CPSC 340: Machine Learning and Data Mining

More PCA

Fall 2018

1. Decision trees
2. Naïve Bayes classification
3. Ordinary least squares regression
4. Logistic regression
5. Support vector machines
6. Ensemble methods
7. Clustering algorithms
8. Principal component analysis
9. Singular value decomposition
10. Independent component analysis (bonus)

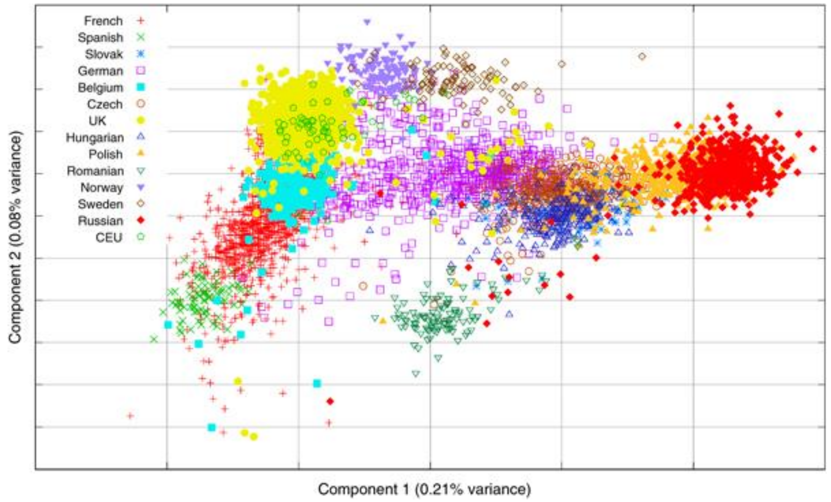
http://www.kdnuggets.com/2016/08/10-algorithms-machine-learning-engineers.html

Last Time: Latent-Factor Models

- Latent-factor models take input data ‘X’ and output a basis ‘Z’:

$$X \longrightarrow \boxed{\text{Latent-factor model}} \longrightarrow Z$$

  – Usually, ‘Z’ has fewer features than ‘X’.
- Uses: dimensionality reduction, visualization, factor discovery.



Trait	Description
Openness	Being curious, original, intellectual, creative, and open to new ideas.
Conscientiousness	Being organized, systematic, punctual, achievement-oriented, and dependable.
Extraversion	Being outgoing, talkative, sociable, and enjoying social situations.
Agreeableness	Being affable, tolerant, sensitive, trusting, kind, and warm.
Neuroticism	Being anxious, irritable, temperamental, and moody.

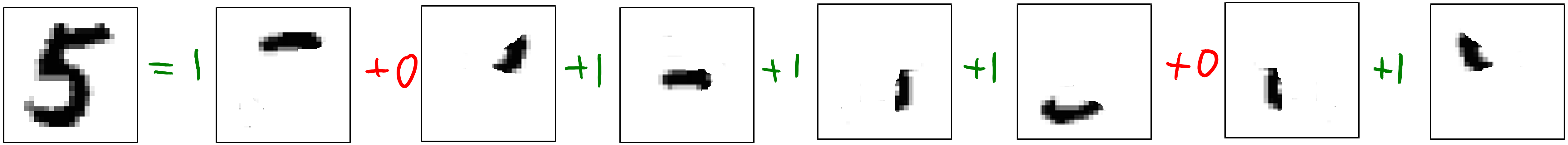
http://infoproc.blogspot.ca/2008/11/european-genetic-substructure.html
https://new.edu/resources/big-5-personality-traits

Last Time: Principal Component Analysis

- Principal component analysis (PCA) is a linear latent-factor model:
  - These models "factorize" matrix X into matrices Z and W:

$$\underset{n \times d}{X} \approx \underset{n \times k}{Z}\,\underset{k \times d}{W} \qquad x_i \approx W^T z_i \qquad x_{ij} \approx \langle w^j, z_i \rangle$$

  - We can think of rows w_c of W as 'k' fixed "part" (used in all examples).
  - z_i is the "part weights" for example x_i: "how much of each part w_c to use".

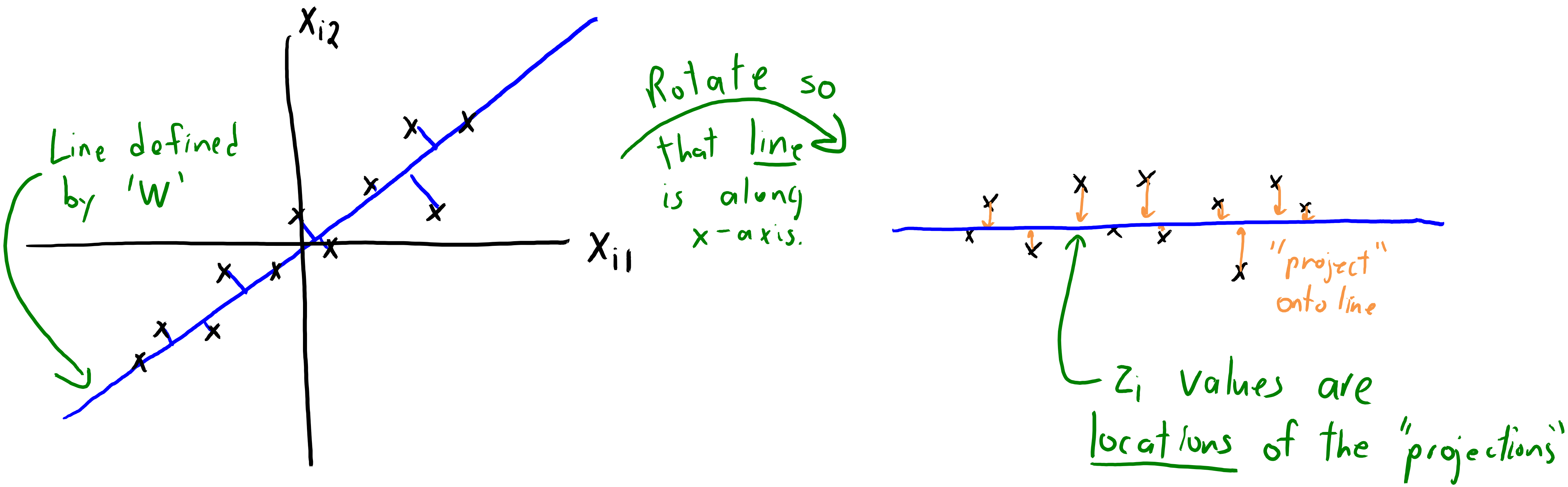


$$\hat{x}_i = z_{i1} w_1 + z_{i2} w_2 + z_{i3} w_3 + z_{i4} w_4 + z_{i5} w_5 + z_{i6} w_6 + z_{i7} w_7$$

"parts" are called "principal components" or "factors"

