CPSC 340: Machine Learning and Data Mining

Principal Component Analysis

Last Time: MAP Estimation

- MAP estimation maximizes posterior:

$$\underbrace{p(w \mid X, y)}_{\text{"posterior"}} \propto \underbrace{p(y \mid X, w)}_{\text{"likelihood"}} \underbrace{p(w)}_{\text{"prior"}}$$

- Likelihood measures probability of labels 'y' given parameters 'w'.
- Prior measures probability of parameters 'w' before we see data.
- For IID training data and independent priors, equivalent to using:

$$f(w) = -\sum_{i=1}^{n} \log(p(y_i \mid x_i, w)) - \sum_{j=1}^{d} \log(p(w_j))$$

- So log-likelihood is an error function, and log-prior is a regularizer.
  - Squared error comes from Gaussian likelihood.
  - L2-regularization comes from Gaussian prior.

The Story So Far…

- Part 1: Supervised Learning.
  - Methods based on counting and distances.
- Part 2: Unsupervised Learning.
  - Methods based on counting and distances.
- Part 3: Supervised Learning (just finished).
  - Methods based on linear models and gradient descent.
- Part 4: Unsupervised Learning (today).
  - Methods based on linear models and gradient descent.

Motivation: Human vs. Machine Perception

- Huge difference between what we see and what computer sees:

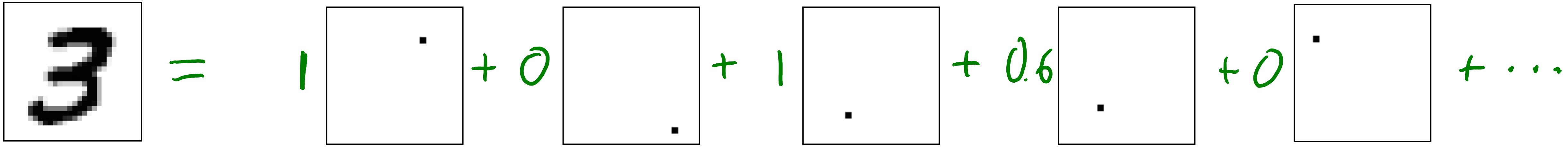
What we see:

What the computer "sees":

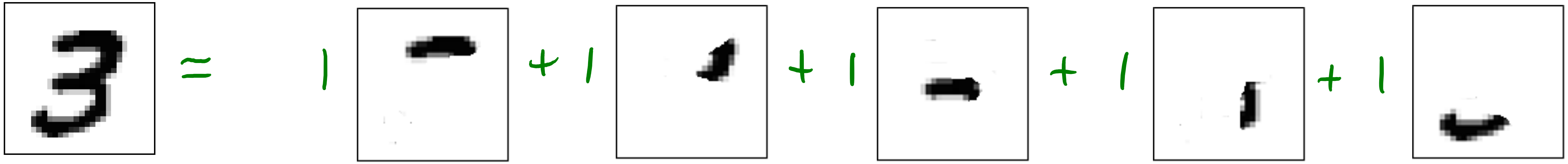
- But maybe images shouldn't be written as combinations of pixels.
  - Can we learn a better representation?
  - In other words, can we learn good features?

Motivation: Pixels vs. Parts

- Can view 28x28 image as weighted sum of "single pixel on" images:



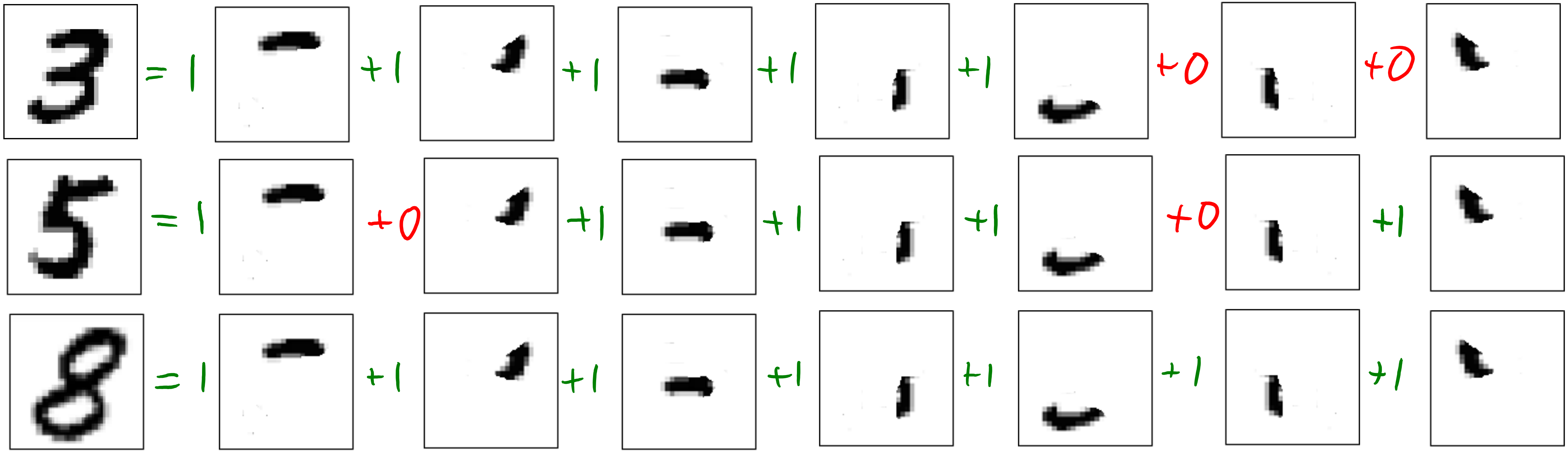
  - We have one image/feature for each pixel.
  - The weights specify "how much of this pixel is in the image".
    - A weight of zero means that pixel is white, a weight of 1 means it's black.
- This is non-intuitive, isn't a "3" made of small number of "parts"?



  - Now the weights are "how much of this part is in the image".

Motivation: Pixels vs. Parts

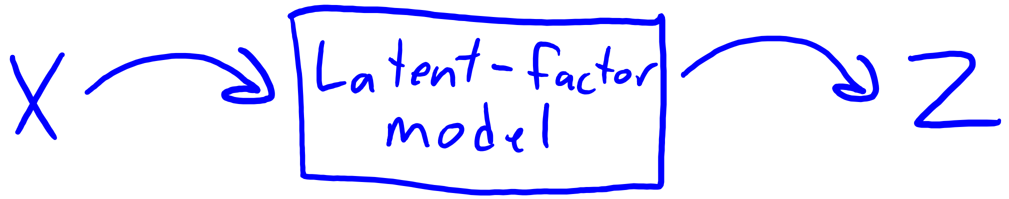
- We could represent other digits as different combinations of "parts":



- Consider replacing images x_i by the weights z_i of the different parts:
  - The 784-dimensional x_i for the "5" image is replaced by 7 numbers: z_i = [1 0 1 1 1 0 1].
  - Features like this could make learning much easier.

Part 4: Latent-Factor Models

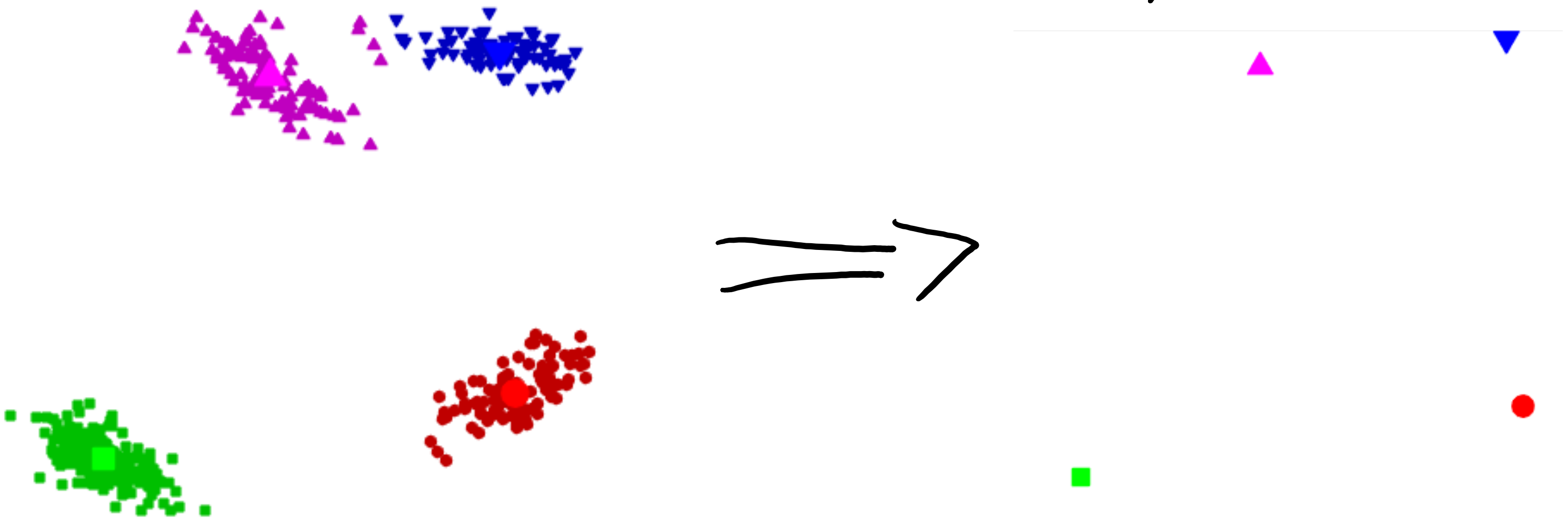
- The "part weights" are a change of basis from x_i to some z_i.
  - But in high dimensions, it can be hard to find a good basis.
- Part 4 is about learning the basis from the data.



