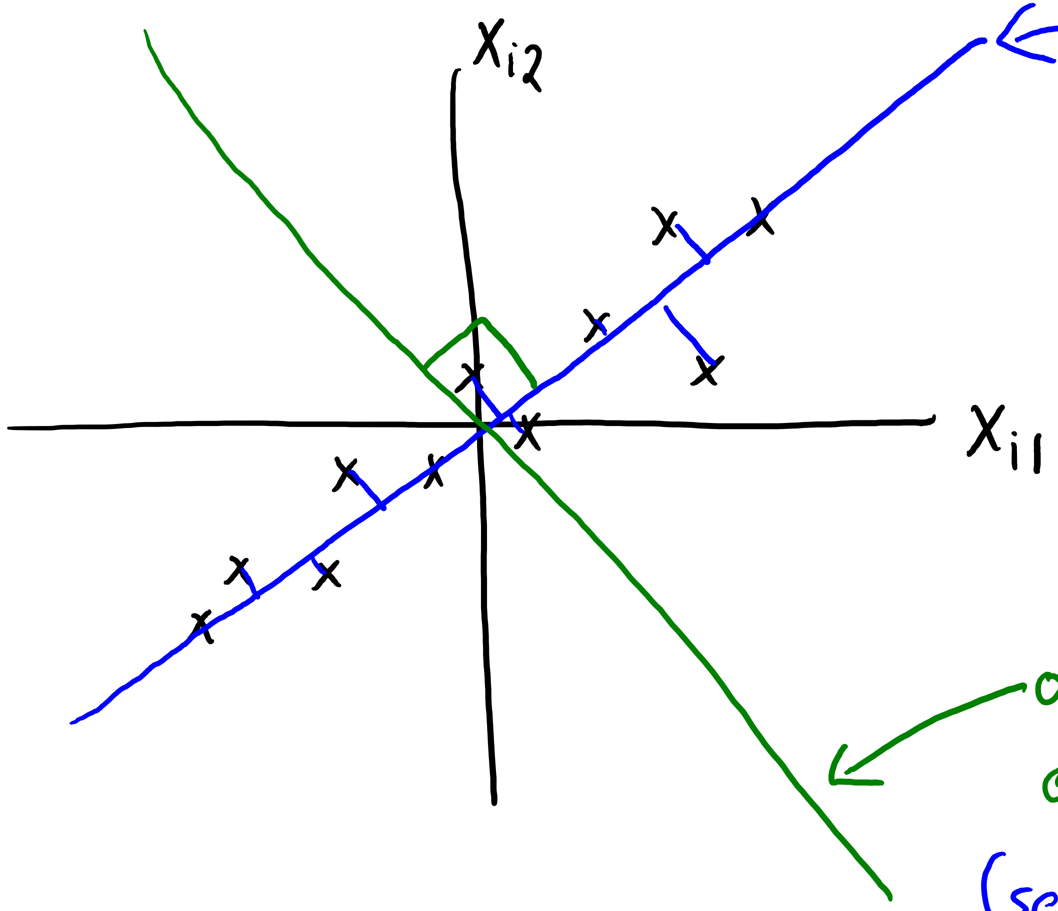
I can get 0 error on every data point.



An orthogonal solution (PCs are not redundant)

but PCs have nothing to do with data

Basis, Orthogonality, Sequential Fitting



optimal solution with one PC ("first" PC)

optimal solution that is orthogonal to "first" PC (sequential fitting of PCs makes directions unique)

http://setosa.io/ev/principal-component-analysis

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:

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

$$WW^T = \begin{bmatrix} - & w_1 & - \\ - & w_2 & - \\ & \vdots & \\ - & w_k & - \end{bmatrix} \begin{bmatrix} | & | & & | \\ w_1^T & w_2^T & \cdots & w_k^T \\ | & | & & | \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & & 0 \\ 0 & & \ddots & & 0 \\ \vdots & & & & \\ 0 & \cdots & & 0 & 1 \end{bmatrix} = I$$

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.

  - These other methods typically don't enforce the uniqueness "constraints".
    - 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, "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:

$$f(W,Z) = \sum_{i=1}^{n} \sum_{j=1}^{d} (\langle w^j, z_i \rangle - x_{ij})^2$$

- In k-means we tried to optimize 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:

$$f(W,Z) = \sum_{i=1}^{n}\sum_{j=1}^{d}(\langle w^j, z_i\rangle - x_{ij})^2$$

- In PCA we can also use alternating minimization:
  - Fix "features" Z, find optimal "factors" W.
  - Fix "factors" W, find optimal "features" 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:

$$f(W,Z) = \sum_{i=1}^{n} \sum_{j=1}^{d} (\langle w^j, z_i \rangle - x_{ij})^2$$

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

$$\nabla_W f(W,Z) = Z^T Z W - Z^T X \quad \text{so} \quad W = (Z^T Z)^{-1}(Z^T X)$$

(writing gradient as a matrix)

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

$$\nabla_Z f(W,Z) = Z W W^T - X W^T \quad \text{so} \quad Z = X W^T (W W^T)^{-1}$$

These are usually invertible since $k \ll n$ and $k \ll d$

PCA Computation: Alternating Minimization

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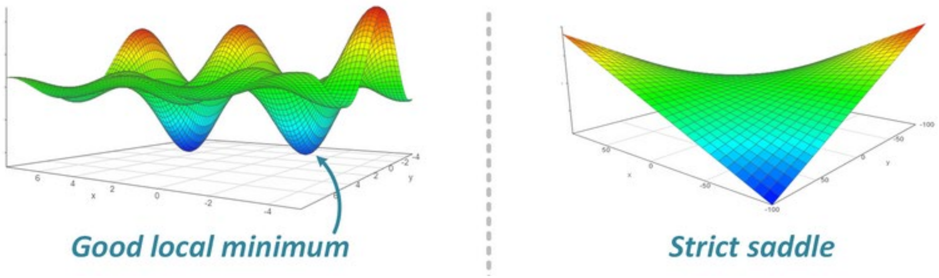
$$f(W,Z) = \sum_{i=1}^{n} \sum_{j=1}^{d} (\langle w^j, z_i \rangle - x_{ij})^2$$



- 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.

http://www.offconvex.org/2018/11/07/optimization-beyond-landscape/

PCA Computation: Stochastic Gradient

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

$$f(W,Z) = \sum_{i=1}^{n}\sum_{j=1}^{d}(\langle w^j, z_i\rangle - x_{ij})^2 = \sum_{(i,j)} \underbrace{(\langle w^j, z_i\rangle - x_{ij})^2}_{f(w^j, z_i, x_{ij})}$$

On each iteration, pick a random example 'i' and feature 'j':

→ Set w^j to $w^j - \alpha^t \nabla_{w^j} f(w^j, z, x_{ij})$

→ Set z_i to $z_i - \alpha^t \nabla_{z_i} f(w^j, z_i, x_{ij})$

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

PCA Computation: Prediction

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

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

means of training data

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

$$\tilde{Z} = \tilde{X}\underbrace{W^T(WW^T)^{-1}}_{\text{(could just store this } d \times k \text{ matrix)}}$$

PCA Computation: Prediction

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

$$\|\underbrace{\tilde{Z}W}_{\hat{X}} - \tilde{X}\|_F^2$$

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_{ij}.

$$Var(x_{ij}) = E[(x_{ij} - \mu_{ij})^2] = E[x_{ij}^2] = \frac{1}{nd}\sum_{i=1}^{n}\sum_{j=1}^{d} x_{ij}^2 = \frac{1}{nd}\|X\|_F^2$$

definition of variance

assumed to be zero

definition of expectation

Frobenius norm

  - For a given ‘k’ we compute (variance of errors)/(variance of x_{ij}):

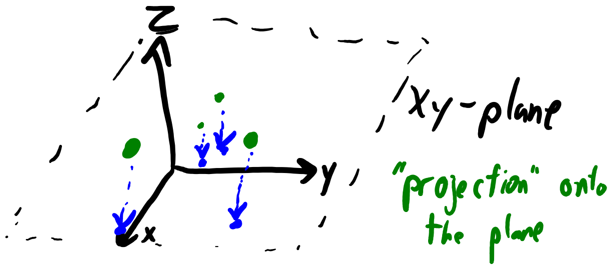
$$\frac{\|ZW - X\|_F^2}{\|X\|_F^2}$$

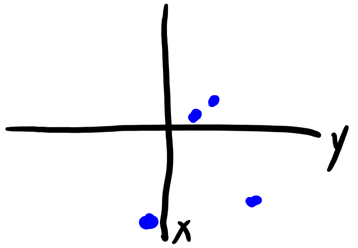
centered version

  - 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:

$$\frac{\|ZW - X\|_F^2}{\|X\|_F^2}$$

$\|ZW - X\|_F^2$ ← Variance in z-dimension (variance in x- and y-dimensions fully captured by overhead map)