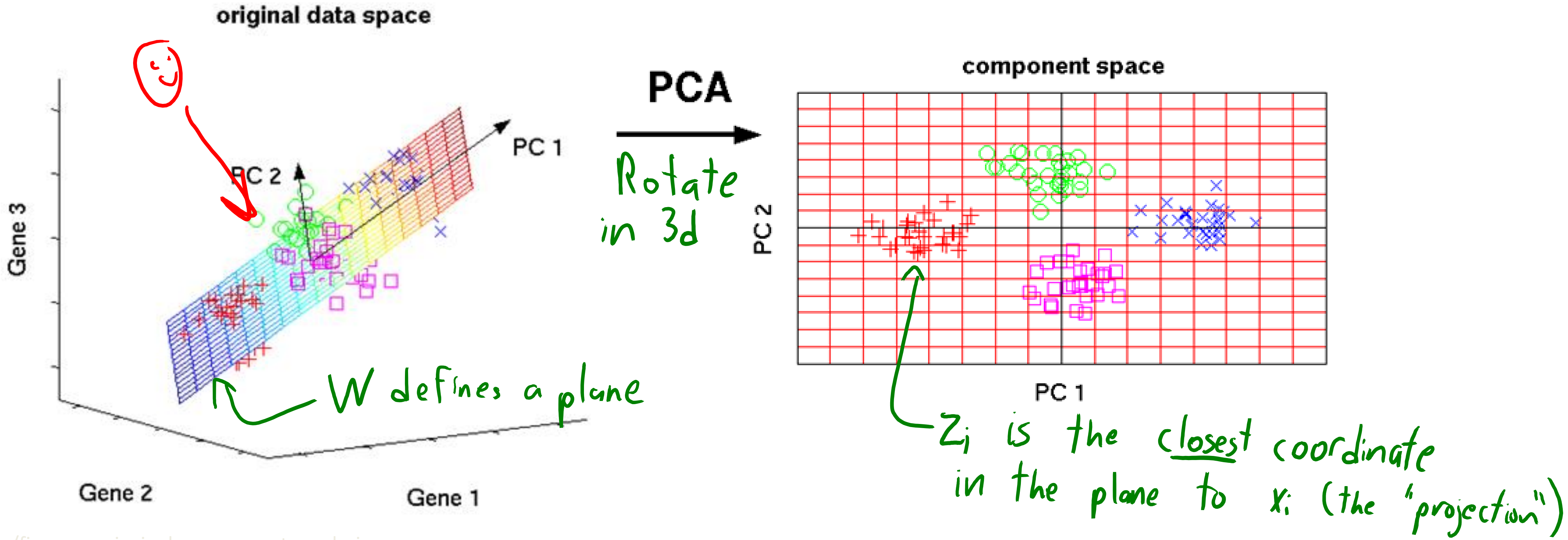
Last Time: PCA Geometry

- When k=1, the W matrix defines a line:
  - We choose 'W' as the line minimizing squared distance to the data.
  - Given 'W', the z_i are the coordinates of the x_i "projected" onto the line.



Last Time: PCA Geometry

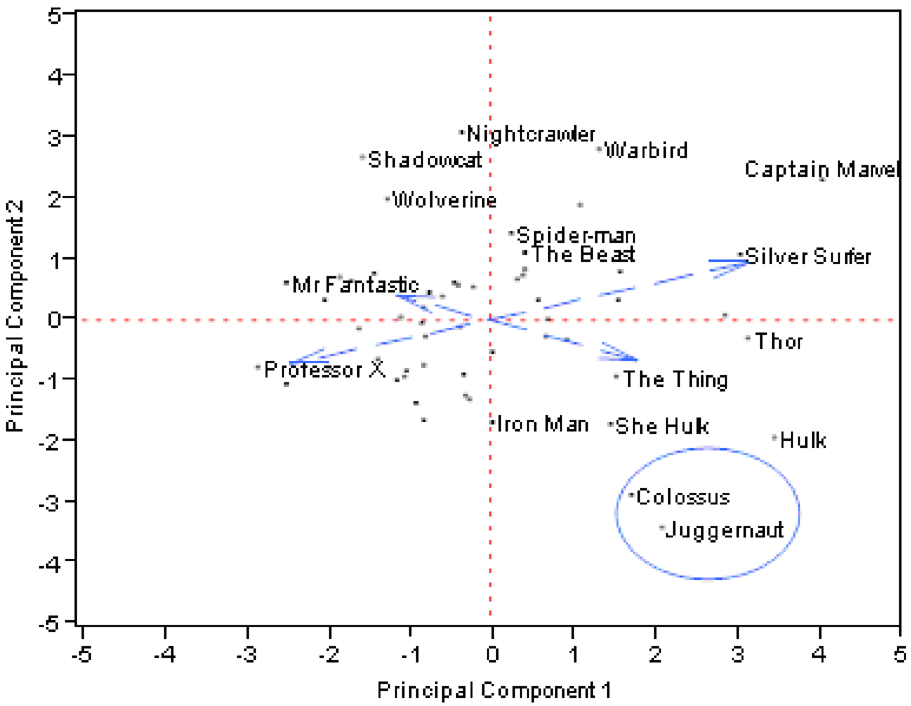
- When k=2, the W matrix defines a plane:
  - We choose 'W' as the plane minimizing squared distance to the data.
  - Given 'W', the z_i are the coordinates of the x_i "projected" onto the plane.

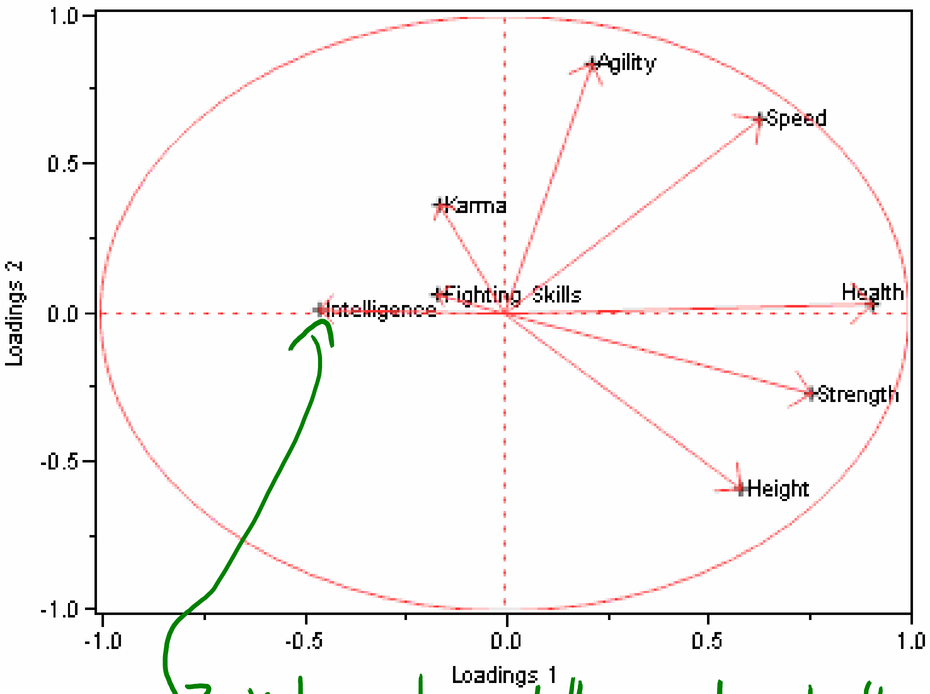


http://www.nlpca.org/fig_pca_principal_component_analysis.png

Last Time: PCA Geometry

- When $k=2$, the W matrix defines a plane:
  - Even if the original data is high-dimensional, we can visualize data “projected” onto this plane.





z_i value when intelligence $=1$ and other $x_{ij}=0$

http://www.prismtc.co.uk/superheroes-pca/

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 means/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 'j' of 'X' from the basis z_i.
    - The output "y_i" we try to predict here is actually the features "x_i".
    - So we have 'd' sums inside the sum over 'n'.
  - And we are also learning the features z_i.
    - Each z_i say how to mix the mean/factor w_c to approximation example 'i'.

Principal Component Analysis (PCA)

- Different ways to write the PCA objective function:

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

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

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

- We're picking Z and W to approximate the original data X.
  - It won't be perfect since usually k is much smaller than d.