- Why?
  - Supervised learning: we could use "part weights" as our features.
  - Outlier detection: it might be an outlier if isn't a combination of usual parts.
  - Dimension reduction: compress data into limited number of "part weights".
  - Visualization: if we have only 2 "part weights", we can view data as a scatterplot.
  - Interpretation: we can try and figure out what the "parts" represent.

Previously: Vector Quantization

- Recall using k-means for vector quantization:
  - Run k-means to find a set of "means" w_c.
  - This gives a cluster $\hat{y}_i$ for each object 'i'.
  - Replace features x_i by mean of cluster: $\hat{x}_i \approx w_{\hat{y}_i}$



- This can be viewed as a (really bad) latent-factor model.

Vector Quantization (VQ) as Latent-Factor Model

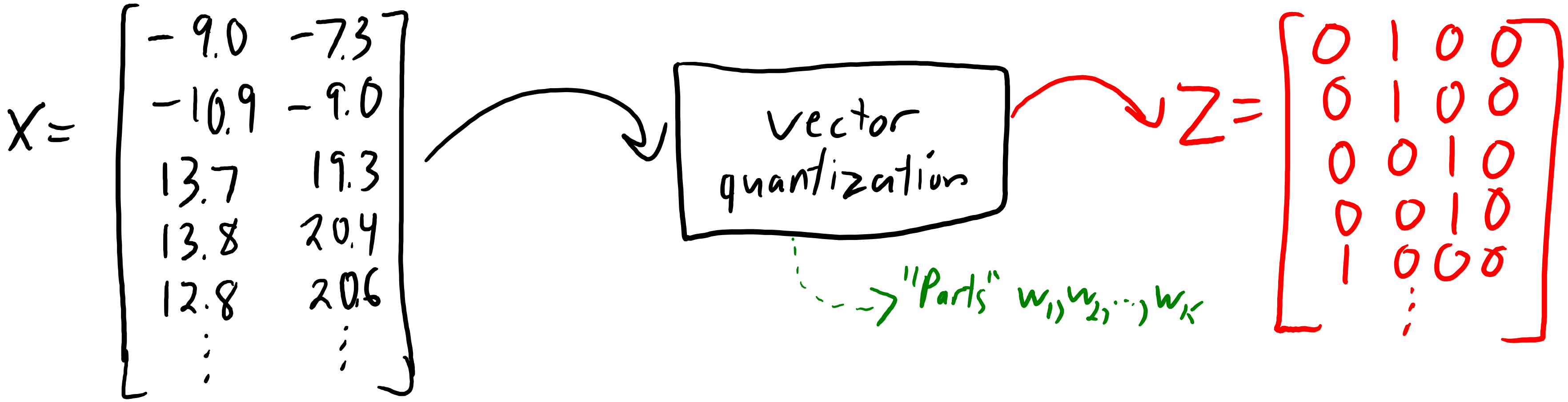
- If x_i is in cluster 2, VQ approximates x_i by mean w_2 of cluster 2:

$$x_i \approx w_2 = 0w_1 + 1w_2 + 0w_3 + 0w_4$$

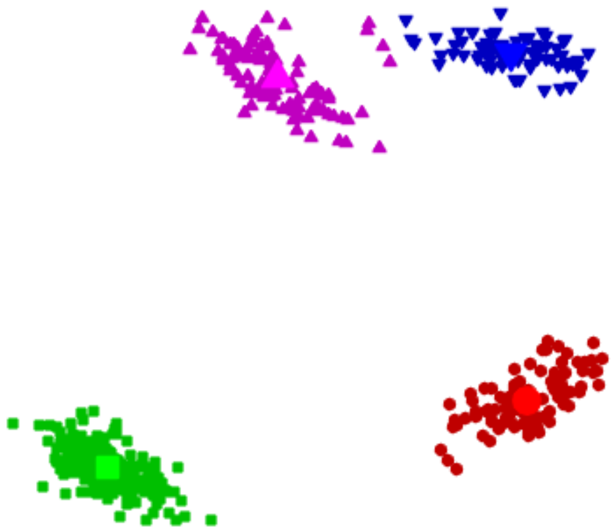
- So in this example we would have z_i = [0 1 0 0].
  - The "parts" are the means from k-means.
  - VQ only uses one part (the "part" from the cluster).

Vector Quantization vs. PCA

- Viewing vector quantization as a latent-factor model:

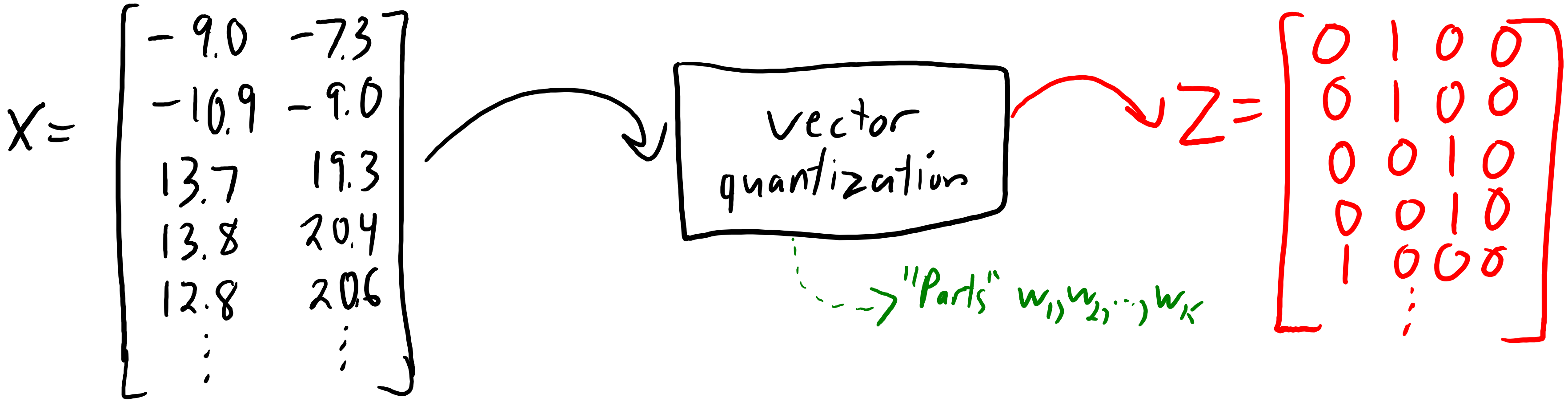


- Suppose we're doing supervised learning, and the colours are the true labels 'y':
  - Classification would be really easy with this "k-means features" 'Z'.

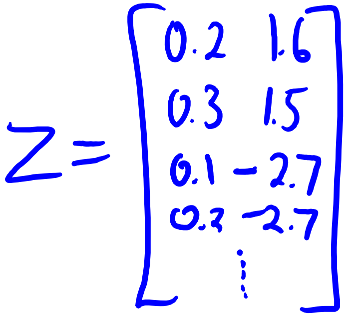


Vector Quantization vs. PCA

- Viewing vector quantization as a latent-factor model:



- But it only uses 1 part, it's just memorizing 'k' points in x_i space.
  - What we want is combinations of parts.
- PCA is a generalization that allows continuous 'z_i':
  - It can have more than 1 non-zero.
  - It can use fractional weights and negative weights.



Principal Component Analysis (PCA) Applications

- Principal component analysis (PCA) has been invented many times:

PCA was invented in 1901 by Karl Pearson,[1] as an analogue of the principal axis theorem in mechanics; it was later independently developed (and named) by Harold Hotelling in the 1930s.[2] Depending on the field of application, it is also named the discrete Kosambi-Karhunen–Loève transform (KLT) in signal processing, the Hotelling transform in multivariate quality control, proper orthogonal decomposition (POD) in mechanical engineering, singular value decomposition (SVD) of $\mathbf{X}$ (Golub and Van Loan, 1983), eigenvalue decomposition (EVD) of $\mathbf{X}^T\mathbf{X}$ in linear algebra, factor analysis (for a discussion of the differences between PCA and factor analysis see Ch. 7 of [3]), Eckart–Young theorem (Harman, 1960), or Schmidt–Mirsky theorem in psychometrics, empirical orthogonal functions (EOF) in meteorological science, empirical eigenfunction decomposition (Sirovich, 1987), empirical component analysis (Lorenz, 1956), quasiharmonic modes (Brooks et al., 1988), spectral decomposition in noise and vibration, and empirical modal analysis in structural dynamics.

standard deviation of 3 in roughly the (0.878, 0.478) direction and of 1 in th orthogonal direction. The vectors shown are the eigenvectors of the covariance matrix scaled by the squa root of the corresponding eigenvalue, and shifted so their tails are at the mean.