$\|X\|_F^2$ ← Variance of goat pos. in 3-dimensions

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

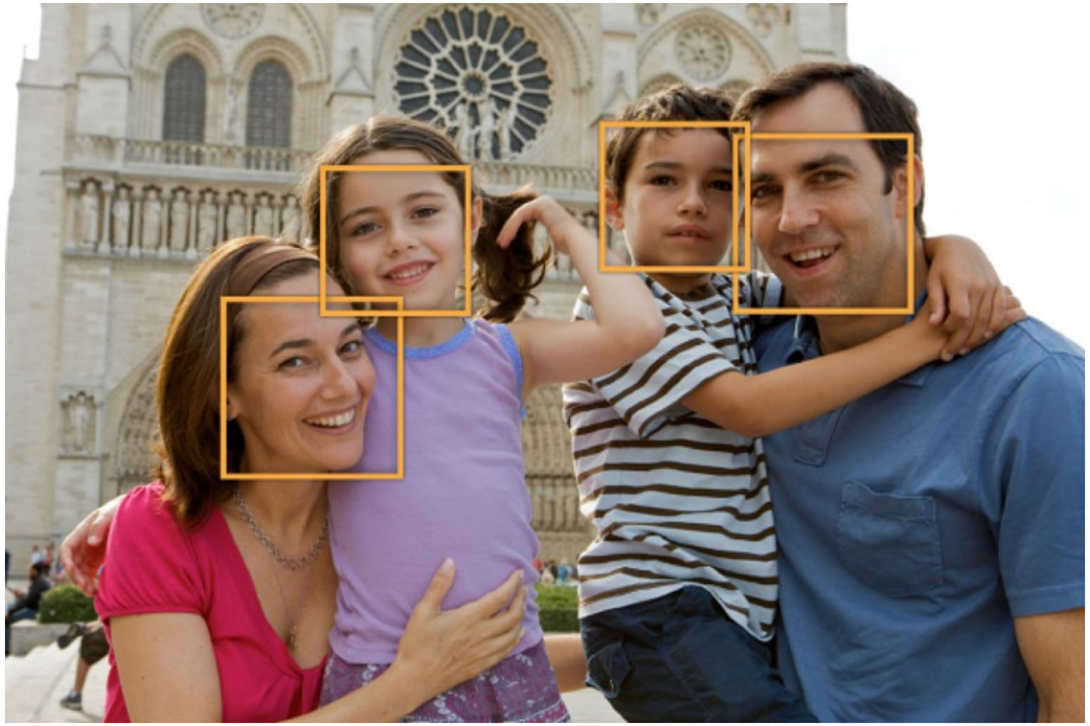
https://en.wikipedia.org/wiki/Doom_(1993_video_game)
https://forum.minetest.net/viewtopic.php?f=5&t=9666

Coming Up Next

EIGENFACES

Application: Face Detection

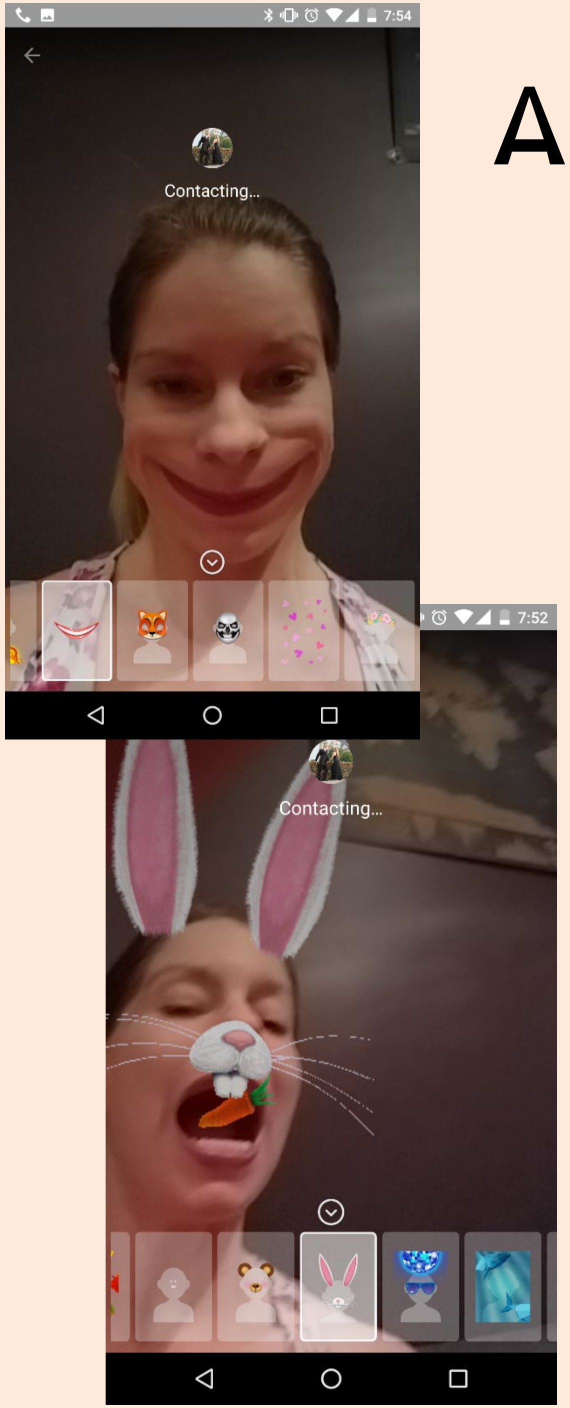
- Consider problem of face detection:

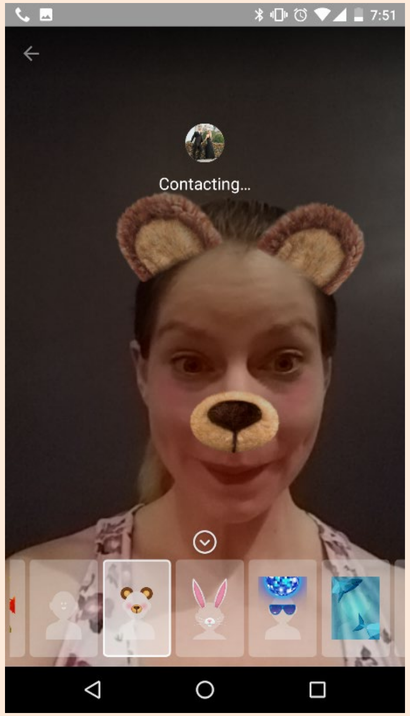


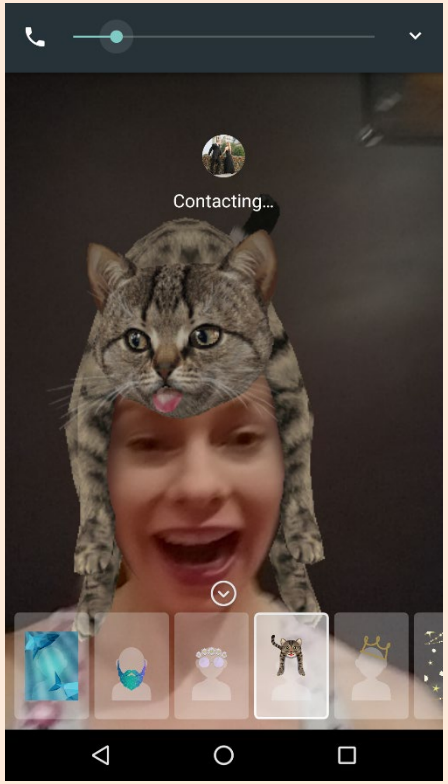
- Classic methods use "eigenfaces" as basis:
  - PCA applied to images of faces.

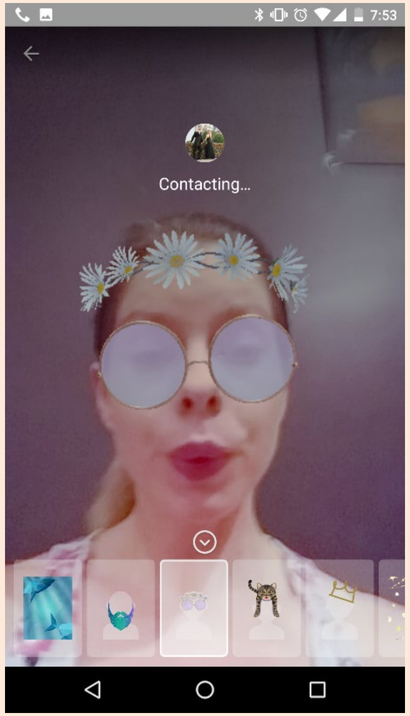
https://developer.apple.com/library/content/documentation/GraphicsImaging/Conceptual/CoreImaging/ci_detect_faces/ci_detect_faces.html

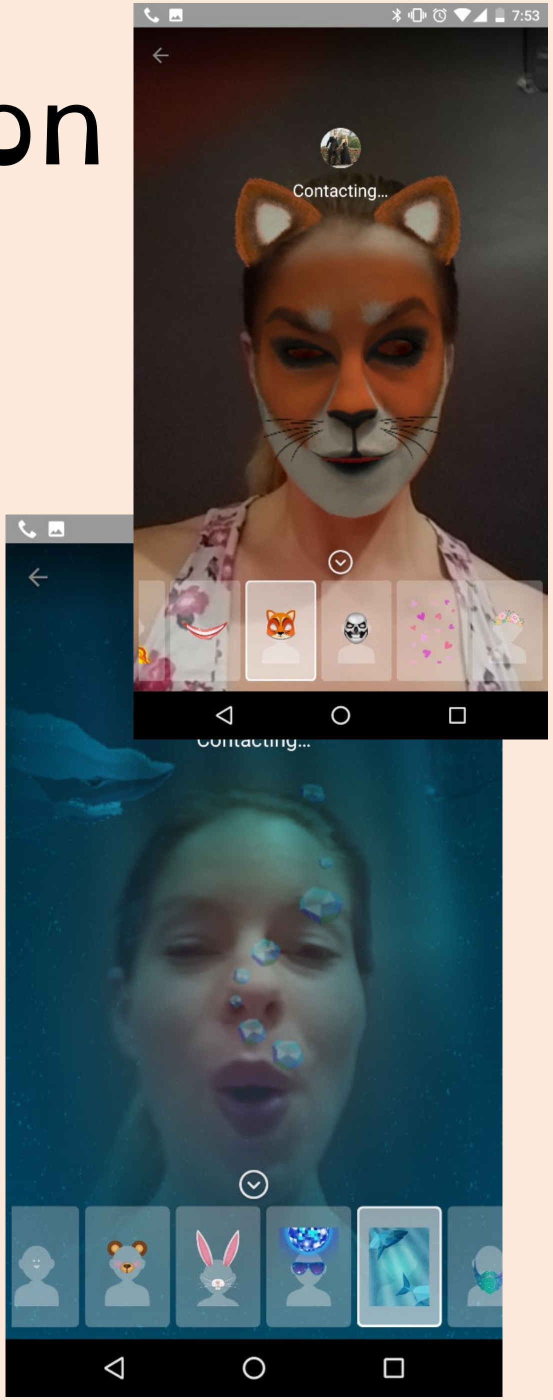
Application: Face Detection











Eigenfaces

- Collect a bunch of images of faces under different conditions:

Each row of X will be pixels in one image:

$X =$

If have 'n' images that are 'm' by 'm' then X is 'n' by m^2.