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.

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.
  - Notice that this means that PCA is parametric (don't need 'Z' at test time).

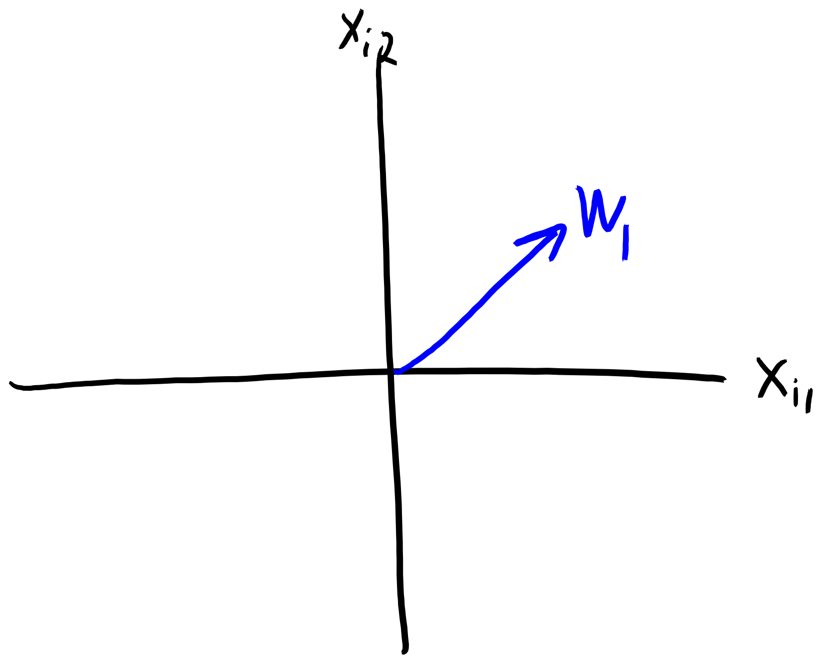
(pause)

Non-Uniqueness of PCA

- Unlike k-means, we can efficiently find global optima of f(W,Z).
  - Algorithms coming later.
- Unfortunately, there never 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.

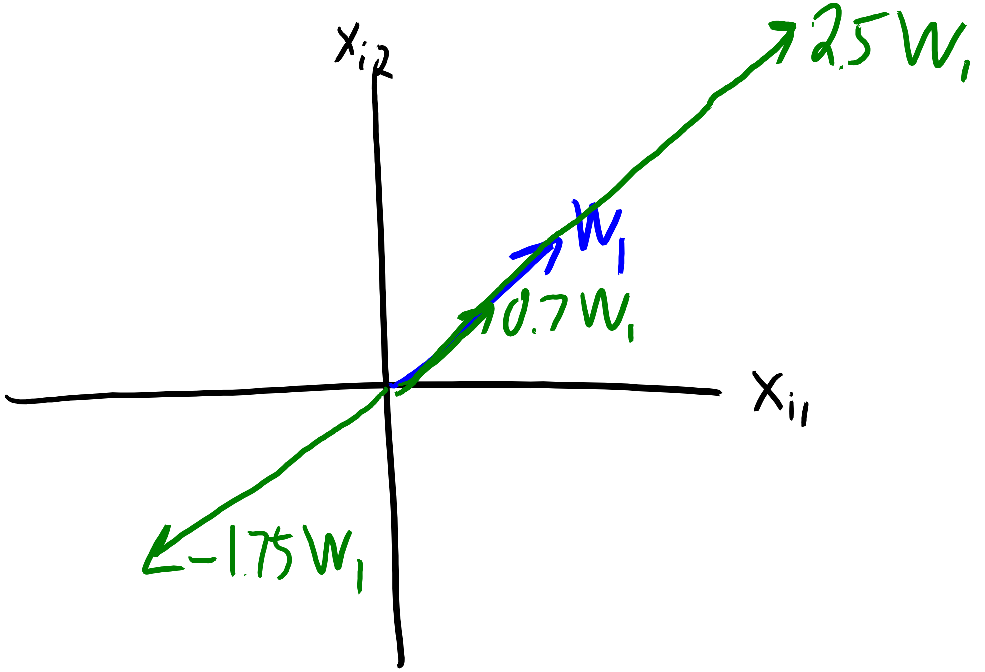
Span of 1 Vector

- 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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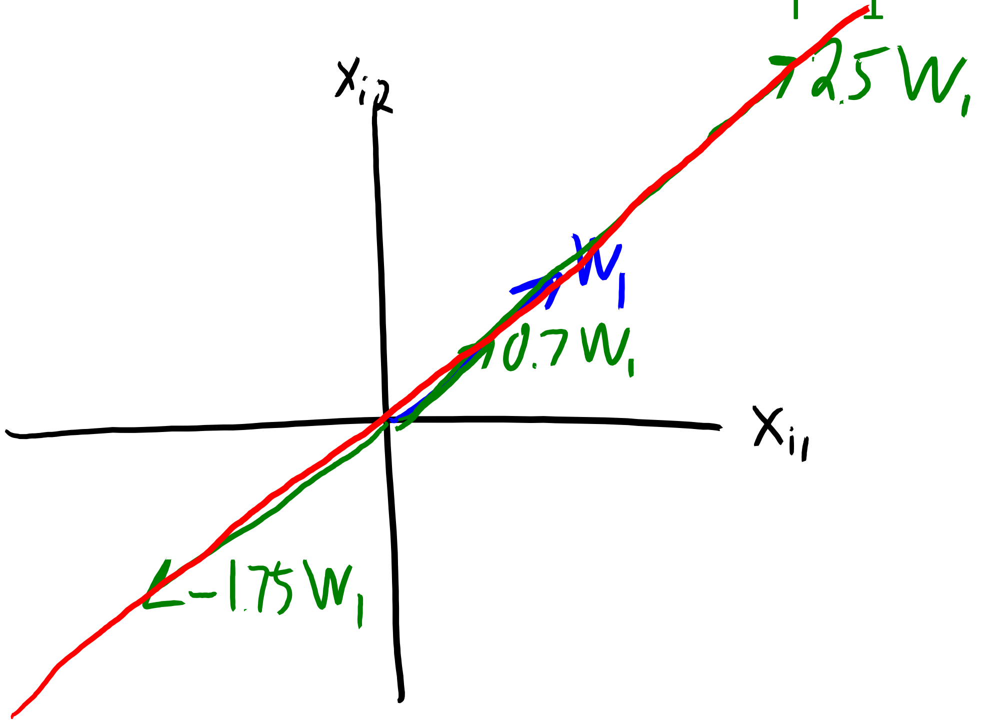
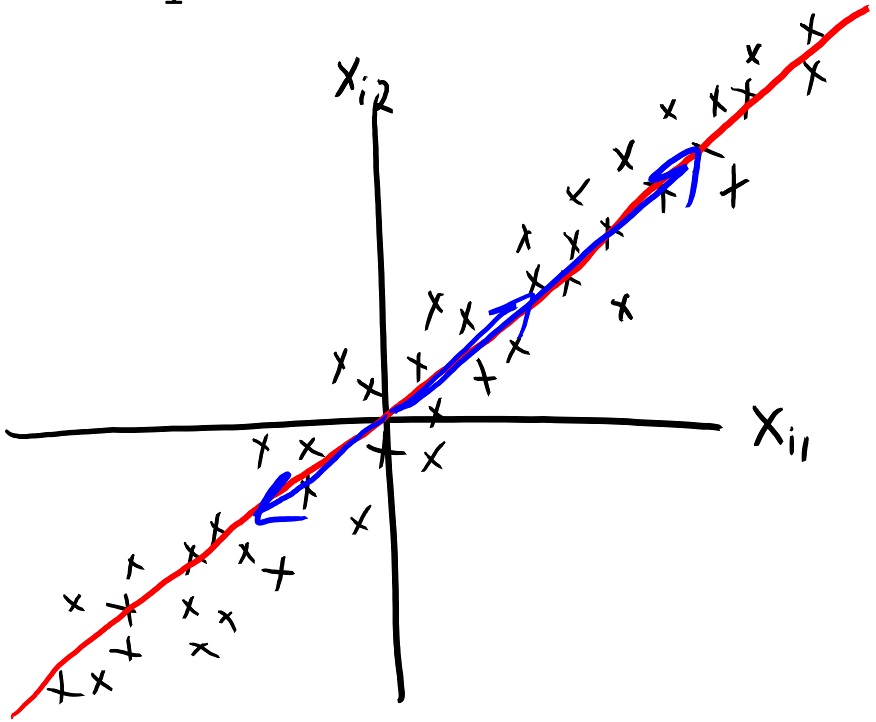