Principal Component Analysis (a Recent Review)

Principal component analysis

Michael Greenacre, Patrick J. F. Groenen, Trevor Hastie, Alfonso Iodice D'Enza, Angelos Markos & Elena Tuzhilina

Nature Reviews Methods Primers **2**, Article number: 100 (2022) | Cite this article

A Publisher Correction to this article was published on 08 March 2023

This article has been updated

Abstract

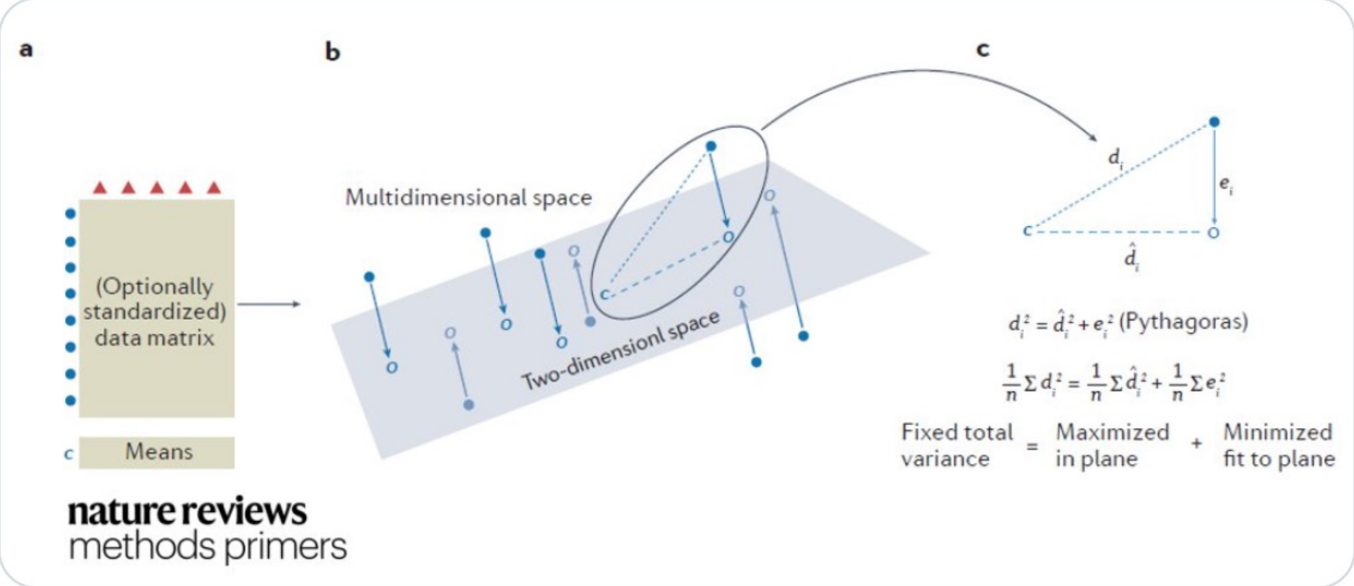
Principal component analysis is a versatile statistical method for reducing a cases-by-variables data table to its essential features, called principal components. Principal components are a few linear combinations of the original variables that maximally explain the variance of all the variables. In the process, the method provides an approximation of the original data table using only these few major components. This Primer presents a

Principal Component Analysis (a Recent Review)

Nature Reviews Methods Primers
@MethodsPrimers

This Primer describes how principle component analysis can be used for data analysis, explaining the mathematical background, analytical workflows, how to interpret a biplot and variants of the method.

go.nature.com/3BsYSxn



1:30 AM · Feb 21, 2023 · **39.5K** Views

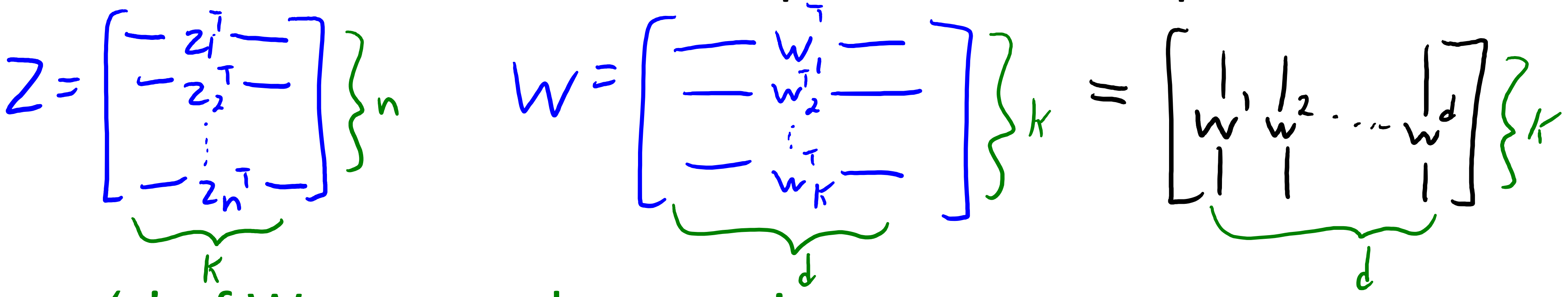
Principal Component Analysis (a Recent Review)

Outlook

PCA has been, and will remain, the workhorse of exploratory data analysis and unsupervised machine learning, while also being at the heart of many real-life research problems. The future of PCA is its increasing application to a wide range of problems and sometimes unexpected areas of research. This section mentions some recent innovations in which PCA and its core algorithm, the SVD, play an important part, especially in the analysis of very large challenging datasets from genetics, ecology, linguistics, business, finance and signal processing. Some of these have already been described, such as sparse PCA and matrix completion. Images, physical objects, and functions are non-standard data objects, to which PCA can be applied after using clever ways of coding the data in the form of a data matrix.

PCA Notation (MEMORIZE)

- PCA takes in a matrix 'X' and an input 'k', and outputs two matrices:



- For row 'c' of W, we use the notation w_c.
  - Each w_c is a "part" (also called a "principal axis", "factor", or "principal component").
- For row 'i' of Z, we use the notation z_i.
  - Each z_i is a set of "part weights" (or "low-dimensional repr." or "features").
- For column 'j' of W, we use the notation w^j.
  - Index 'j' of all the 'k' "parts" (value of pixel 'j' in all the different parts).

PCA Notation (MEMORIZE)

- PCA takes in a matrix ‘X’ and an input ‘k’, and outputs two matrices:

$$\underbrace{Z = \begin{bmatrix} — z_1^T — \\ — z_2^T — \\ \vdots \\ — z_n^T — \end{bmatrix}}_{k}\Big\}n \qquad \underbrace{W = \begin{bmatrix} — w_1^T — \\ — w_2^T — \\ \vdots \\ — w_k^T — \end{bmatrix}}_{d}\Big\}k = \underbrace{\begin{bmatrix} | & | & & | \\ w^1 & w^2 & \cdots & w^d \\ | & | & & | \end{bmatrix}}_{d}\Big\}k$$

- With this notation, we can write approximation of the vector x_i as:

$$\underset{d \times 1}{\hat{x}_i} \approx \begin{bmatrix} \langle w^1, z_i \rangle \\ \langle w^2, z_i \rangle \\ \vdots \\ \langle w^d, z_i \rangle \end{bmatrix} = \underset{d \times k}{W^T} \underset{k \times 1}{z_i}$$

PCA Notation (MEMORIZE)

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$$Z = \underbrace{\begin{bmatrix} - & z_1^T & - \\ - & z_2^T & - \\ & \vdots & \\ - & z_n^T & - \end{bmatrix}}_{k} \Big\} n \qquad W = \underbrace{\begin{bmatrix} - & w_1^T & - \\ - & w_2^T & - \\ & \vdots & \\ - & w_k^T & - \end{bmatrix}}_{d} \Big\} k = \underbrace{\begin{bmatrix} | & | & & | \\ w^1 & w^2 & \cdots & w^d \\ | & | & & | \end{bmatrix}}_{d} \Big\} k$$

- We can write our approximation of one x_{ij} as:

$$\hat{x}_{ij} = z_{i1} w_{1j} + z_{i2} w_{2j} + \cdots + z_{ik} w_{kj} = \sum_{c=1}^{k} z_{ic} w_{cj} = (w^j)^T z_i = \langle w^j, z_i \rangle$$

(NEW NOTATION)

  - K-means: "take index 'j' of closest mean".
  - PCA: "z_i gives weights for index 'j' of all factors".

Different views (MEMORIZE)

- PCA approximates each x_{ij} by the inner product $\langle w^j, z_i \rangle$.
- PCA approximates each x_i by the matrix-vector product $W^T z_i$.
- PCA approximates matrix 'X' by the matrix-matrix product ZW.

$$\underset{n \times d}{X} \approx \underset{n \times k}{Z}\,\underset{k \times d}{W}$$

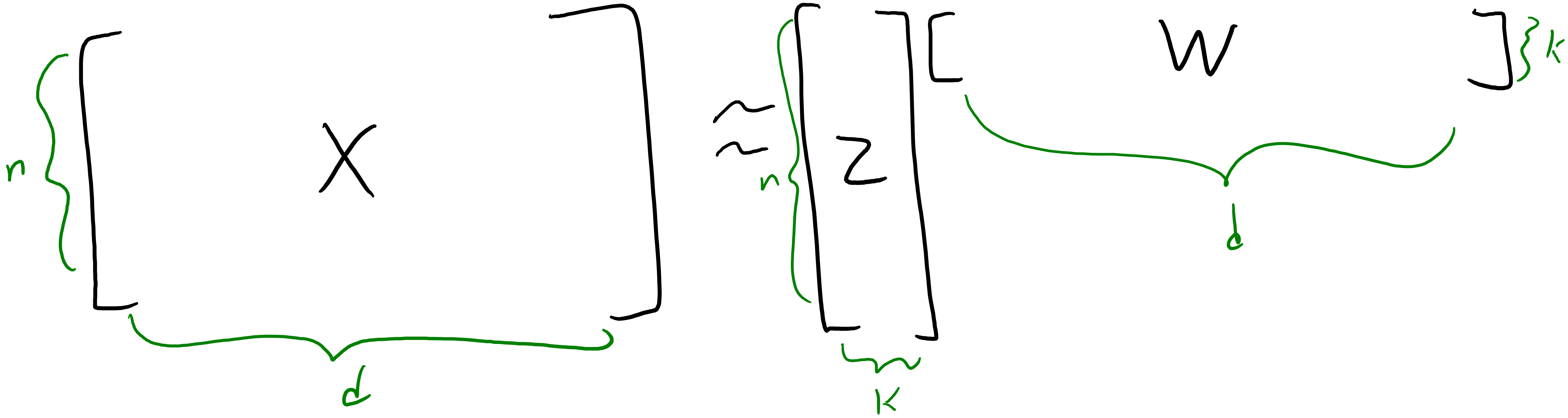
  – PCA is also called a "matrix factorization" model.
  – Both 'Z' and 'W' are variables.