Eigenfaces

Compute mean μ_j of each column.

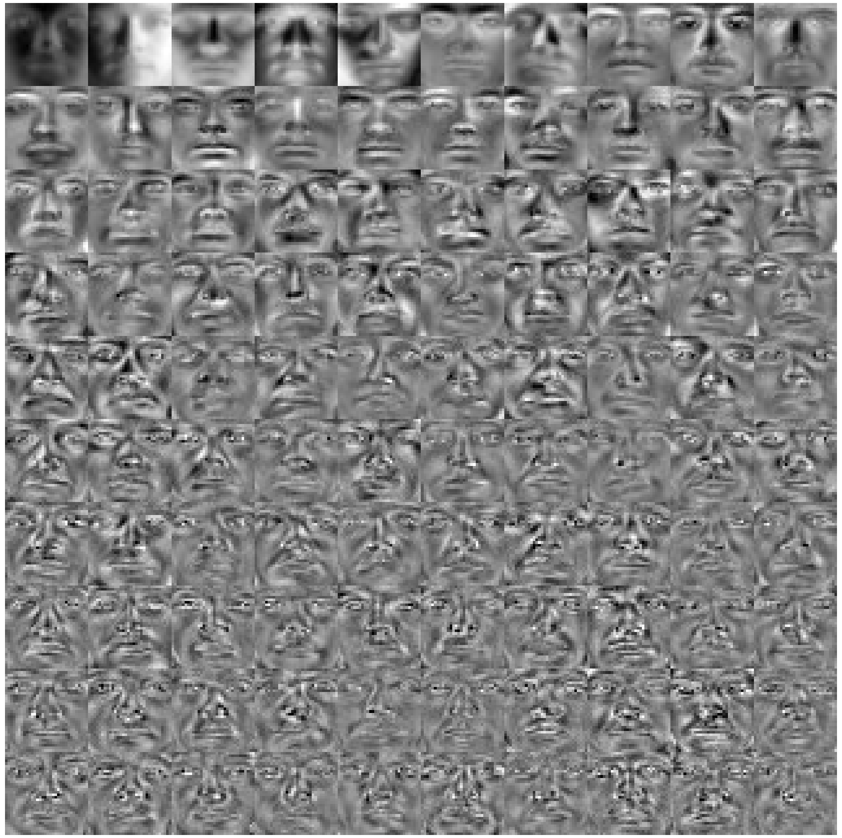
Replace each x_{ij} by $x_{ij} - \mu_j$

Each row of X will be pixels in one image:

$$X = \begin{bmatrix} — & x_1 - \mu & — \\ — & x_2 - \mu & — \\ & \vdots & \\ — & x_n - \mu & — \end{bmatrix}$$

Eigenfaces

Compute top 'k' PCs on centered data:

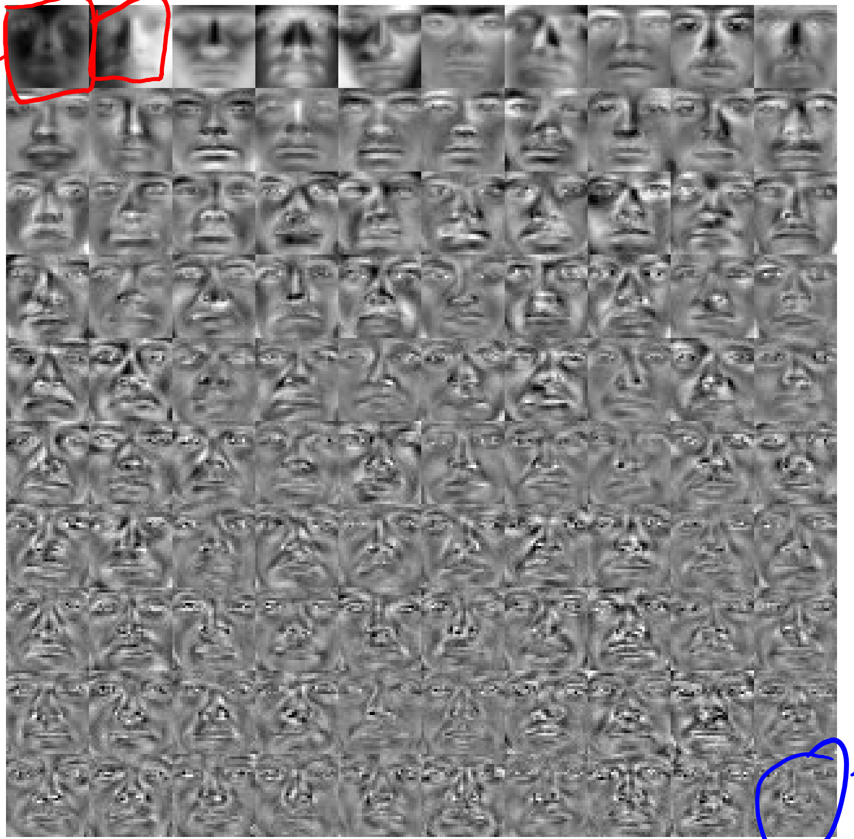


Each row of X will be pixels in <u>one</u> image:

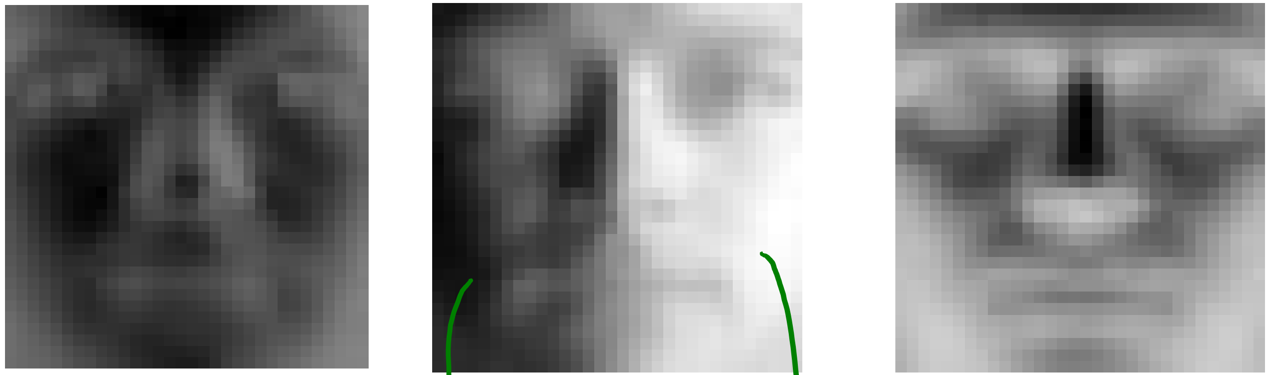
$$X = \begin{bmatrix} \text{---} & x_1 - \mu & \text{---} \\ \text{---} & x_2 - \mu & \text{---} \\ & \vdots & \\ \text{---} & x_n - \mu & \text{---} \end{bmatrix}$$

Eigenfaces

Compute top 'k' PCs on centered data:



Note that these are "signed" images.



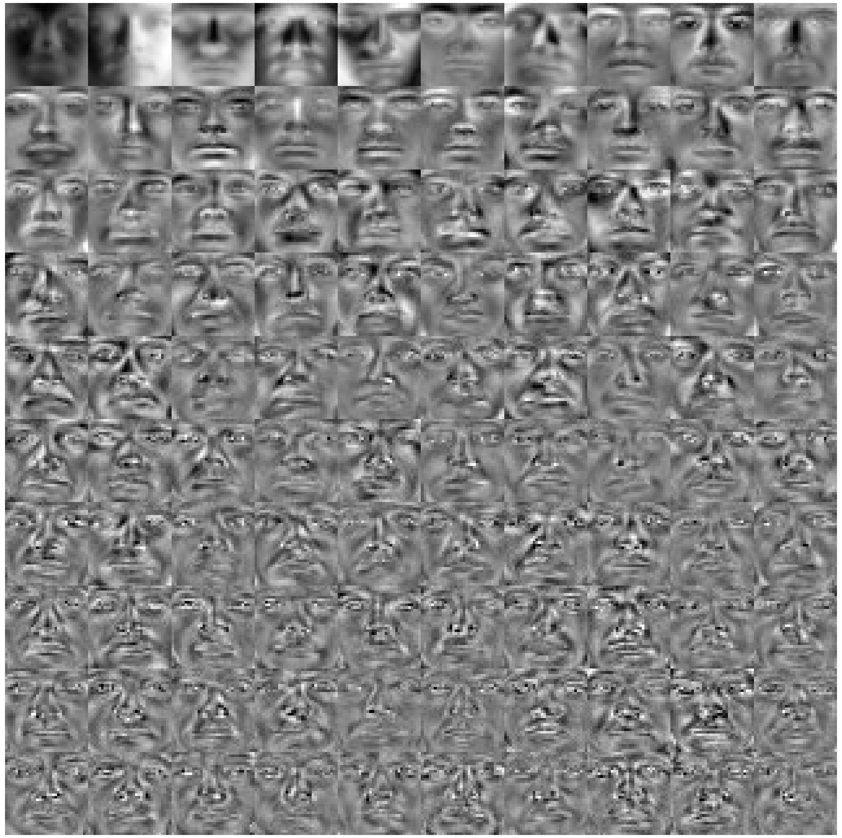
"gray" represents values close to 0.