- If $w_1 \neq 0$, this forms a line.

Span of 1 Vector

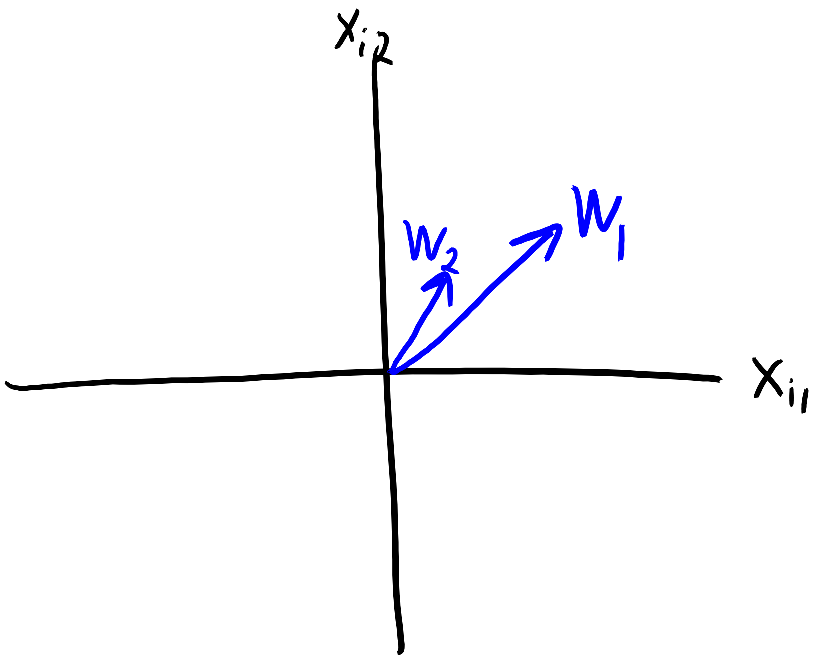
- But note that the "span" of many different vectors gives same line.
  - Mathematically: αw_1 defines the same line as w_1 for any scalar $\alpha \neq 0$.



  - 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. $\|(\alpha W)(\frac{1}{\alpha}Z)-X\|_F^2 = \|WZ-X\|_F^2$

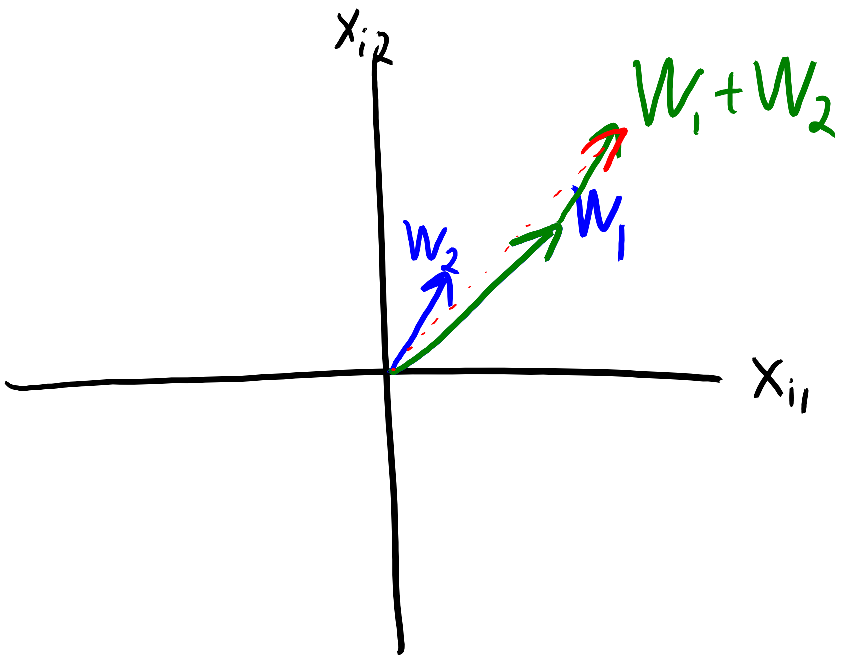
Span of 2 Vectors

- 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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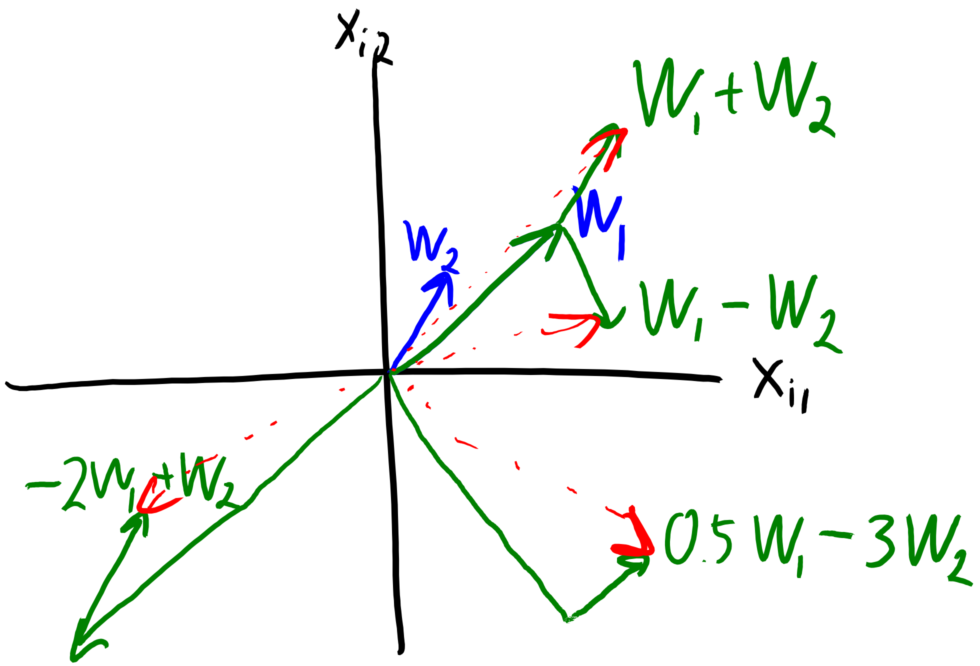