- This can be viewed as a "change of basis" from x_i to z_i values.
  – The "basis vectors" are the rows of W, the w_c.
  – The "coordinates" in the new basis of each x_i are the z_i.

Next Topic: PCA Applications

PCA Applications

- Applications of PCA:
  - Dimensionality reduction: replace 'X' with lower-dimensional 'Z'.
    - If k << d, then compresses data.
    - Often better approximation than vector quantization.



PCA Applications

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$$\underbrace{\begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ 2 & 4 & 6 & 8 & 10 & 12 & 14 & 16 \\ 3 & 6 & 9 & 12 & 15 & 18 & 21 & 24 \\ 4 & 8 & 12 & 16 & 20 & 24 & 28 & 32 \\ 5 & 10 & 15 & 20 & 25 & 30 & 35 & 40 \\ 6 & 12 & 18 & 24 & 30 & 36 & 42 & 48 \\ 7 & 14 & 21 & 28 & 35 & 42 & 49 & 56 \\ 8 & 16 & 24 & 32 & 40 & 48 & 56 & 64 \end{bmatrix}}_{X} \approx \underbrace{\begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \end{bmatrix}}_{Z} \underbrace{\begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \end{bmatrix}}_{W}$$

Compresses 64 elements of ‘X’ down to 16 elements of ‘Z’ and ‘W’

(can predict all x_i values from one z_i value)

PCA Applications

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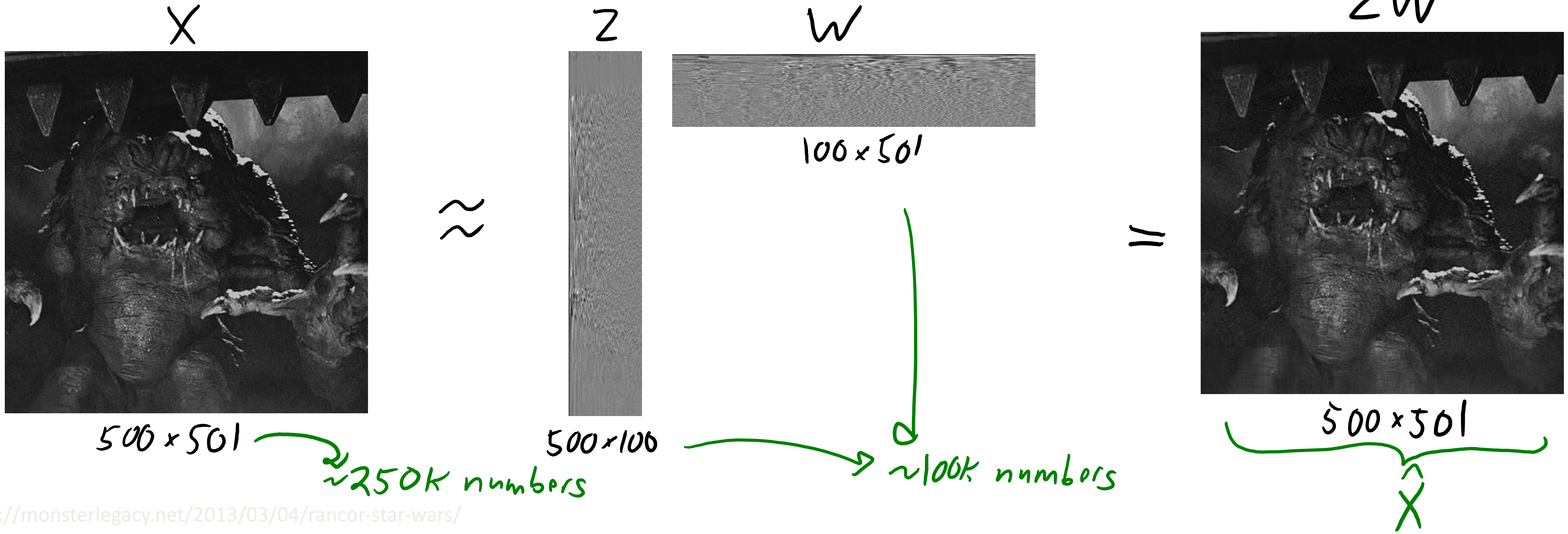

https://monsterlegacy.net/2013/03/04/rancor-star-wars/

PCA Applications

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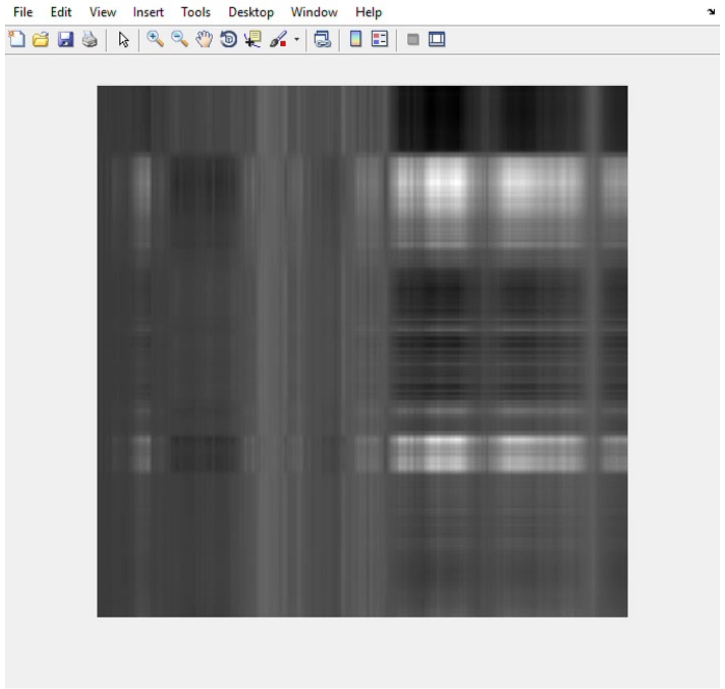


https://monsterlegacy.net/2013/03/04/rancor-star-wars/

PCA Applications

- An essential step for scRNA-seq data analysis

Perform linear dimensional reduction

Next we perform PCA on the scaled data. By default, only the previously determined variable features are used as input, but can be defined using `features` argument if you wish to choose a different subset (if you do want to use a custom subset of features, make sure you pass these to `ScaleData` first).

For the first principal components, Seurat outputs a list of genes with the most positive and negative loadings, representing modules of genes that exhibit either correlation (or anti-correlation) across single-cells in the dataset.

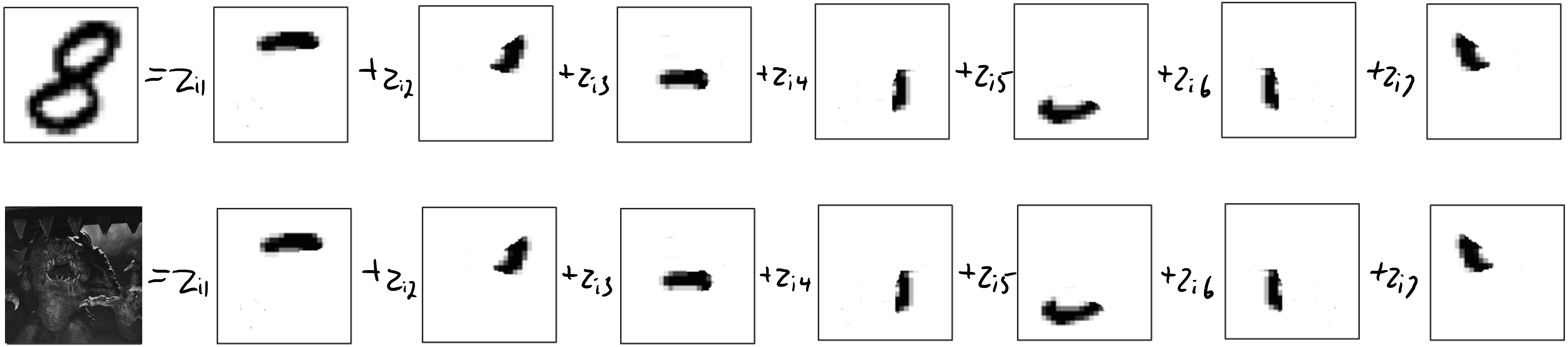
```
pbmc <- RunPCA(pbmc, features = VariableFeatures(object = pbmc))
```

Seurat provides several useful ways of visualizing both cells and features that define the PCA, including `VizDimReduction()`, `DimPlot()`, and `DimHeatmap()`

```
# Examine and visualize PCA results a few different ways
print(pbmc[["pca"]], dims = 1:5, nfeatures = 5)
```

PCA Applications

- Applications of PCA:
  - Outlier detection: if PCA gives poor approximation of x_i, could be ‘outlier’.
    - Though due to squared error PCA is sensitive to outliers.