"dark" represents negative values

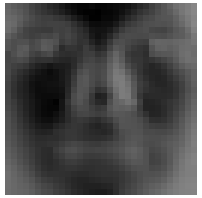
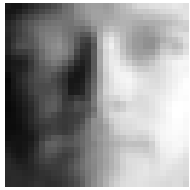
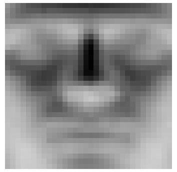
"bright" represents positive values

Eigenfaces

Compute top 'k' PCs on centered data:



"Eigenface" representation:

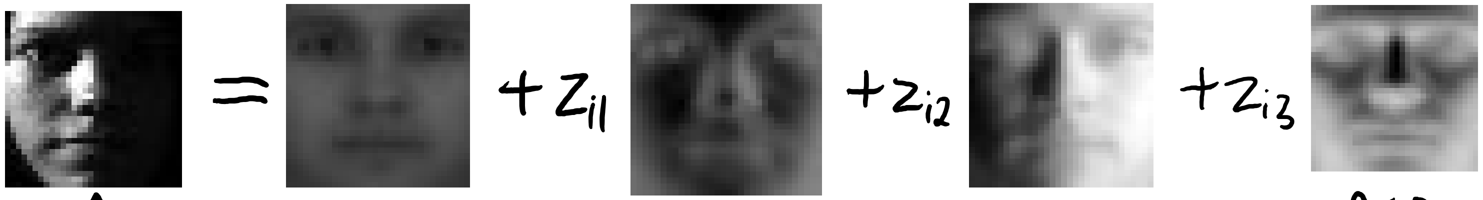
 $=$  $+ z_{i1}$  $+ z_{i2}$  $+ z_{i3}$  $+ \dots$

$\hat{x}_i$ $\qquad \mu$ $\qquad$ PC1 (first row of W) $\qquad$ PC2 $\qquad$ PC3

Eigenfaces

100 of the original faces:

"Eigenface" representation:

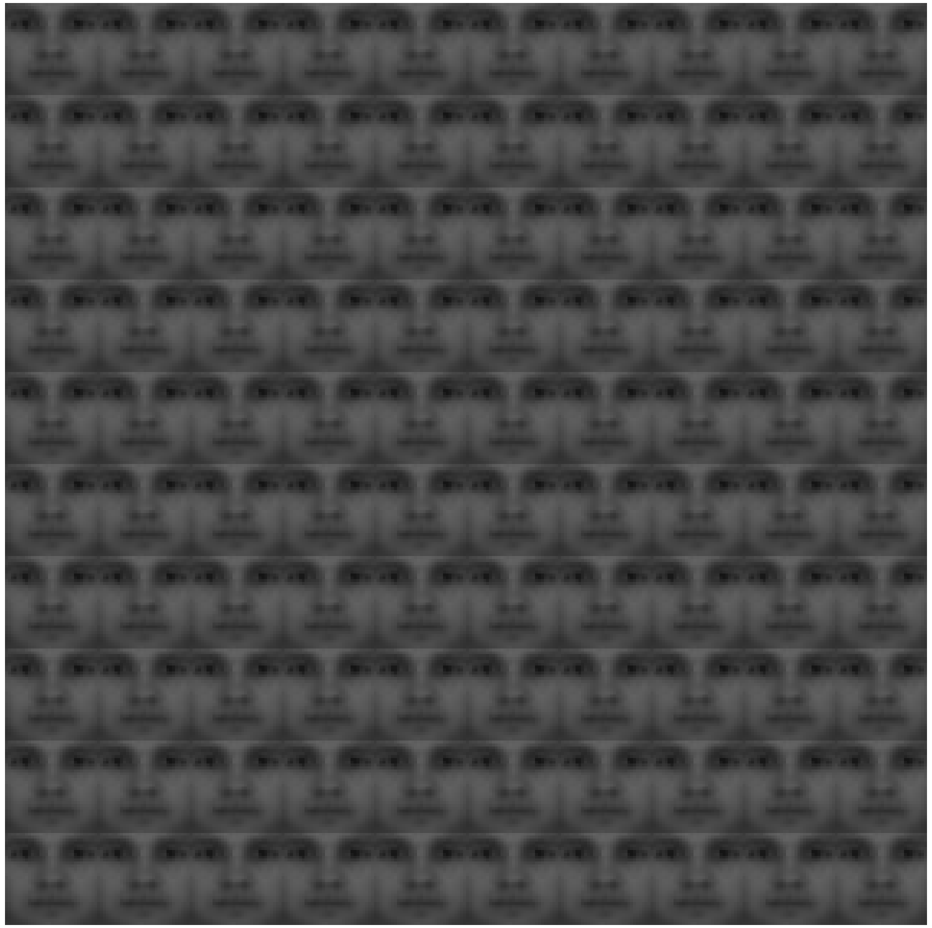


$\hat{x}_i = \mu + z_{i1}\,\text{PC1} + z_{i2}\,\text{PC2} + z_{i3}\,\text{PC3} + \cdots$

$\hat{x}_i$ μ PC1 (first row of W) PC2 PC3

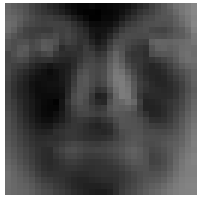
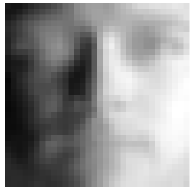
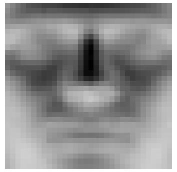
Eigenfaces

Reconstruction with $k = 0$



Variance explained: 0%

"Eigenface" representation:

 =  $+ z_{i1}$  $+ z_{i2}$  $+ z_{i3}$  + ...

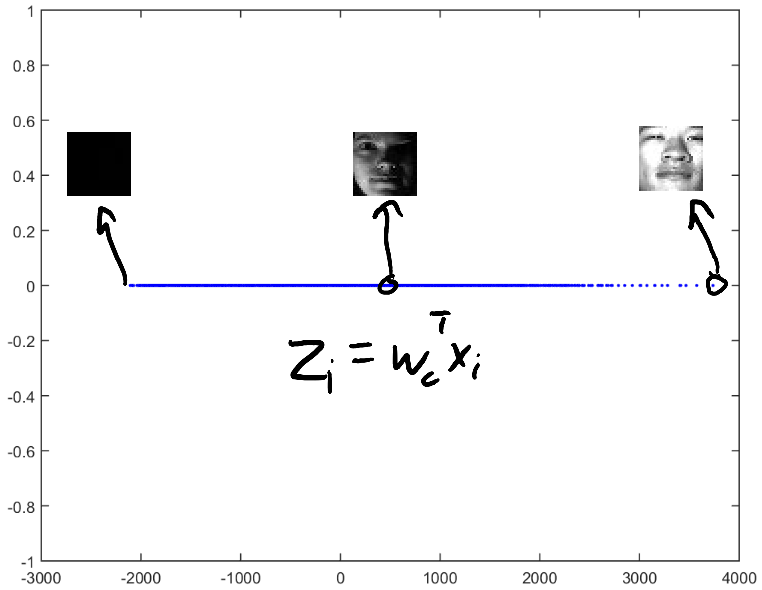
$\hat{x}_i$ μ PC1 (first row of W) PC2 PC3

Eigenfaces

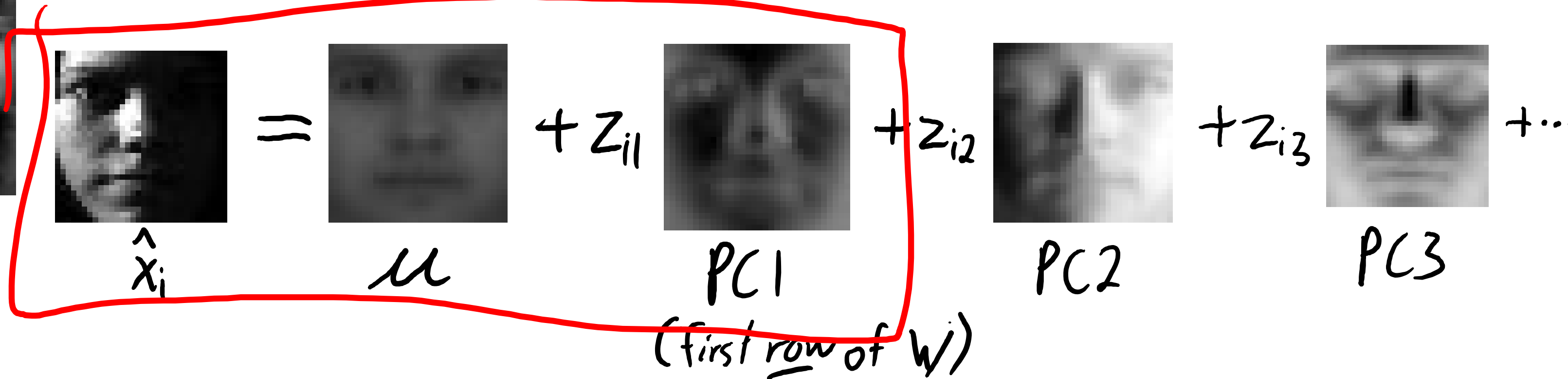
Reconstruction with k=1

Variance explained: 36%

PCA Visualization:



"Eigenface" representation:

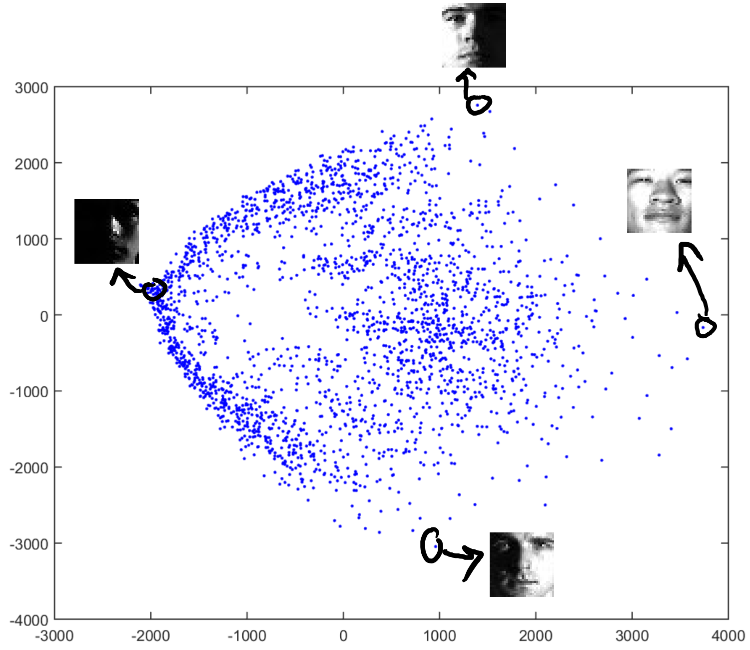


Eigenfaces

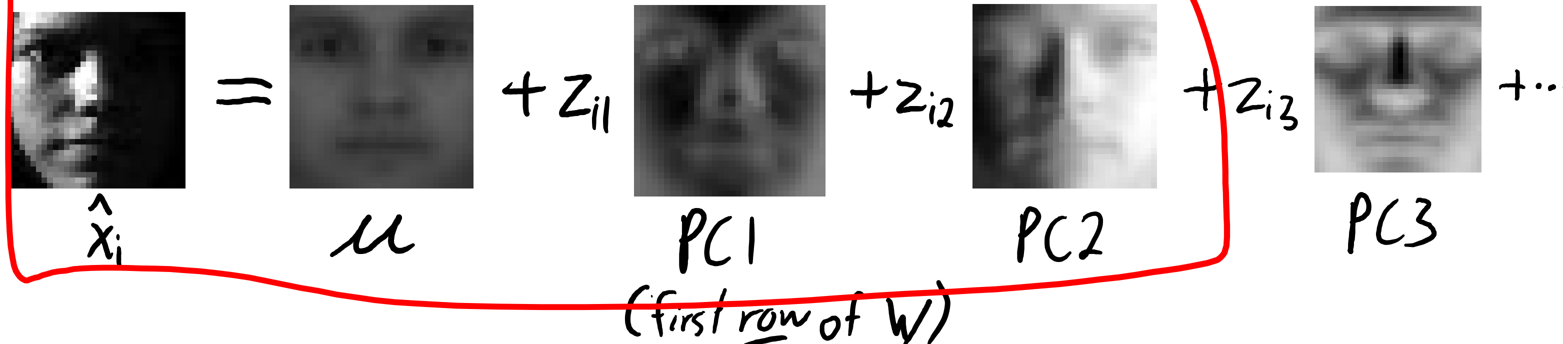
Reconstruction with $k=2$

Variance explained: 71%

PCA Visualization:



"Eigenface" representation:

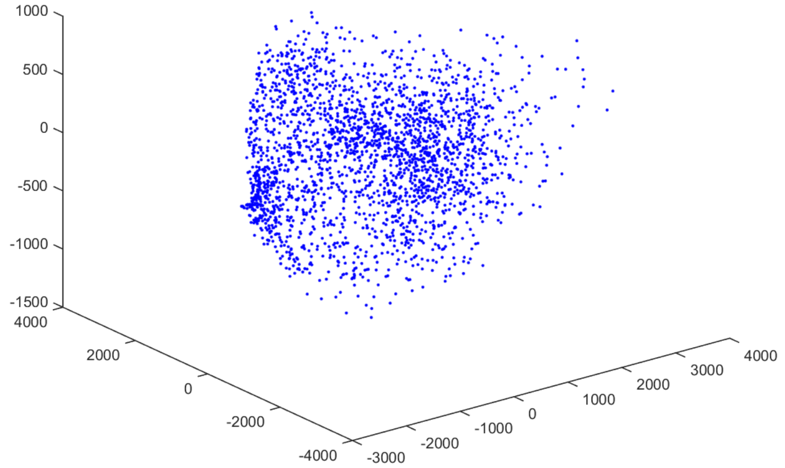


Eigenfaces

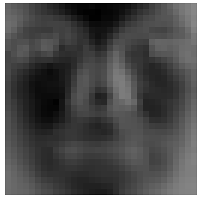
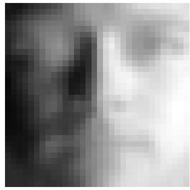
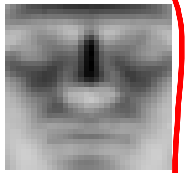
Reconstruction with $k=3$

Variance explained: 76%

PCA Visualization:



"Eigenface" representation:

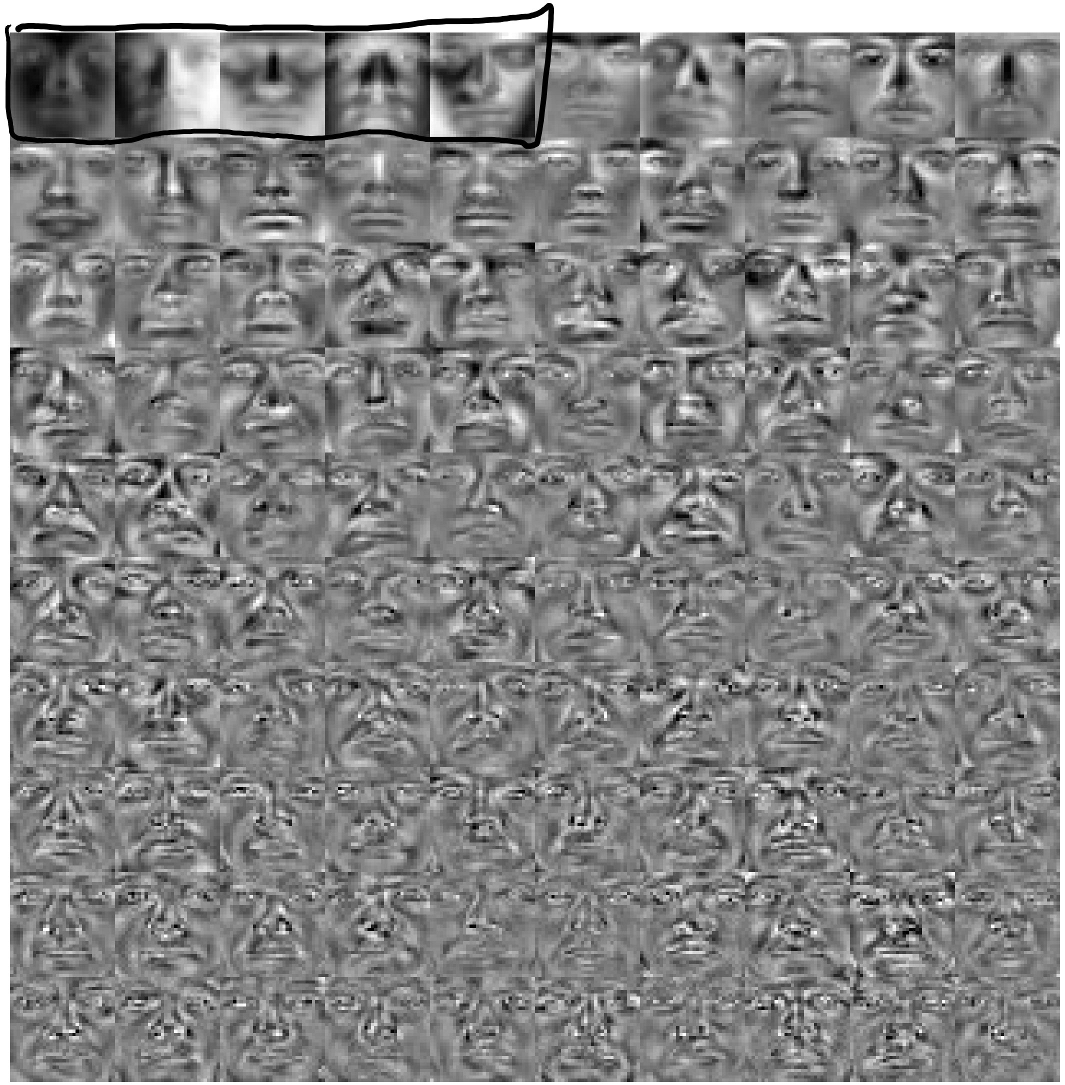
 =  $+ z_{i1}$  $+ z_{i2}$  $+ z_{i3}$  $+ \dots$