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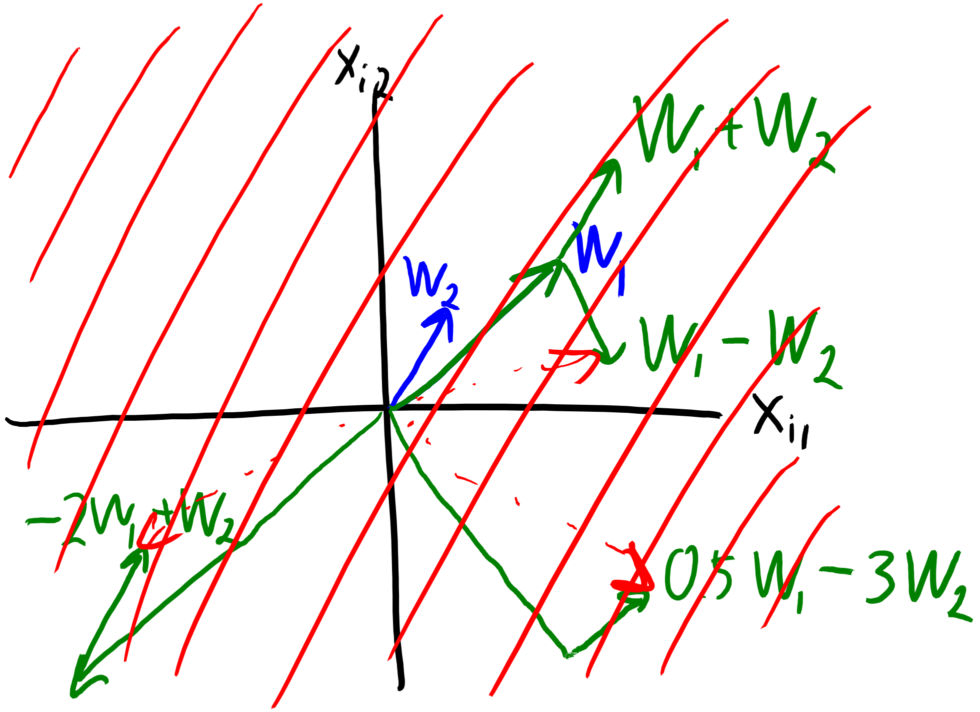

  - For most non-zero 2d vectors, span(w_1,w_2) is a plane.
    - In the case of two vectors in R^2, the plane will be *all* of R^2.

Span of 2 Vectors

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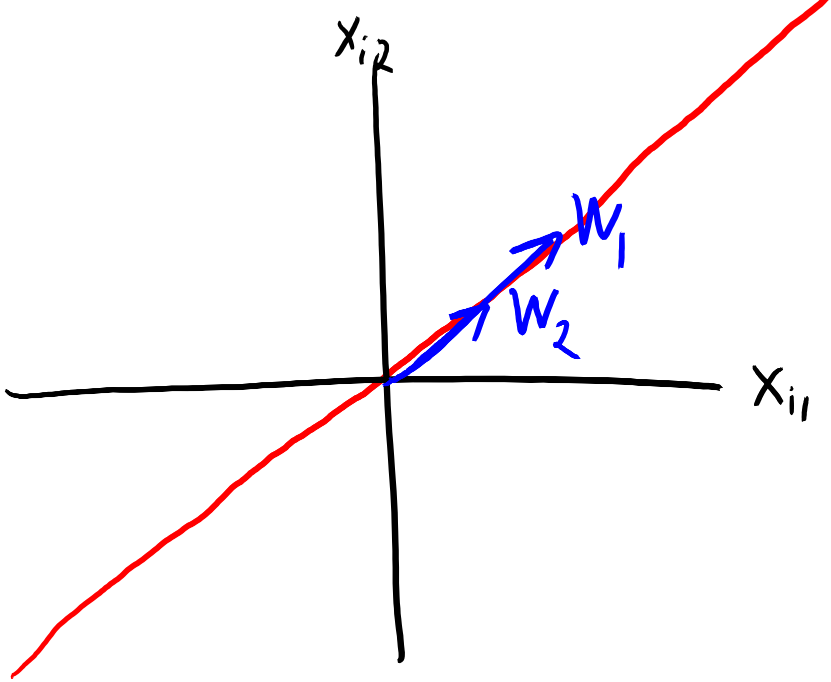
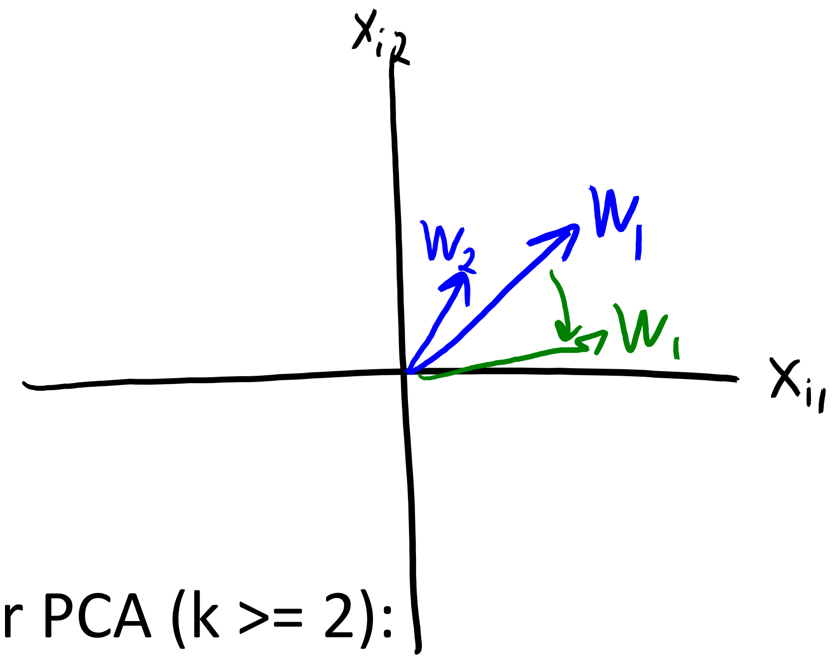


  - For most non-zero 2d vectors, span(w_1,w_2) is plane.
    - Exception is if w_2 is in span of w_1 ("collinear"), then span(w_1,w_2) is just a line.

Span of 2 Vectors

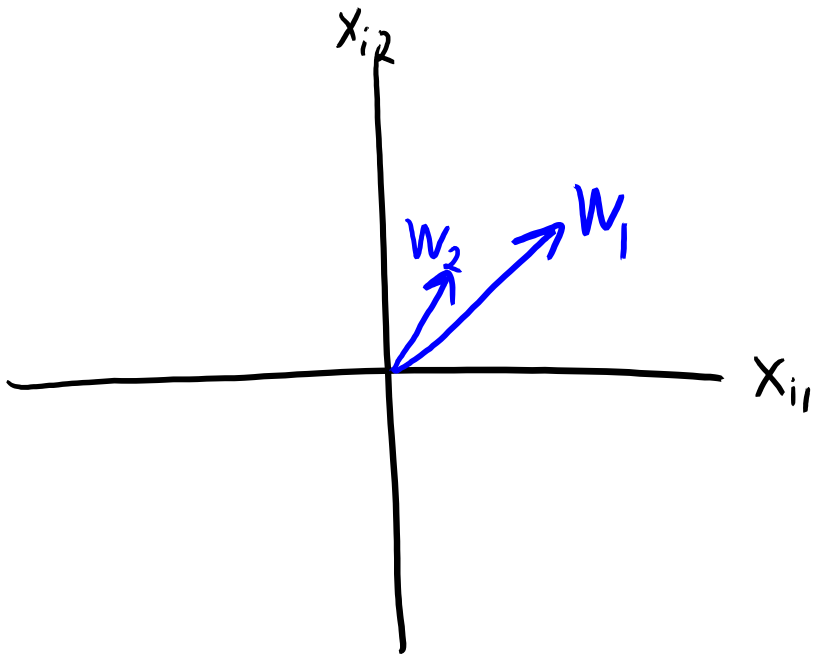
- Consider two vector w_1 and w_2 (k=2).
  - The span(w_1,w_2) is all vectors of form $z_{i1}w_1 + z_{i2}w_2$ for a scalars z_{i1} and z_{i2}.



