CS 540 Introduction to Artificial Intelligence

Linear Algebra & PCA

University of Wisconsin-Madison

Spring 2023

Linear Algebra: What is it good for?

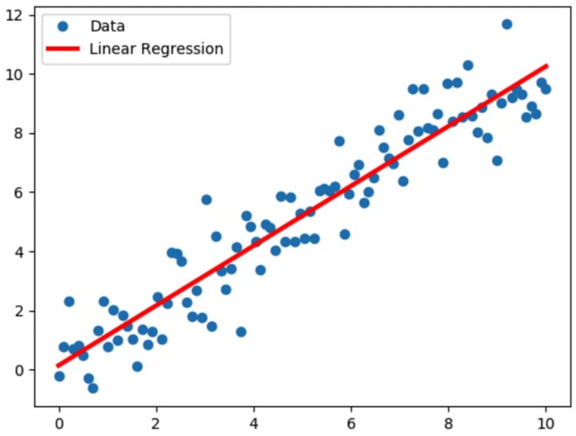
- Almost everything is a **function**
  - Multiple inputs and outputs

- Linear functions
  - Simple, tractable
- Study of linear functions

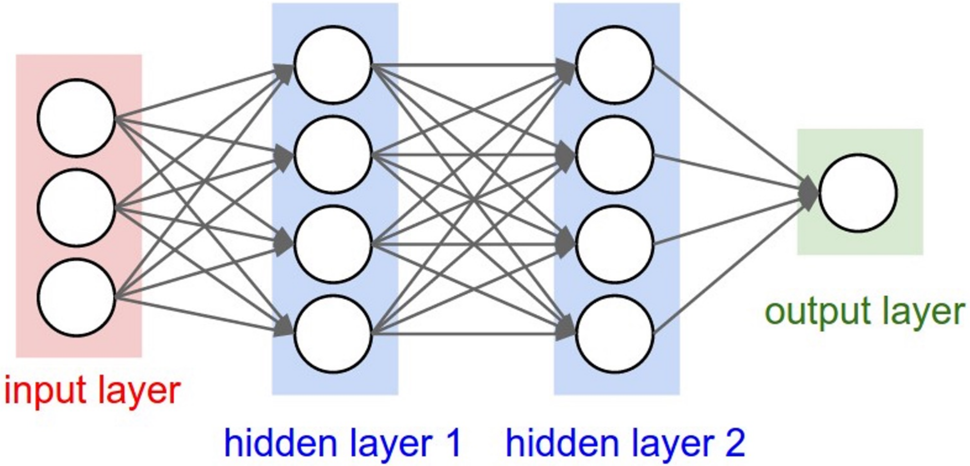
In AI/ML Context

Building blocks for **all models**

- E.g., linear regression; part of neural networks



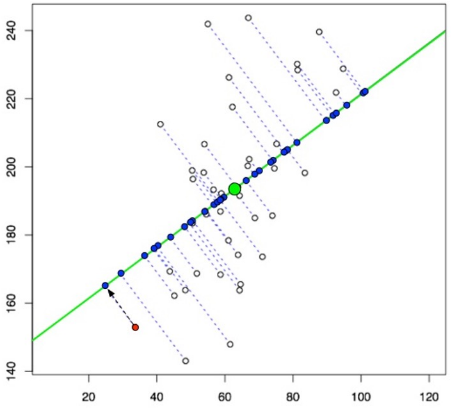
Hieu Tran



Stanford CS231n

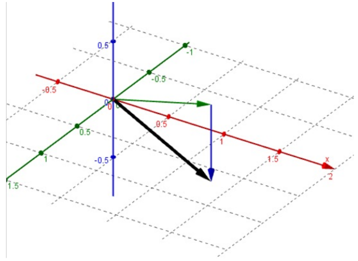
Outline

- Basics: vectors, matrices, operations
- Dimensionality reduction
- Principal Components Analysis (PCA)