$\hat{x}_i$ $\quad \mu \quad$ PC1 (first row of W) $\quad$ PC2 $\quad$ PC3

Eigenfaces

Reconstruction with $k=5$

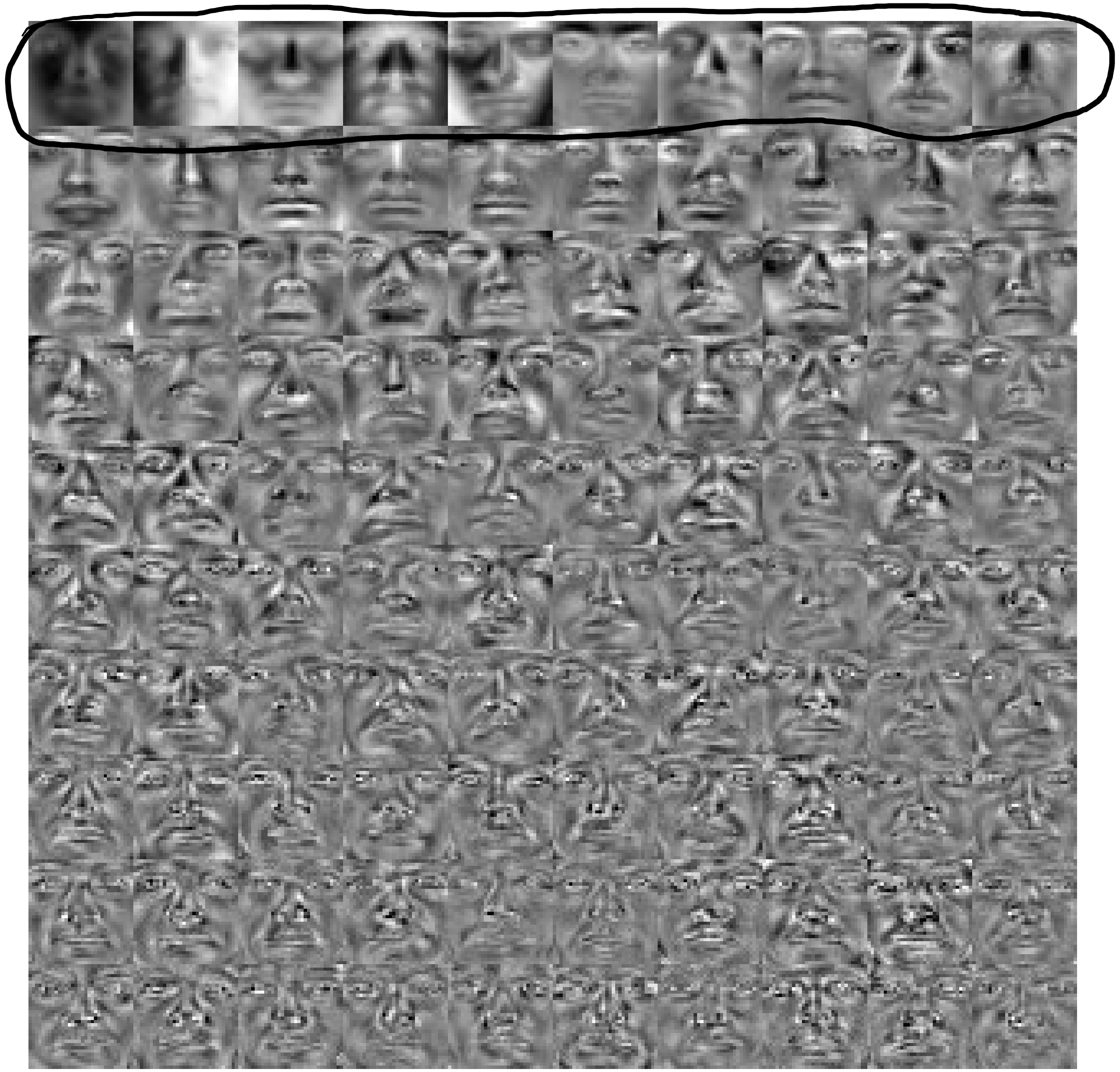
Variance explained: 80%



Eigenfaces

Reconstruction with k=10

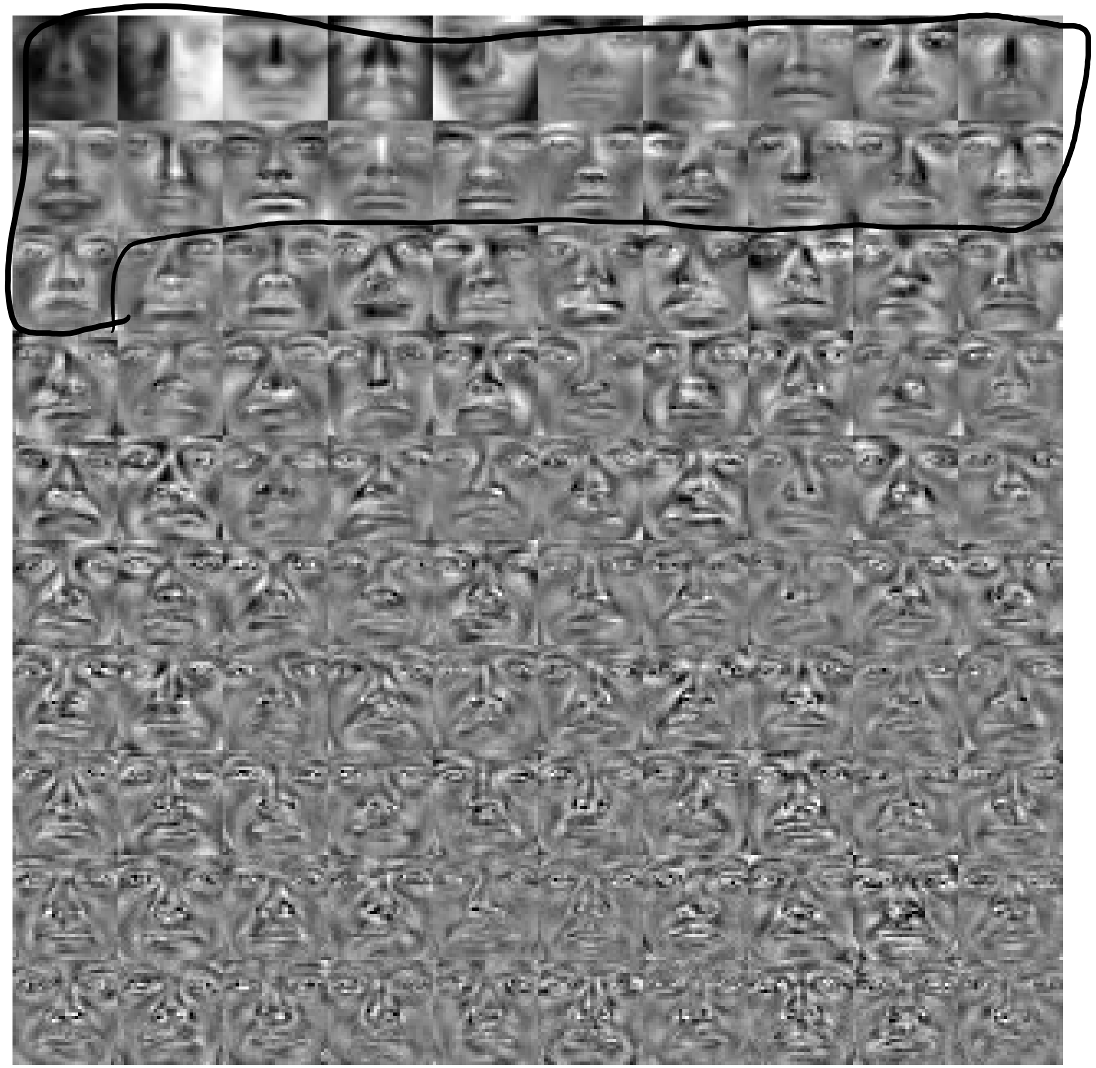
Variance explained: 85%



Eigenfaces

Reconstruction with k=21

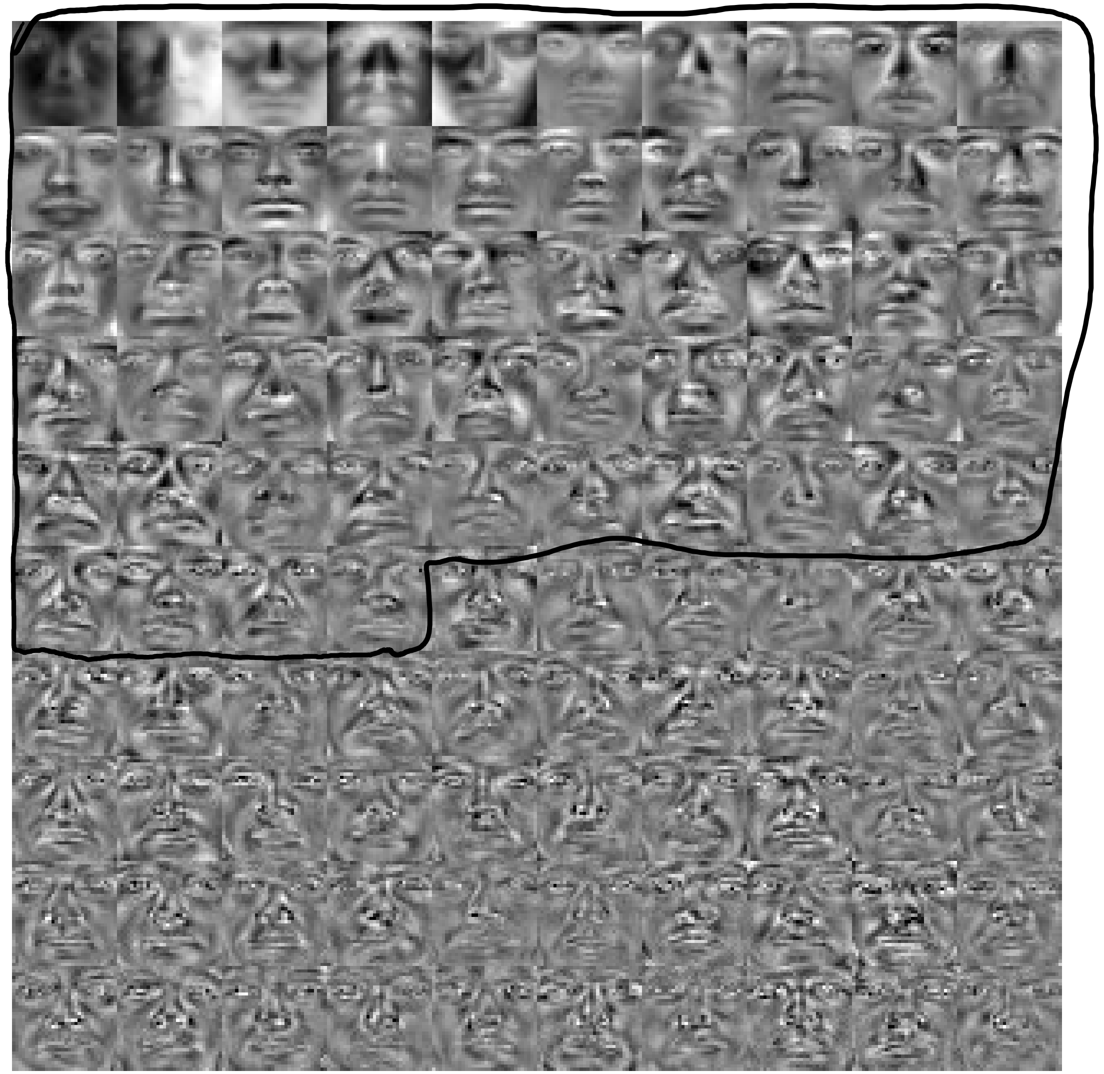
Variance explained: 90%



Eigenfaces

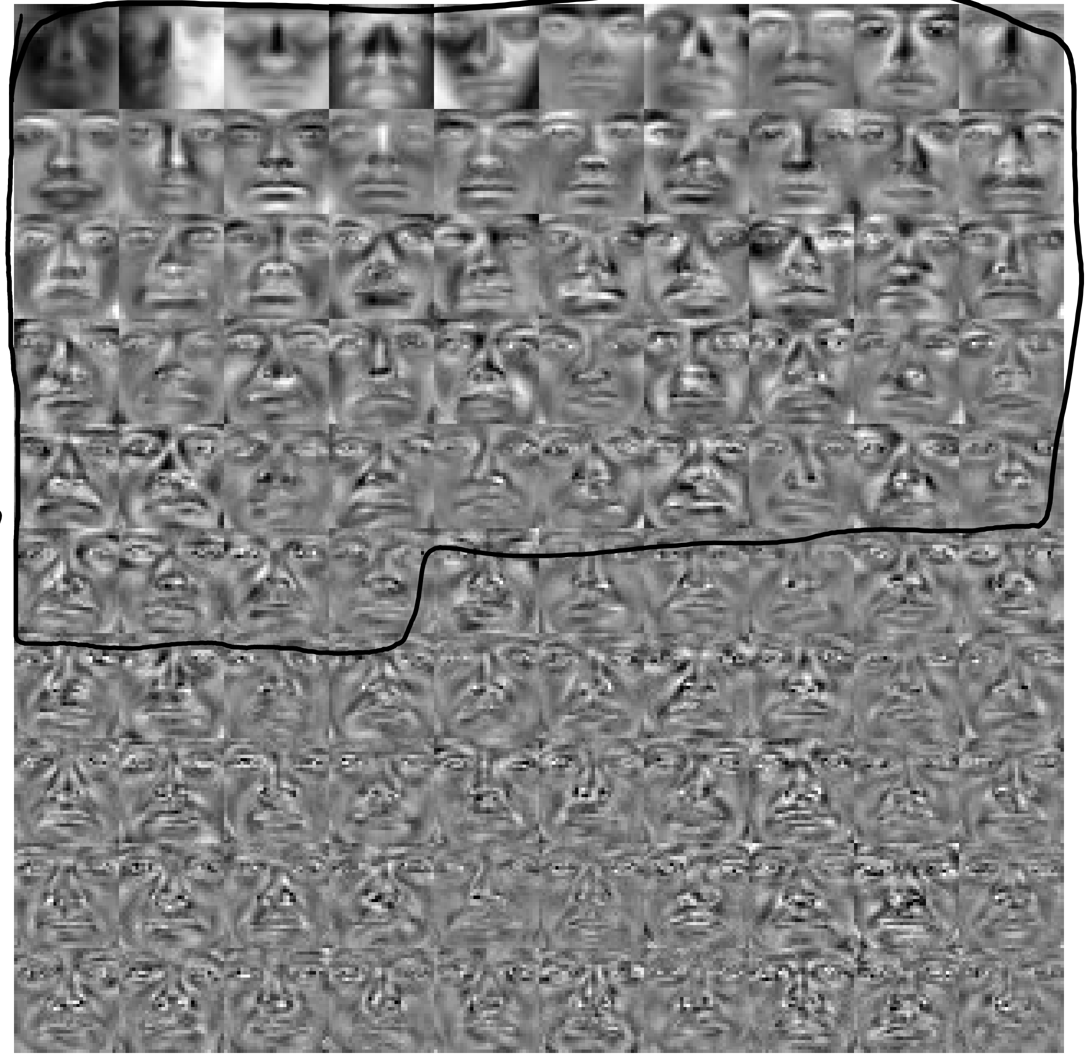
Reconstruction with $k = 54$

Variance explained: 95%



Eigenfaces

Original Images again:



Plus these "eigenfaces" and the mean.