  - 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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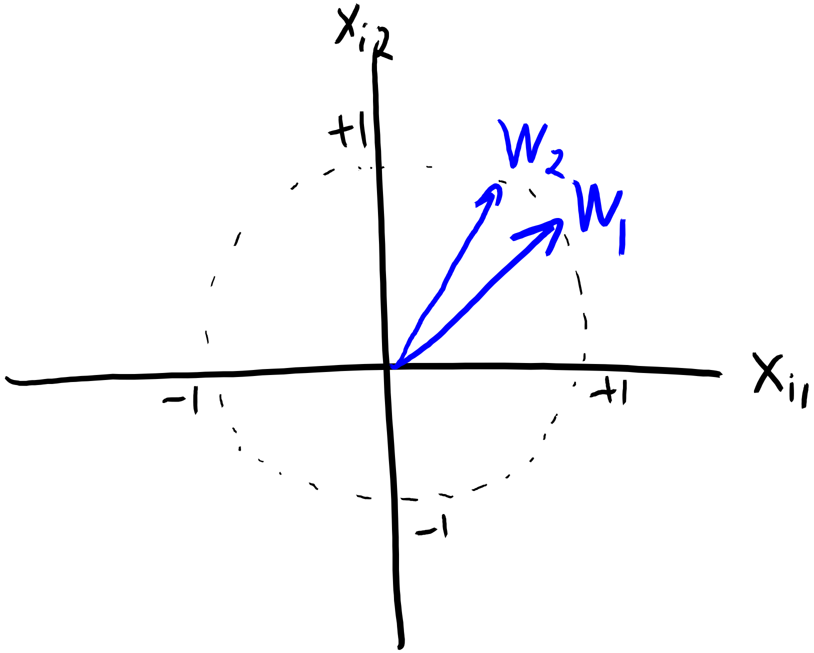
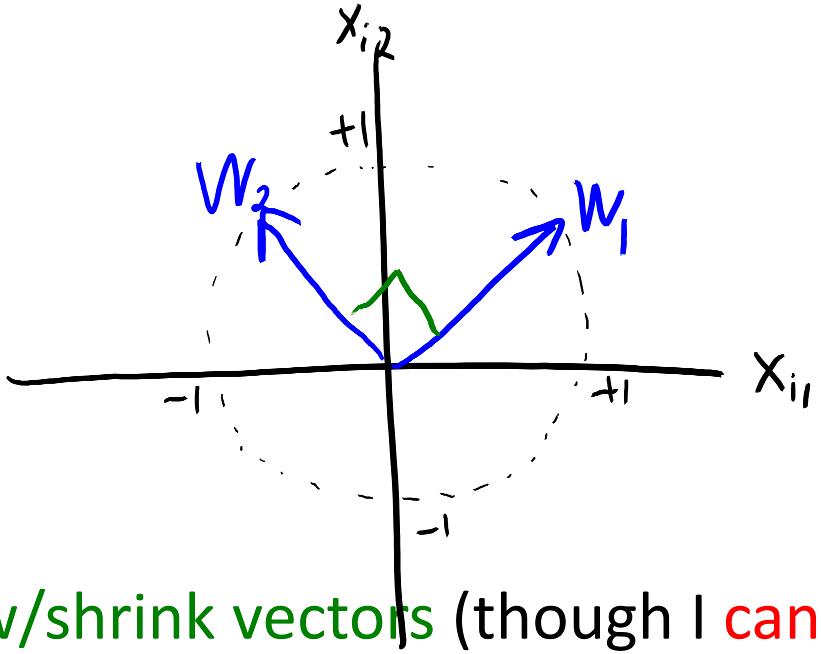


Span of 2 Vectors

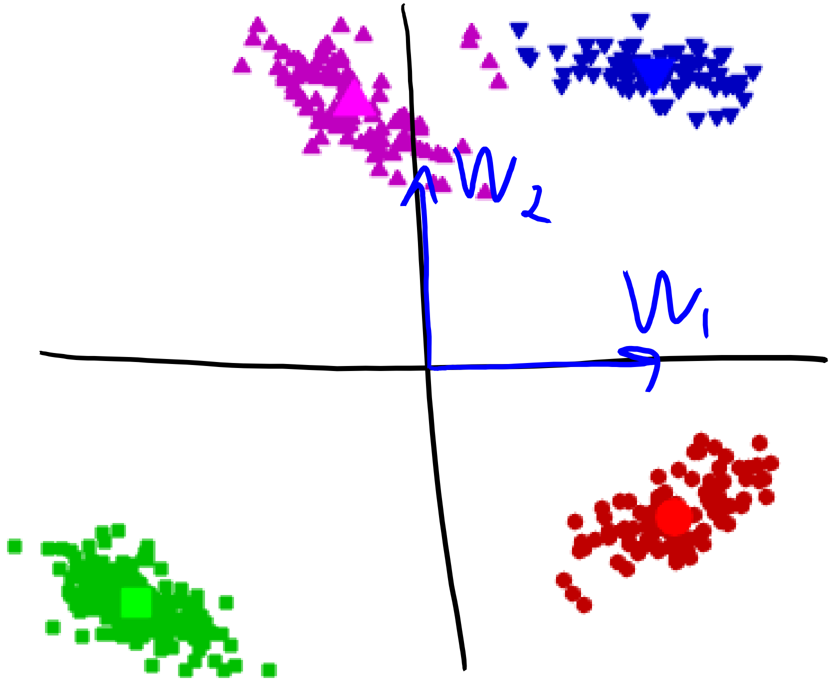
- 2 tricks to make vectors defining a plane "more unique":
  - Normalization: enforce that $||w_1|| = 1$ and $||w_2|| = 1$.
  - Orthogonality: enforce that $w_1^T w_2 = 0$ ("perpendicular").



  - 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 $k \leq d$

- 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 just set Z=X and W=I to get ZW=X (error of 0).