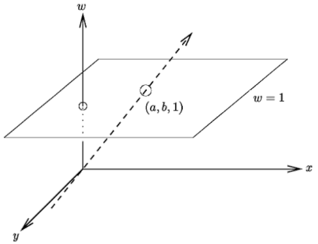
Lior Pachter

Basics: Vectors



Vectors

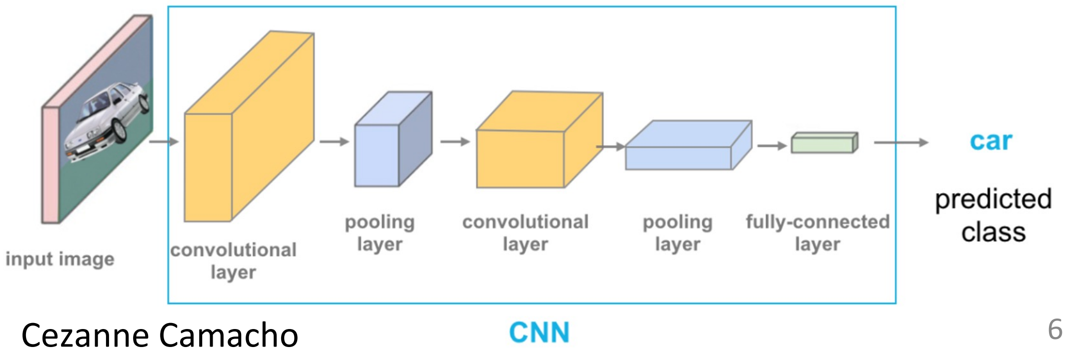
- Many interpretations
  - Physics: magnitude + direction
  - Point in a space
  - List of values (represents information)



$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix}$$

Basics: **Vectors**

- Dimension
  - Number of values $x \in \mathbb{R}^d$
  - Higher dimensions: richer but more complex
- AI/ML: often use **very high dimensions**:
  - Ex: images!



Cezanne Camacho

Basics: **Matrices**

- Again, many interpretations
  - Represent linear transformations
  - Apply to a vector, get another vector
  - Also, list of vectors

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix}$$

- Not necessarily square
  - Indexing! $A \in \mathbb{R}^{c \times d}$
  - Dimensions: #rows x #columns

Basics: Transposition

- Transposes: flip rows and columns
  - Vector: standard is a column. Transpose: row
  - Matrix: go from *m x n* to *n x m*

$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \quad x^T = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}$$

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \end{bmatrix} \quad A^T = \begin{bmatrix} A_{11} & A_{21} \\ A_{12} & A_{22} \\ A_{13} & A_{23} \end{bmatrix}$$

Matrix & Vector **Operations**

- Vectors
  - Addition: component-wise
    - Commutative
    - Associative

$$x + y = \begin{bmatrix} x_1 + y_1 \\ x_2 + y_2 \\ x_3 + y_3 \end{bmatrix}$$

  - Scalar Multiplication
    - Uniform stretch / scaling

$$cx = \begin{bmatrix} cx_1 \\ cx_2 \\ cx_3 \end{bmatrix}$$

Matrix & Vector **Operations**

- **Vector products.**
  - Inner product (e.g., dot product)

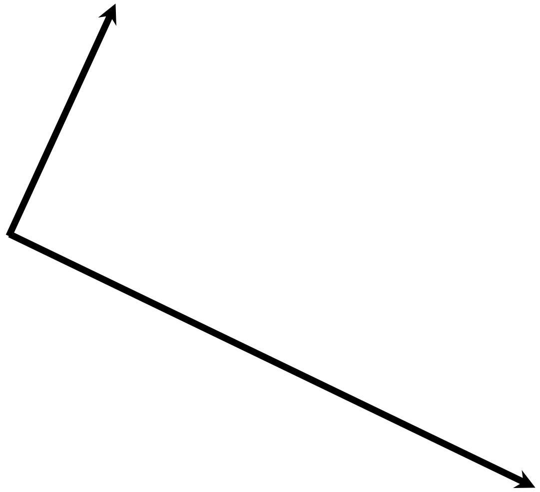
$$< x, y > := x^T y = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = x_1 y_1 + x_2 y_2 + x_3 y_3$$