We can replace 1024 x_i values by 54 z_i 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.

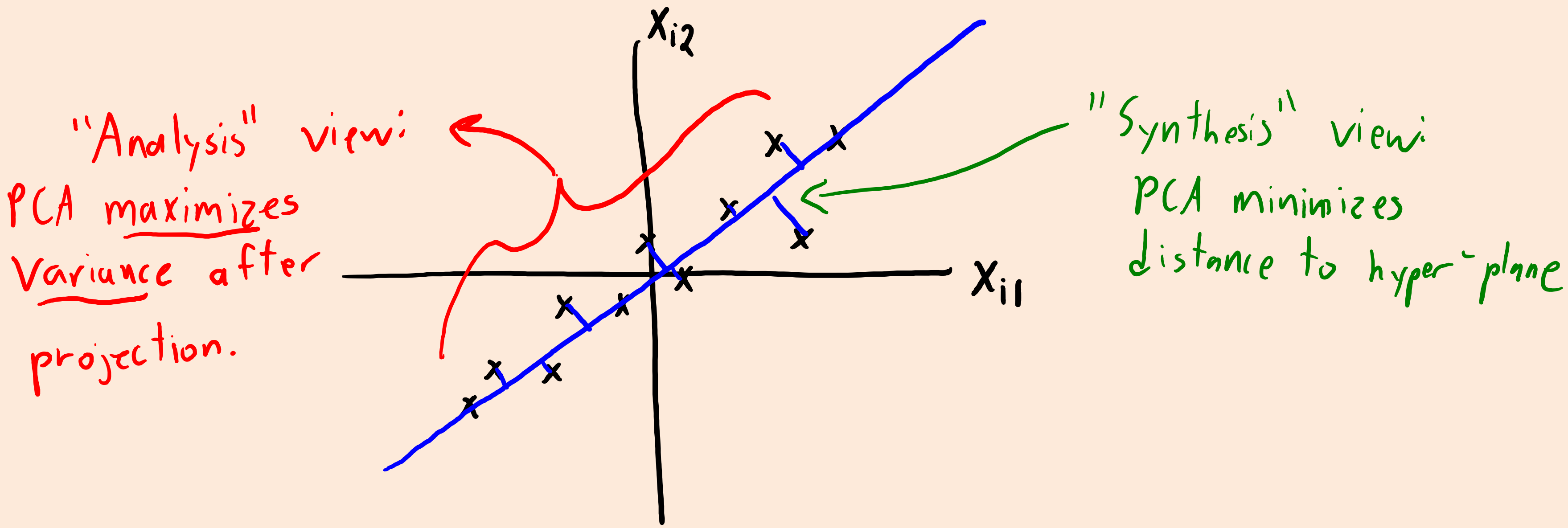
- Next time: cancer signatures and NBA shot charts.

Making PCA Unique

- PCA implementations add constraints to make solution unique:
  - Normalization: we enforce that $||w_c|| = 1$.
  - 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

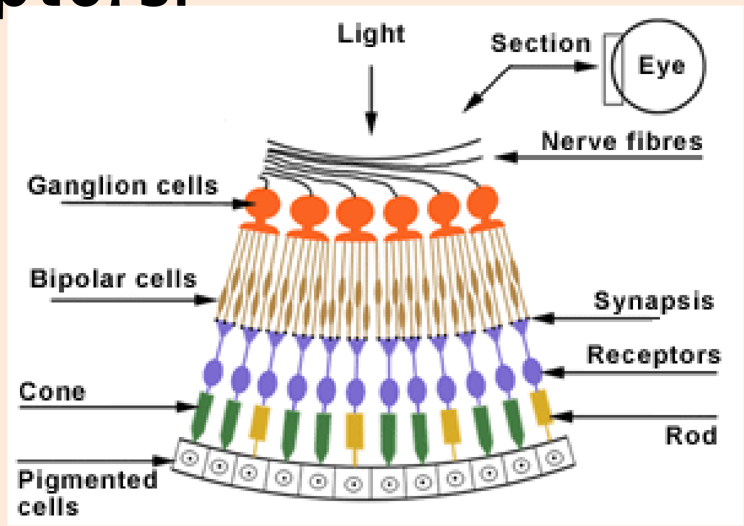
- We said that PCA finds hyper-plane minimizing distance to data x_i.
  - This is the "synthesis" view of PCA (connects to k-means and least squares).