PCA Applications

- Applications of PCA:
  - Partial least squares: uses PCA features as basis for linear model.

Compute approximation $X \approx ZW$

Now use Z as features in a linear model:

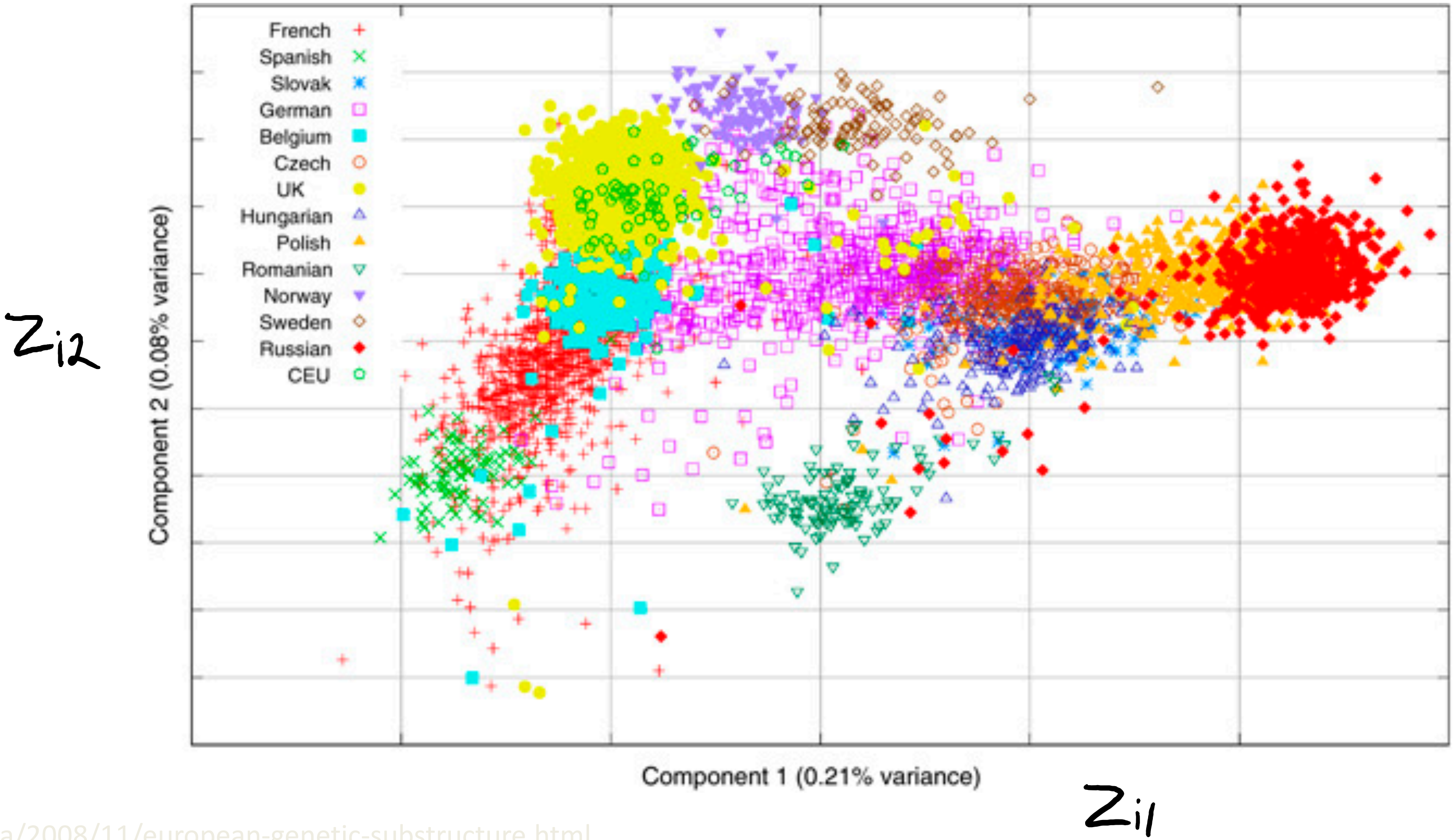
$$y_i = v^T z_i$$

linear regression weights 'v' trained under this change of basis.

lower-dimensional than original features so less overfitting

PCA Applications

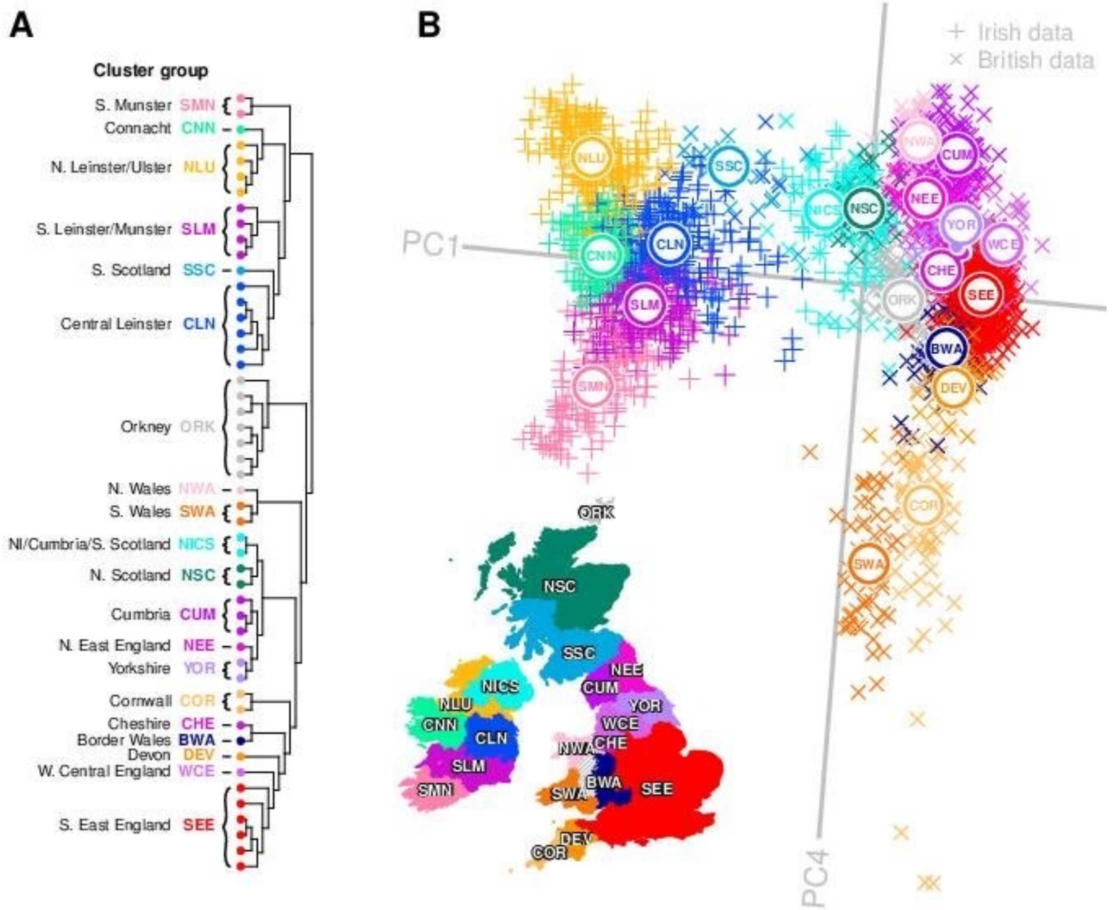
- Applications of PCA:
  - Data visualization: plot z_i with $k = 2$ to visualize high-dimensional objects.



http://infoproc.blogspot.ca/2008/11/european-genetic-substructure.html

PCA Applications

- Applications of PCA:
  - Data visualization: plot z_i with $k = 2$ to visualize high-dimensional objects.
    - Can augment other visualizations:



PCA Applications

- Applications of PCA:
  - Data interpretation: we can try to assign meaning to latent factors w_c.
    - Hidden "factors" that influence all the variables.

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.

https://new.edu/resources/big-5-personality-traits

"Most Personality Quizzes Are Junk Science. I Found One That Isn't."