  - Outer product

$$xy^T = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \begin{bmatrix} y_1 & y_2 & y_3 \end{bmatrix} = \begin{bmatrix} x_1 y_1 & x_1 y_2 & x_1 y_3 \\ x_2 y_1 & x_2 y_2 & x_2 y_3 \\ x_3 y_1 & x_3 y_2 & x_3 y_3 \end{bmatrix}$$

Matrix & Vector **Operations**

- Inner product defines "orthogonality"
  - If $\langle x, y \rangle = 0$



- Vector norms: "length"

$$\|x\|_2 = \sqrt{\sum_{i=1}^{n} x_i^2}$$

Matrix & Vector **Operations**

- Matrices:
  - Addition: Component-wise
  - Commutative, Associative

$$A + B = \begin{bmatrix} A_{11} + B_{11} & A_{12} + B_{12} \\ A_{21} + B_{21} & A_{22} + B_{22} \\ A_{31} + B_{31} & A_{32} + B_{32} \end{bmatrix}$$

  - Scalar Multiplication
  - "Stretching" the linear transformation

$$cA = \begin{bmatrix} cA_{11} & cA_{12} \\ cA_{21} & cA_{22} \\ cA_{31} & cA_{32} \end{bmatrix}$$

Matrix & Vector **Operations**

- Matrix-Vector multiply
  - I.e., linear transformation; plug in vector, get another vector
  - Each entry in *Ax* is the inner product of a row of *A* with *x*

$$Ax = \begin{bmatrix} A_{11}x_1 + A_{12}x_2 + \ldots + A_{1n}x_n \\ A_{21}x_1 + A_{22}x_2 + \ldots + A_{2n}x_n \\ \vdots \\ A_{n1}x_1 + A_{n2}x_2 + \ldots + A_{nn}x_n \end{bmatrix}$$

Matrix & Vector **Operations**

Ex: feedforward neural networks. Input *x*.

- Output of layer k is

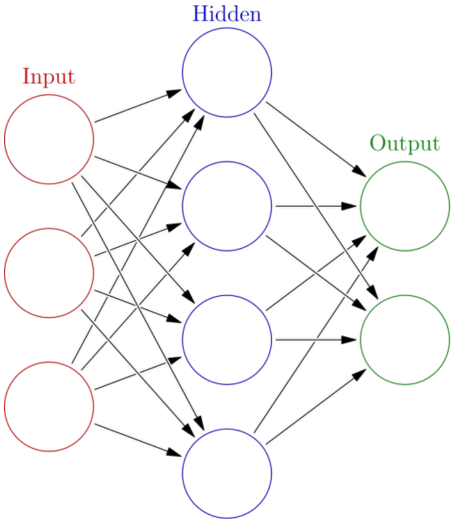
nonlinearity

$$f^{(k)}(x) = \sigma(W_k^T f^{(k-1)}(x))$$

Output of layer k-1: **vector**

Output of layer k: vector

Weight **matrix** for layer k:
Note: linear transformation!