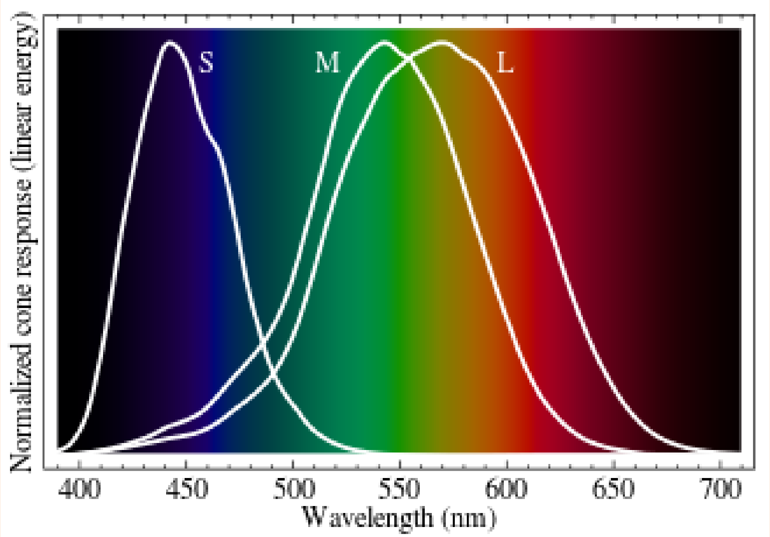
- "Analysis" view when we have orthogonality constraints:
  - PCA finds hyper-plane maximizing variance in z_i space.
  - You pick W to "explain as much variance in the data" as possible.

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).



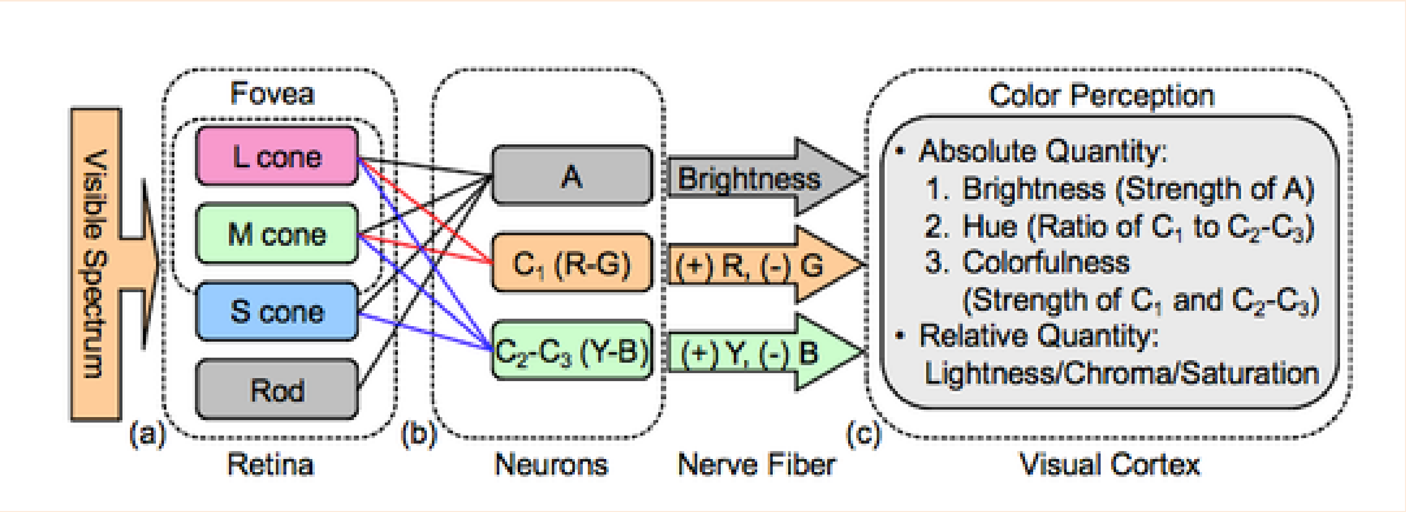
- Two problems with this system:
  - Not orthogonal.
    - High correlation in particular between red/green.
  - We have 4 receptors for 3 colours.

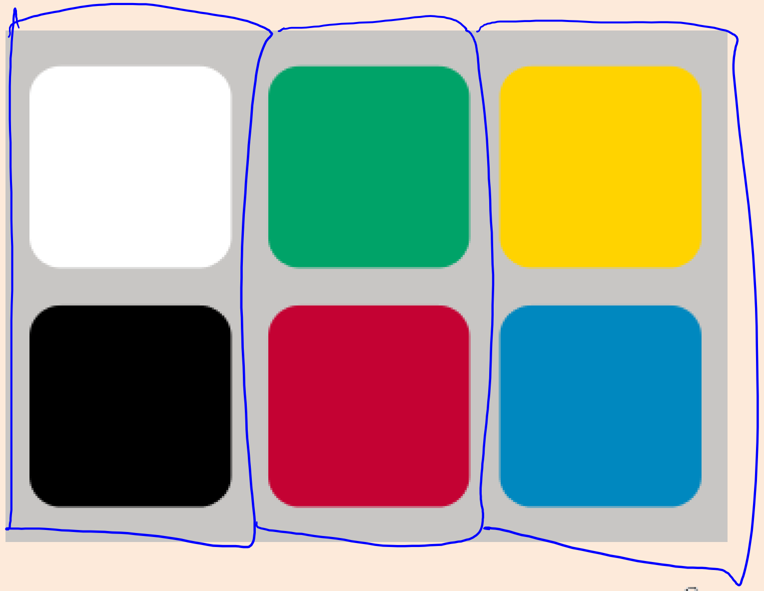


http://oneminuteastronomer.com/astro-course-day-5/
https://en.wikipedia.org/wiki/Color_visio

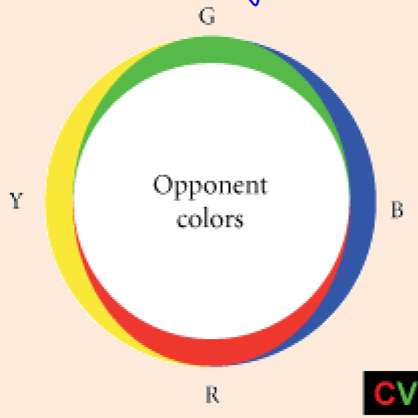
Colour Opponency in the Human Eye

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





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

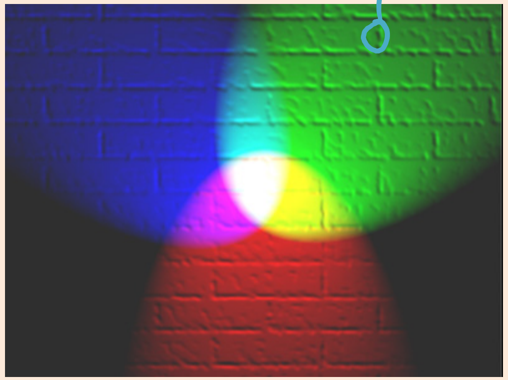


http://oneminuteastronomer.com/astro-course-day-5/
https://en.wikipedia.org/wiki/Color_visio
http://5sensesnews.blogspot.ca/

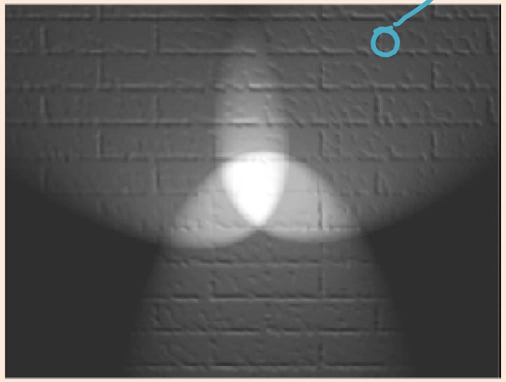
Colour Opponency Representation

For this pixel, eye gets 4 signals

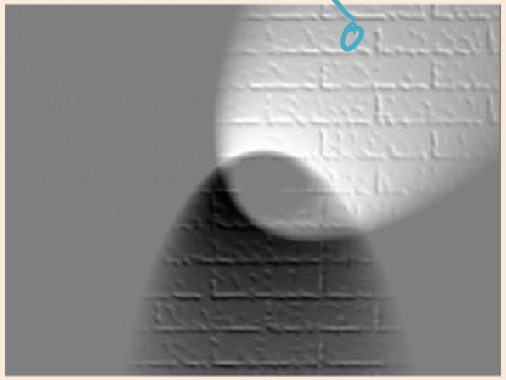
Can represent 4 original values with these 3 z_i values and matrix 'W'



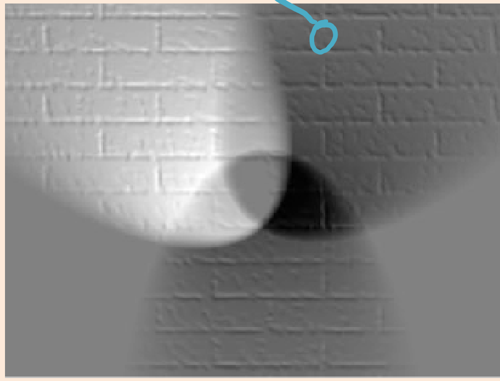
$\approx w_1$



$+w_2$



$+w_3$



First row of W (First PC)

Analogous to means in k-means.

brightness

Second row (4×1)

red/green

Third row (4×1)

blue/yellow

https://en.wikipedia.org/wiki/RGB_color_model