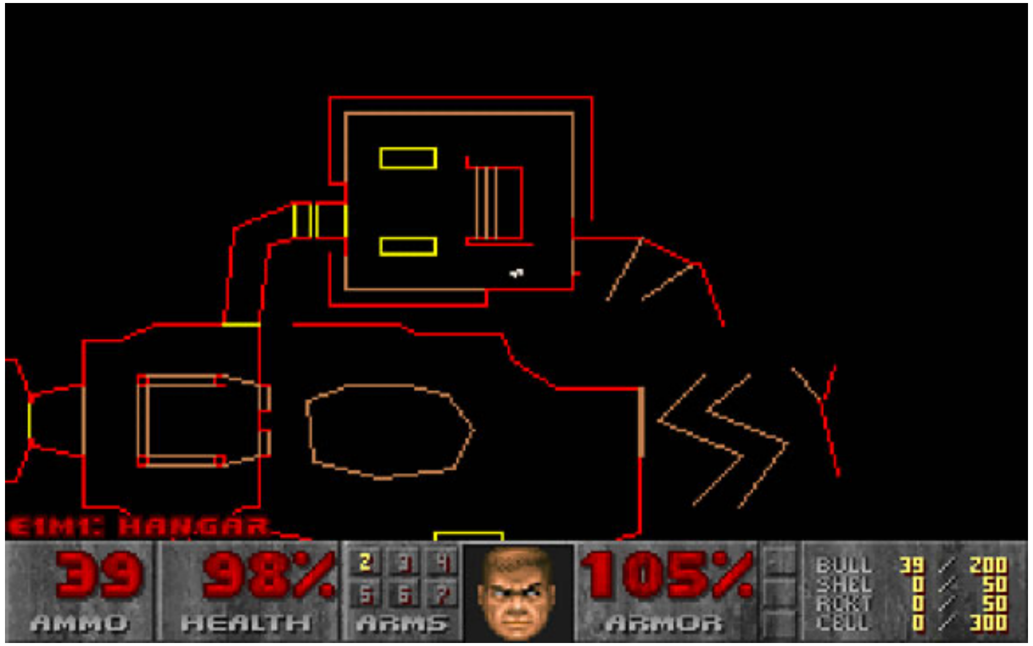
What is PCA actually doing?

When should PCA work well?

Today I just want to show geometry,
we’ll talk about implementation next time.

Doom Overhead Map and Latent-Factor Models

- Original “Doom” video game included an “overhead map” feature:



- This map can be viewed as a latent-factor model of player location.

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

Overhead Map and Latent-Factor Models

- Actual player location at time 'i' can be described by 3 coordinates:

$$x_i = \begin{bmatrix} x_{i1} \\ x_{i2} \\ x_{i3} \end{bmatrix} \begin{matrix} \leftarrow \text{"x" coordinate} \\ \leftarrow \text{"y" coordinate} \\ \leftarrow \text{"z" coordinate} \end{matrix}$$

- The overhead map approximates these 3 coordinates with only 2:

$$z_i = \begin{bmatrix} z_{i1} \\ z_{i2} \end{bmatrix} \begin{matrix} \leftarrow \text{"x" coordinate} \\ \leftarrow \text{"y" coordinate} \end{matrix}$$

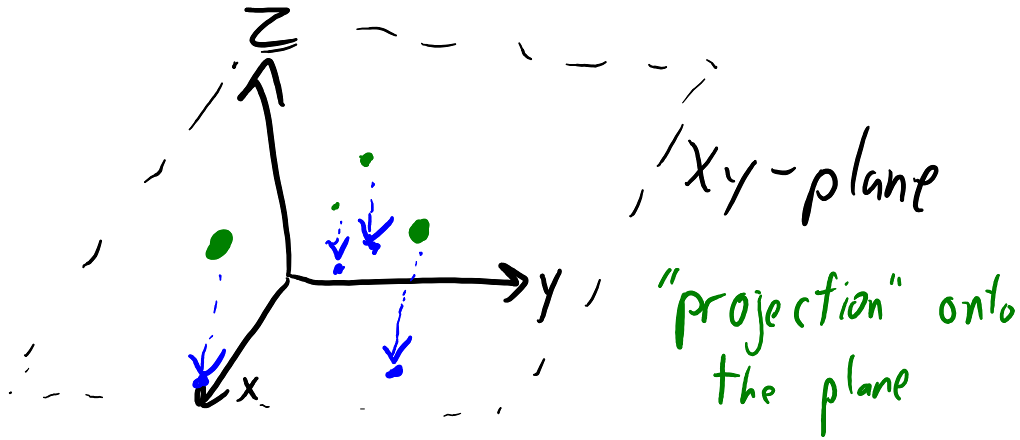
- Our k=2 latent factors are the following:

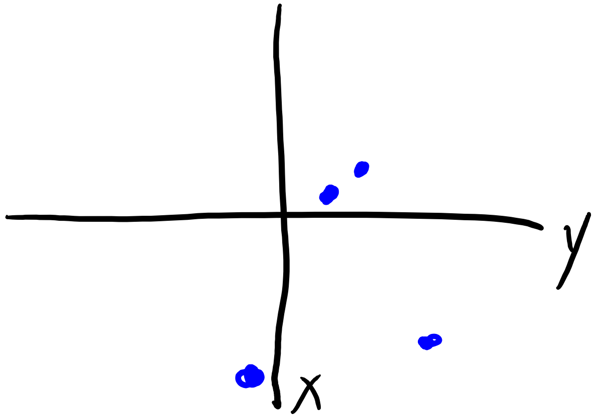
$$W = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

- So our approximation of x_i is: $\hat{x}_i = z_{i1}\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + z_{i2}\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$

Overhead Map and Latent-Factor Models

- The "overhead map" approximation just ignores the "height".



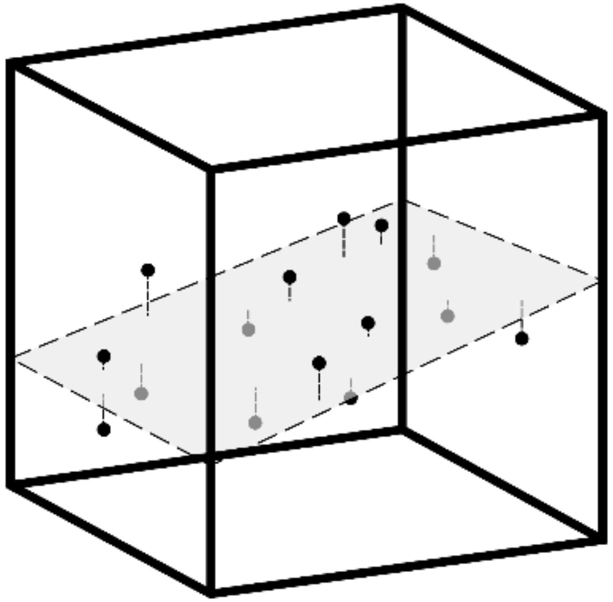


  - This is a good approximation if the world is flat.
    - Even if the character jumps, the first two features will approximate location.

  - But it's a poor approximation if heights are different.

Overhead Map and Latent-Factor Models

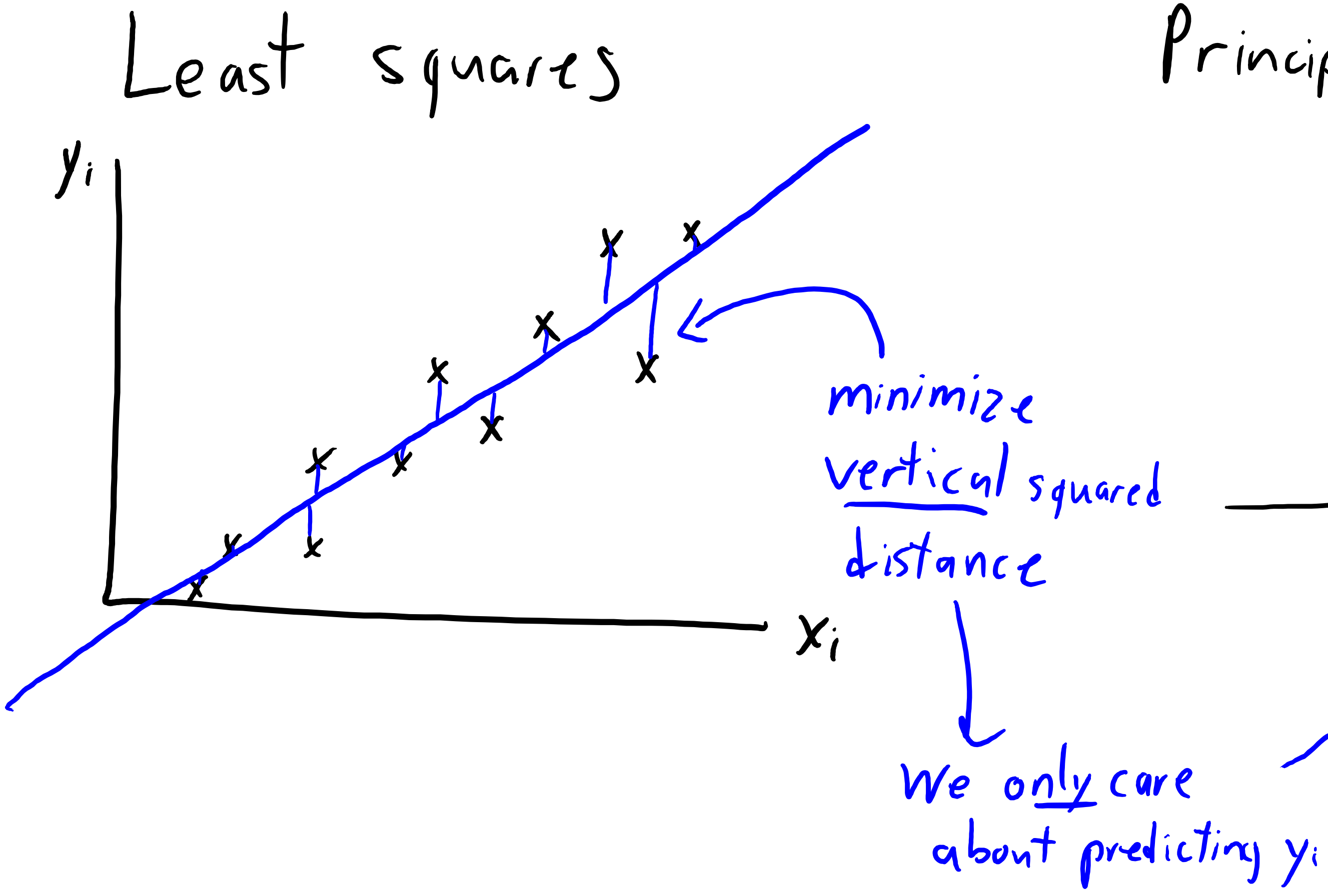
- Consider these crazy goats trying to get some salt:
  - Ignoring height gives poor approximation of goat location.