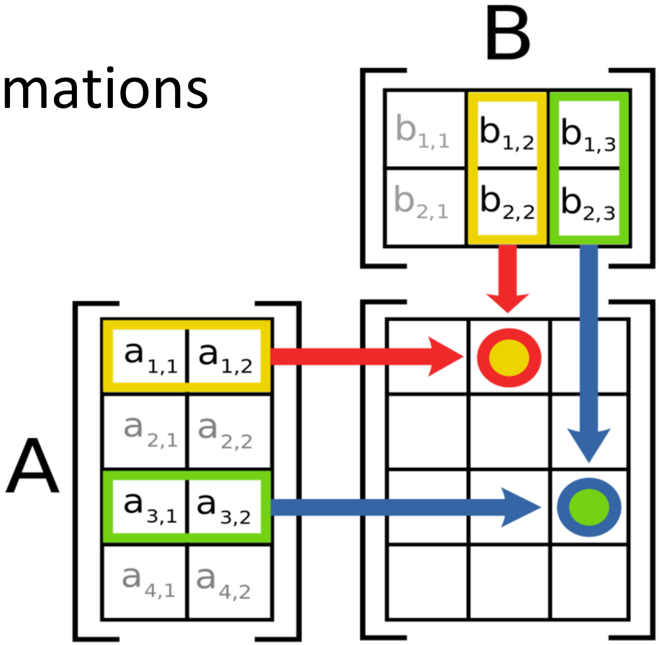


Wikipedia

Matrix & Vector **Operations**

- Matrix multiplication
  - "Composition" of linear transformations
  - **Not commutative** (in general)!

  - Lots of interpretations



Wikipedia

More on Matrix Operations

- Identity matrix:
  - Like "1"
  - Multiplying by it gets back the same matrix or vector
  - Rows & columns are the "**standard basis vectors**" e_i

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

Break & Quiz

- **Q 1.1**: What is $\begin{bmatrix} 1 & 2 \\ 3 & 1 \\ 1 & 1 \end{bmatrix} \times \begin{bmatrix} 0 \\ 1 \end{bmatrix}$?
- A. $[-1\ 1\ 1]^T$
- B. $[2\ 1\ 1]^T$
- C. $[1\ 3\ 1]^T$
- D. $[1.5\ 2\ 1]^T$

Break & Quiz

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- A. [-1 1 1]^T
- **B. [2 1 1]^T**
- C. [1 3 1]^T
- D. [1.5 2 1]^T

Check dimensions: answer must be 3 x 1 matrix (i.e., column vector).

$$\begin{matrix} 1 & 2 \\ 3 & 1 \\ 1 & 1 \end{matrix} \times \begin{matrix} 0 \\ 1 \end{matrix} = \begin{matrix} 0 * 1 + 1 * 2 \\ 0 * 3 + 1 * 1 \\ 0 * 1 + 1 * 1 \end{matrix} = \begin{matrix} 2 \\ 1 \\ 1 \end{matrix}$$

Break & Quiz

- **Q 1.2**: Given matrices $A \in \mathbb{R}^{m \times n}, B \in \mathbb{R}^{d \times m}, C \in \mathbb{R}^{p \times n}$

What are the dimensions of BAC^T

- A. *n x p*
- B. *d x p*
- C. *d x n*
- D. Undefined

Break & Quiz

- **Q 1.2**: Given matrices $A \in \mathbb{R}^{m \times n}, B \in \mathbb{R}^{d \times m}, C \in \mathbb{R}^{p \times n}$

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What are the dimensions of BAC^T

- A. *n x p*
- **B. *d x p***
- C. *d x n*
- D. Undefined

To rule out (D), check that for each pair of adjacent matrices XY, the # of columns of X = # of rows of Y

Then, B has d rows so solution must have d rows. C^T has p columns so solution has p columns.

Break & Quiz

- **Q 1.3**: A and B are matrices, neither of which is the identity. Is $AB = BA$?

- A. Never
- B. Always
- C. Sometimes

Break & Quiz

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Break & Quiz

- **Q 1.3**: A and B are matrices, neither of which is the identity. Is $AB = BA$?

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- **C. Sometimes**

Matrix multiplication is not necessarily commutative.