Span in Higher Dimensions

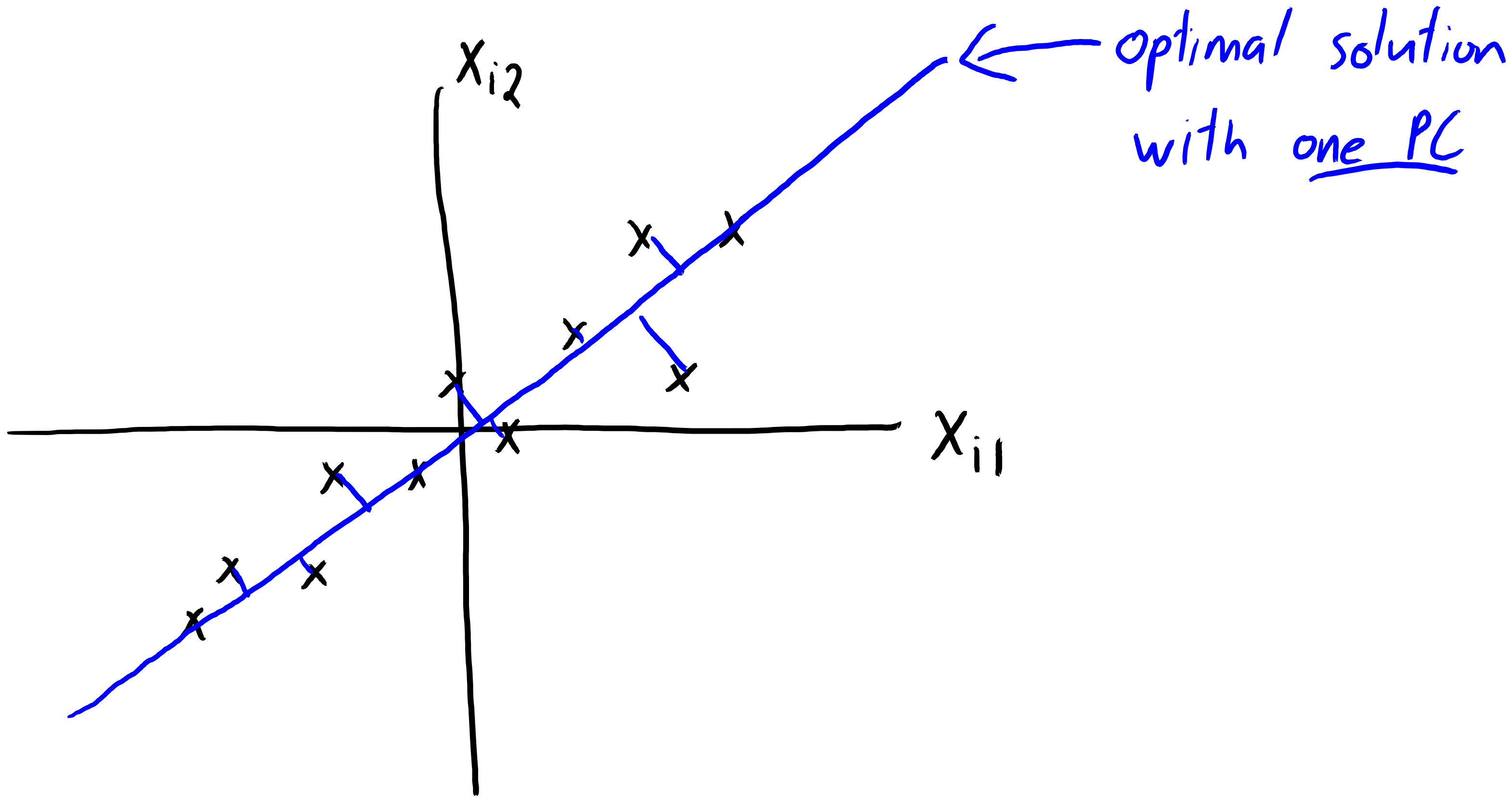
- In higher-dimensional spaces:
  - Span of 1 non-zero vector w_1 is a line.
  - Span of 2 non-zero vectors w_1 and w_2 is a plane (if not collinear).
    - Can be visualized as a 2D plot.
  - Span of 3 non-zeros vectors $\{w_1, w_2, w_3\}$ is a 3d space (if not "coplanar").
  - …
- This is how the W 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:
  - I can multiply any w_c by any non-zero α.
  - I can rotate any w_c almost arbitrarily within the span.
  - I can 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.

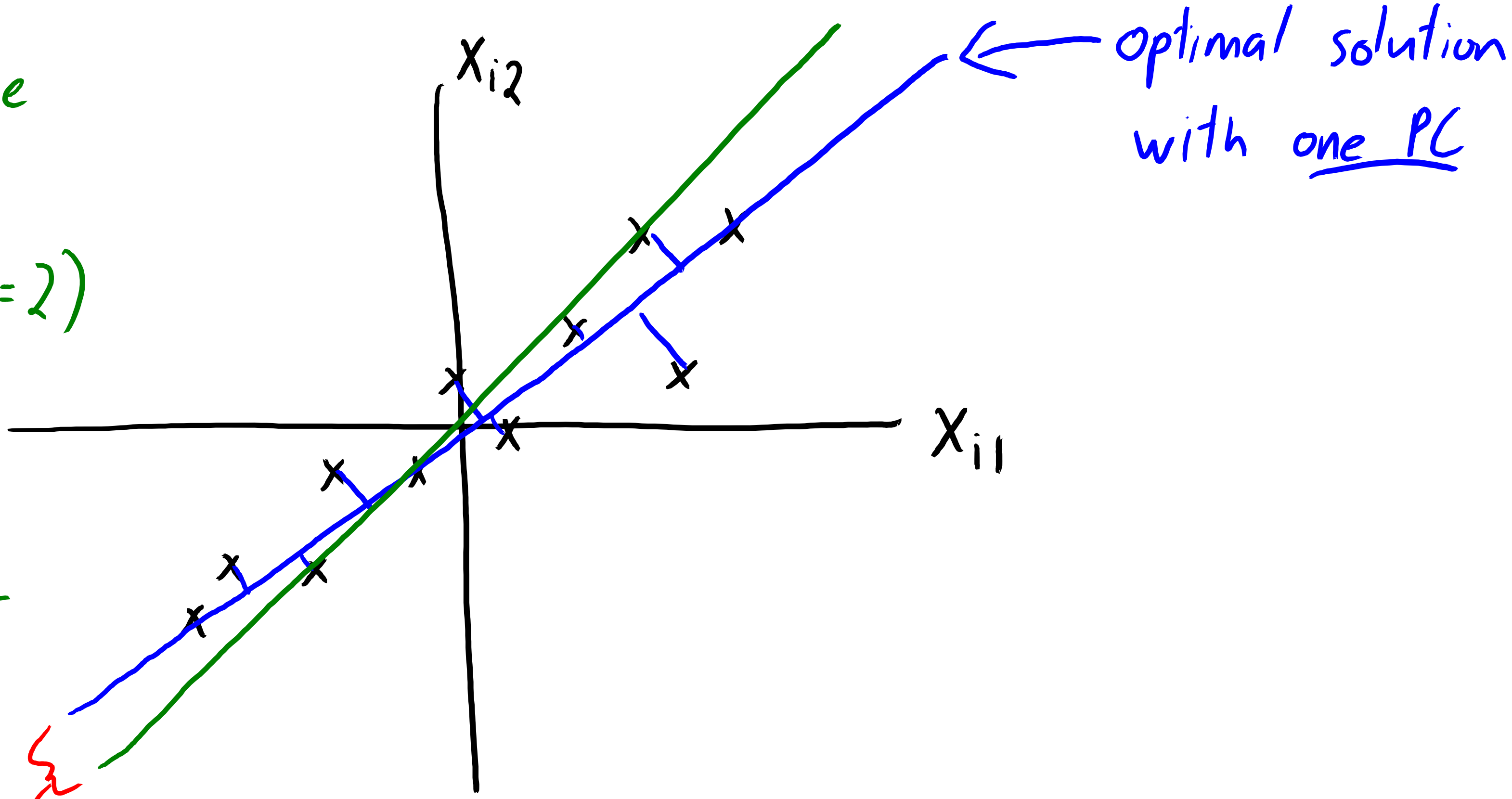
Basis, Orthogonality, Sequential Fitting



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.