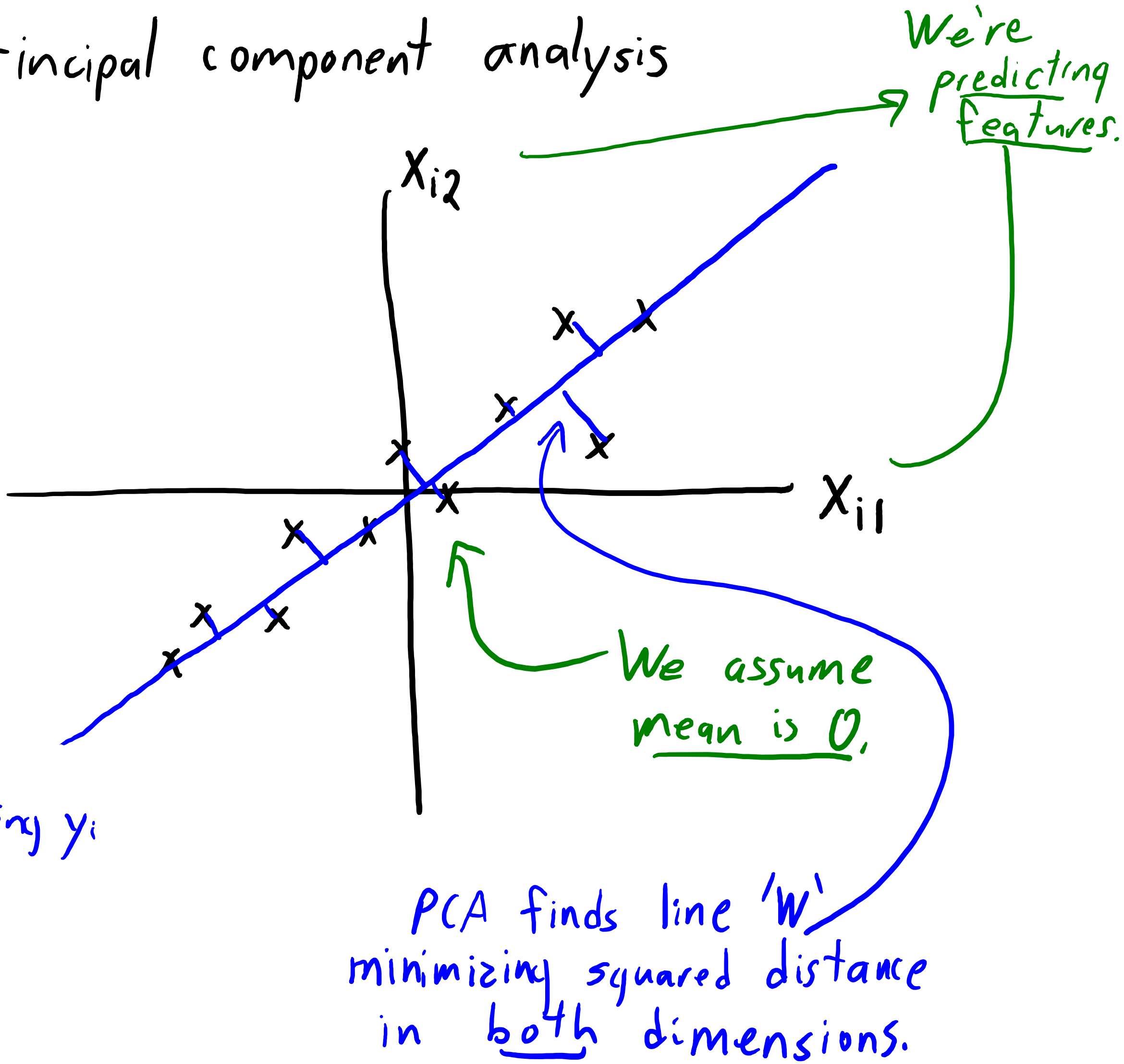


- But the "goat space" is basically a two-dimensional plane.
  - Better k=2 approximation: define 'W' so that combinations give the plane.

www.momtastic.com/webecoist/2010/11/07/some-fine-dam-climbing-goats-scaling-steep-vertical-wall
https://www.quora.com/What-is-a-simplified-explanation-and-proof-of-the-Johnson-Lindenstrauss-lemma

PCA Geometry with d=2 and k =1





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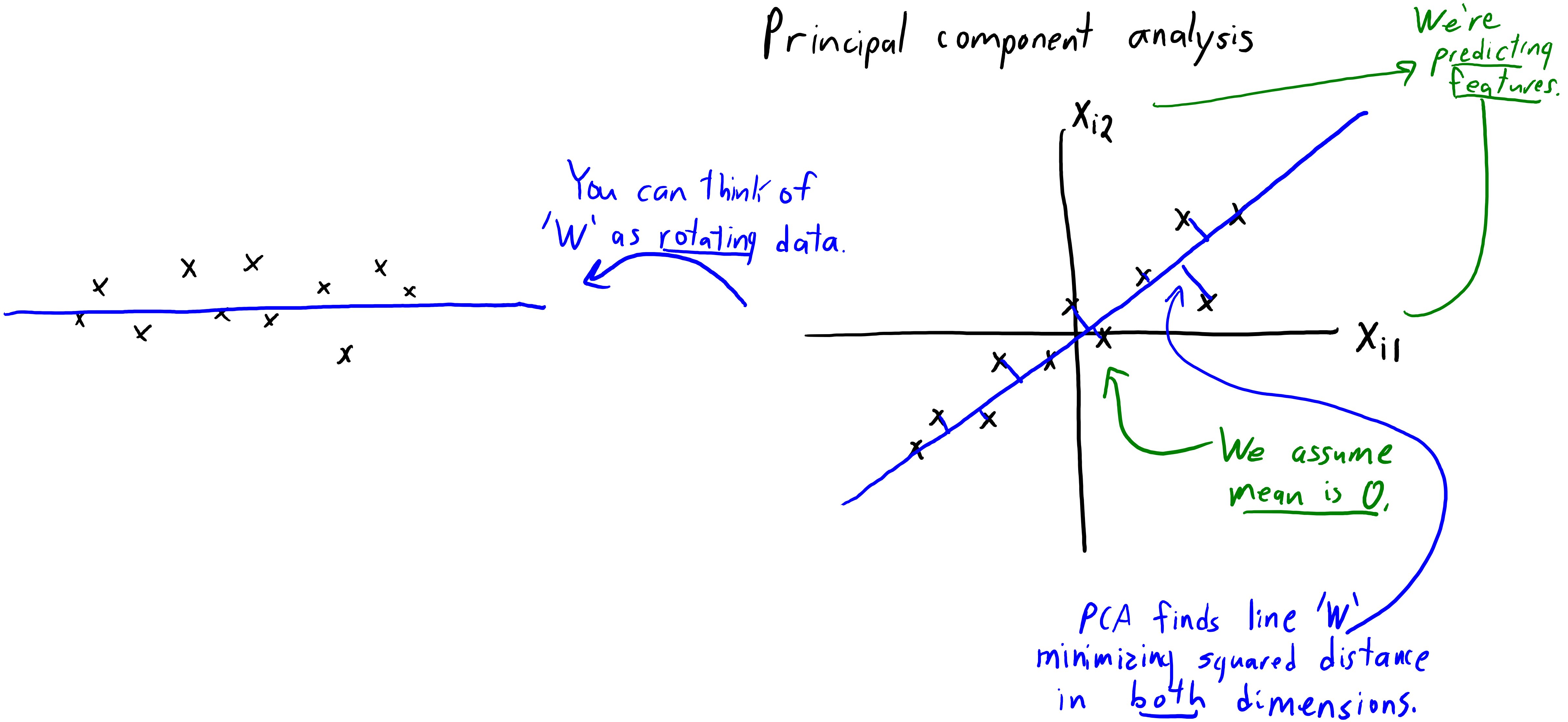