More on Matrices: Inverses

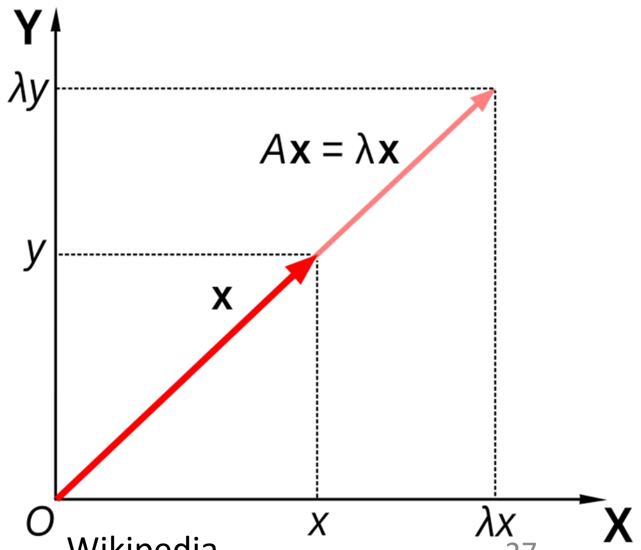
- If for *A* there is a *B* such that $AB = BA = I$
  - Then *A* is invertible/nonsingular, B is its inverse
  - Some matrices are **not** invertible!
  - Usual notation: A^{-1}

$$\begin{bmatrix} 1 & 1 \\ 2 & 3 \end{bmatrix} \times \begin{bmatrix} 3 & -1 \\ -2 & 1 \end{bmatrix} = I$$

Eigenvalues & Eigenvectors

- For a square matrix *A*, solutions to $Av = \lambda v$
  - *v* (nonzero) is a vector: **eigenvector**
  - λ is a scalar: **eigenvalue**

  - Intuition: A is a linear transformation;
  - Can stretch/rotate vectors;
  - E-vectors: only stretched (by e-vals)



Wikipedia

Dimensionality Reduction

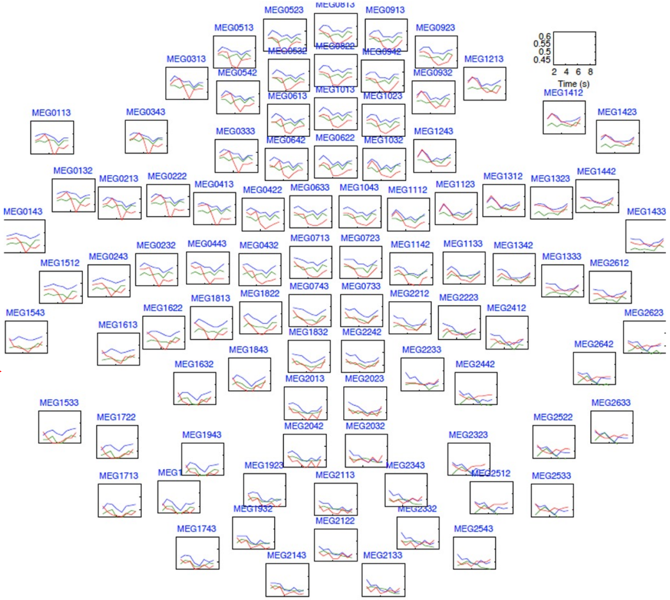
- Vectors used to store features
  - Lots of data -> lots of features!
- Document classification
  - Each doc: thousands of words/millions of bigrams, etc
- Netflix surveys: 480189 users x 17770 movies

	movie 1	movie 2	movie 3	movie 4	movie 5	movie 6
Tom	5	?	?	1	3	?
George	?	?	3	1	2	5
Susan	4	3	1	?	5	1
Beth	4	3	?	2	4	2

Dimensionality Reduction

Ex: MEG Brain Imaging: 120 locations x 500 time points x 20 objects

- Or any image



Dimensionality Reduction

Reduce dimensions

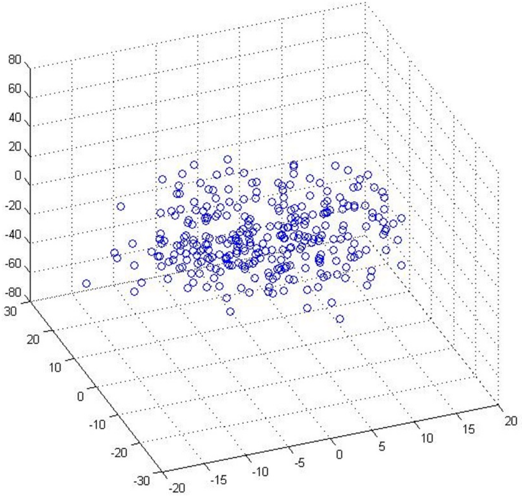
- Why?
  - Lots of features redundant
  - Storage & computation costs