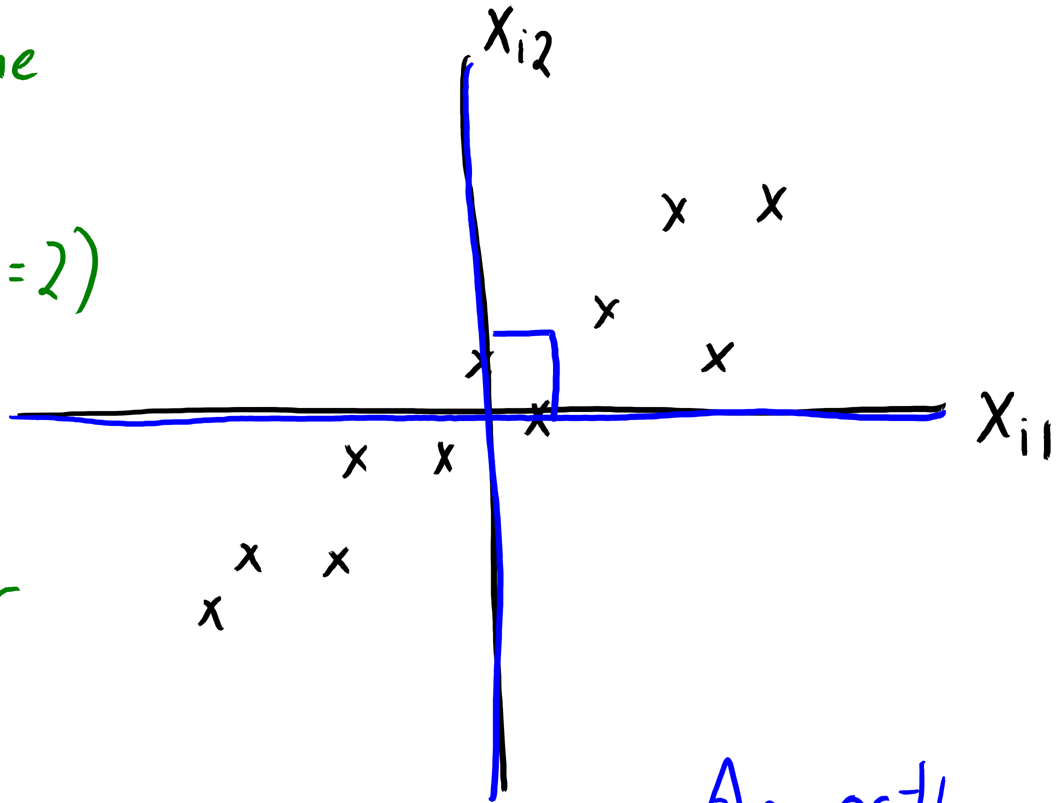
An optimal solution but not orthogonal.

(both PCs give similar information)

Basis, Orthogonality, Sequential Fitting

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

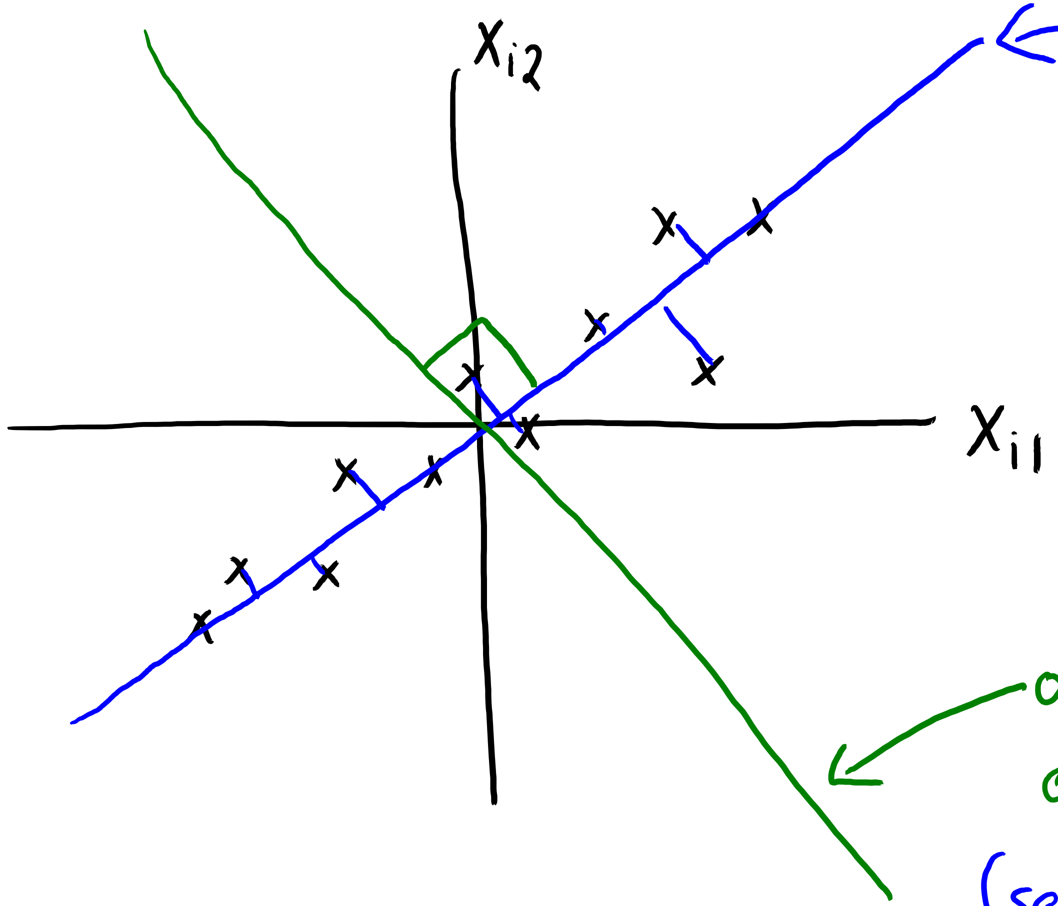
I can get 0 error on every data point.



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.

- 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:

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

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

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

PCA Computation: other methods

- 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 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 "part weights" Z and find the optimal "parts" W.
  - Fix "parts" W and find the optimal "part weights" 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):

$$\nabla_W f(W,Z) = Z^TZW - Z^TX \quad \text{so} \quad W = (\underline{Z^TZ})^{-1}(Z^TX)$$

(writing gradient as a matrix)

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

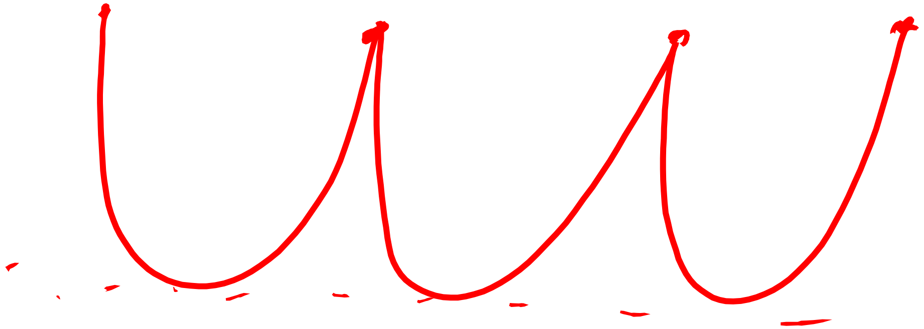
$$\nabla_Z f(W,Z) = ZWW^T - XW^T \quad \text{so} \quad Z = XW^T(\underline{WW^T})^{-1}$$

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

PCA Computation: Alternating Minimization

- With centered data, the PCA objective is:

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



- 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 $W_1 = 0$, 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:

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

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).

Summary

- PCA objective:
  - Minimizes squared error between elements of X and elements of ZW.
- 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 $||w_c|| = 1$.
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  - 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.