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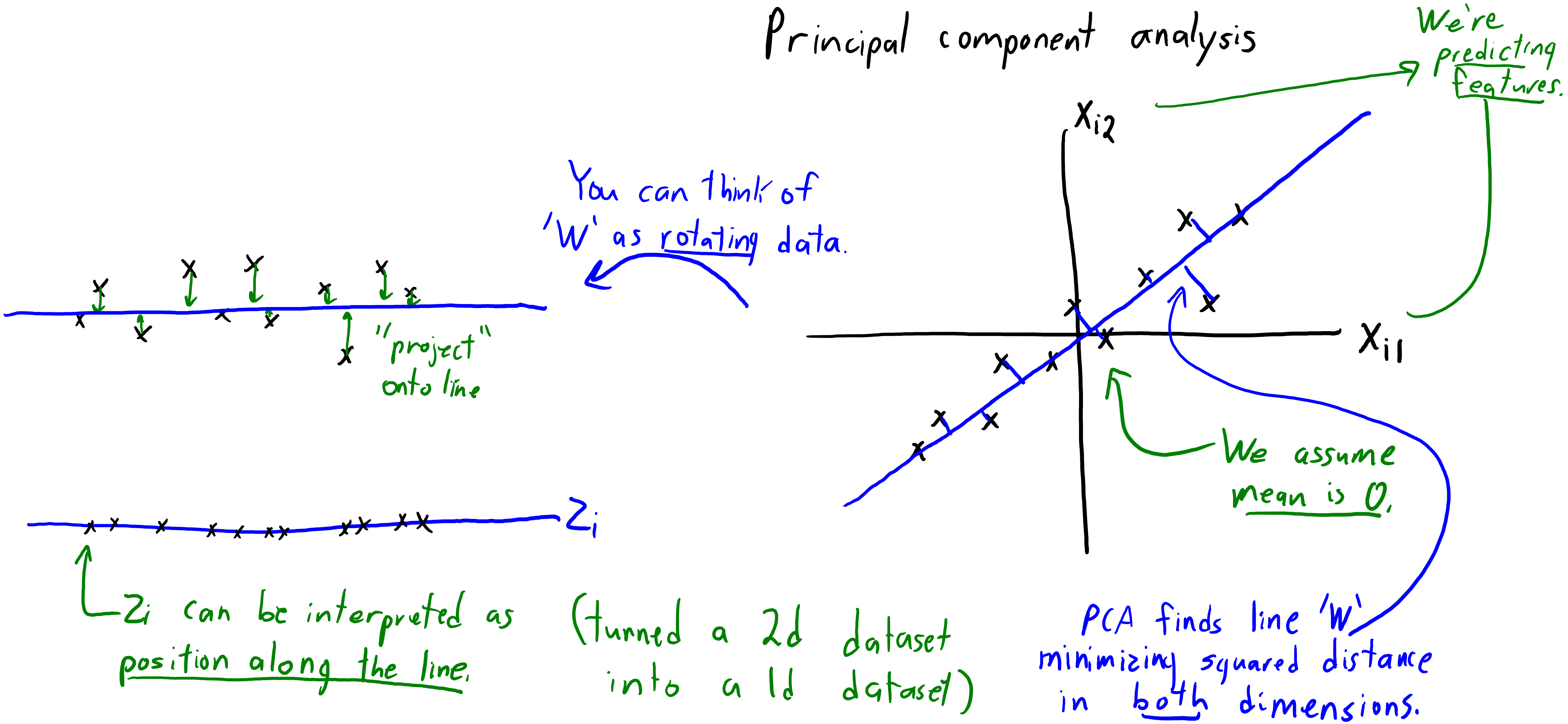
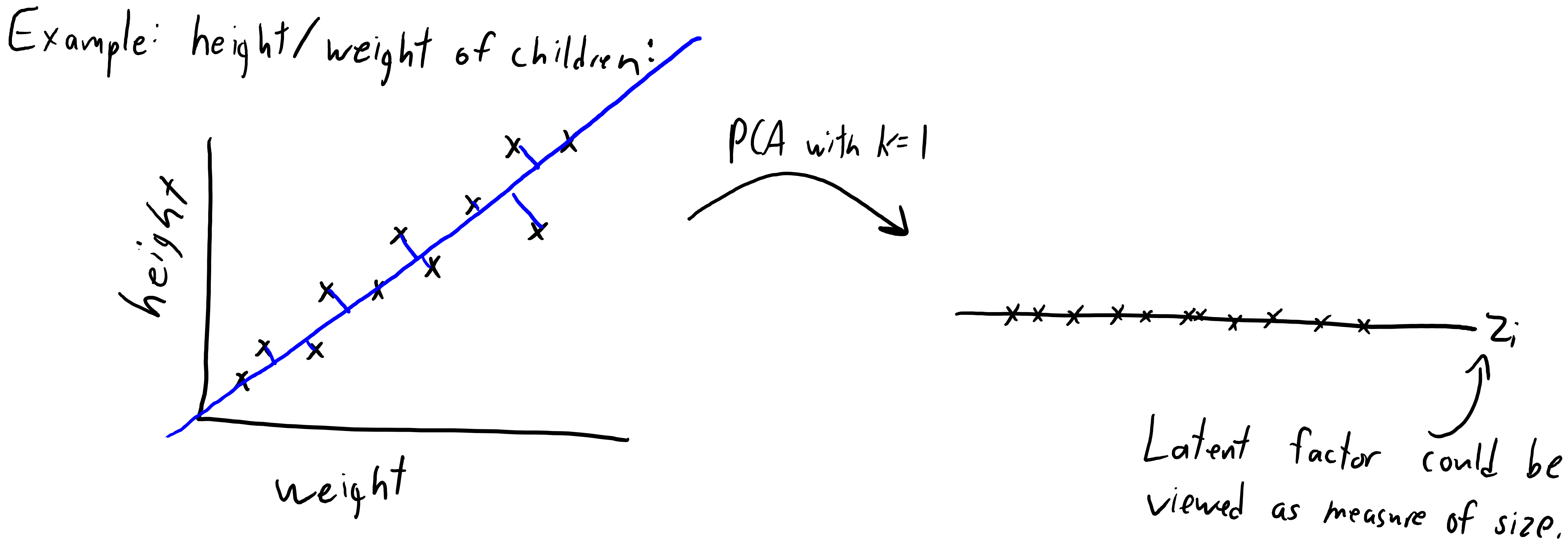
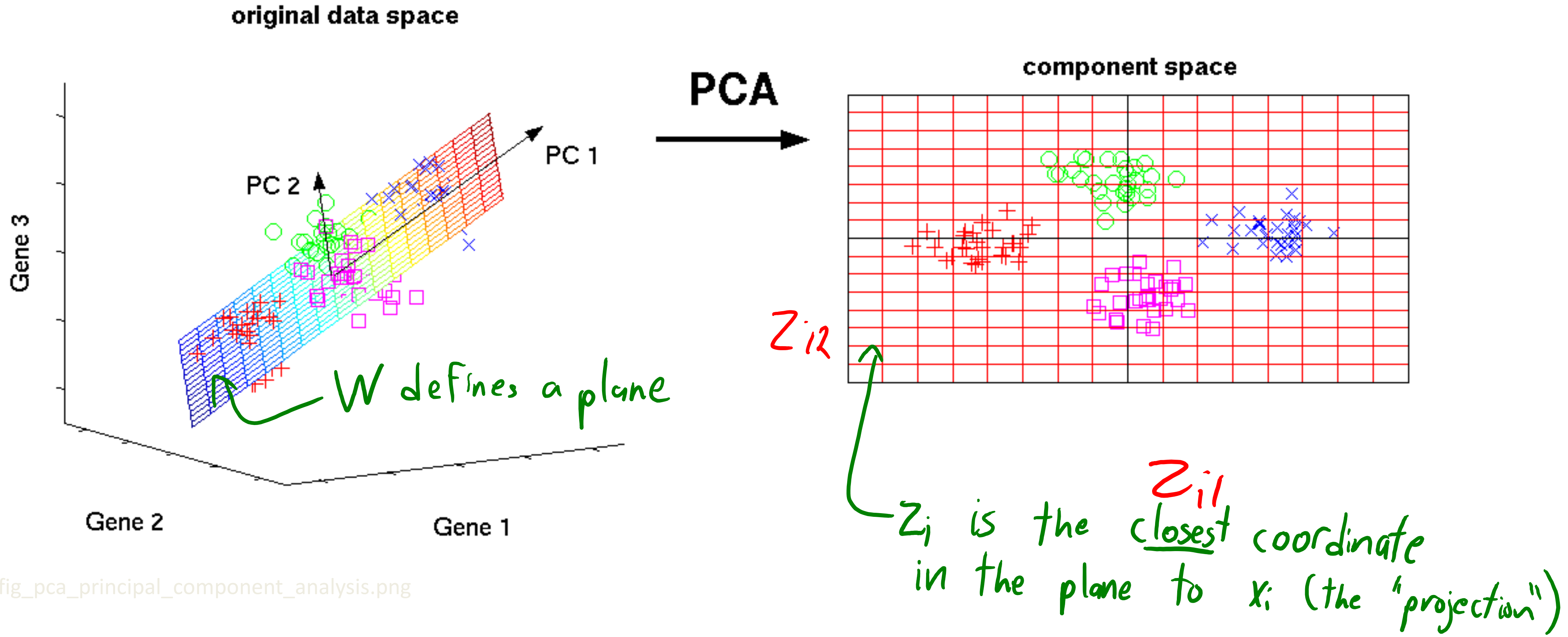


PCA Geometry with d=2 and k =1



PCA Geometry with d=3 and k=2.

- With d=3, PCA (k=1) finds line minimizing squared distance to x_i.
- With d=3, PCA (k=2) finds plane minimizing squared distance to x_i.



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

Summary

- Latent-factor models:
  - Try to learn a low-dimensional matrix Z from training examples X.
  - Usually, the z_i are "part weights" for "parts" w_c.
  - Useful for dimensionality reduction, visualization, factor discovery, etc.
- Principal component analysis:
  - Writes each training examples as linear combination of parts.
    - We learn both the "parts" 'W' and the "features" Z.
  - We can view 'W' as best lower-dim. hyper-plane (a k-dim. subspace in R^d).
  - We can view 'Z' as the coordinates in the lower-dimensional hyper-plane.

- Next time: PCA in 4 lines of code.