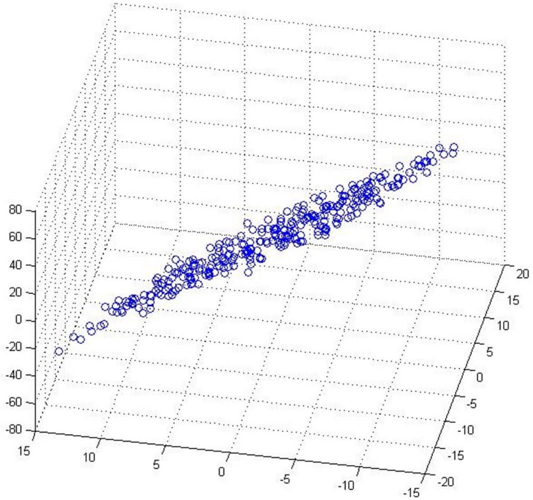
CreativeBlog

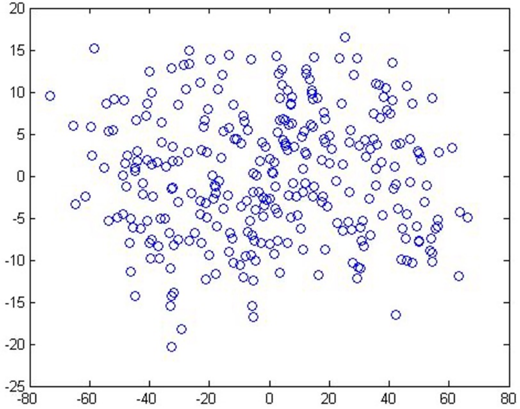
- Goal: take $x \in \mathbb{R}^d \rightarrow x \in \mathbb{R}^r$ for $r << d$
  - But, minimize information loss

Compression

Examples: 3D to 2D







Andrew Ng

Break & Quiz

Q 2.1: What is the inverse of

$$A = \begin{bmatrix} 0 & 2 \\ 3 & 0 \end{bmatrix}$$

A: $$A^{-1} = \begin{bmatrix} -3 & 0 \\ 0 & -2 \end{bmatrix}$$

B: $$A^{-1} = \begin{bmatrix} 0 & \frac{1}{3} \\ \frac{1}{2} & 0 \end{bmatrix}$$

C: Undefined / *A* is not invertible

Break & Quiz

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$$AA^{-1} = \begin{bmatrix} 0 & 2 \\ 3 & 0 \end{bmatrix} \begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} 0 * a + c * 2 & 0 * b + 2 * d \\ 3 * a + c * 0 & 3 * b + 0 * d \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$2c = 1$$
$$3a = 0$$
$$2d = 0$$
$$3b = 1$$

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} 0 & 1/3 \\ 1/2 & 0 \end{bmatrix}$$

Break & Quiz

Q 2.2: What are the eigenvalues of $A = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

A. -1, 2, 4
B. 0.5, 0.2, 1.0
C. 0, 2, 5
D. 2, 5, 1

Break & Quiz

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Solution #1: You may recall from a linear algebra course that the eigenvalues of a diagonal matrix (in which only diagonal entries are non-zero) are just the entries along the diagonal. Hence D is the correct answer.

Break & Quiz

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C. 0, 2, 5
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Solution #2: Use the definition of eigenvectors and values: $Av = \lambda v$

$$\begin{bmatrix} 2 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{matrix} v_1 \\ v_2 \\ v_3 \end{matrix} = \begin{bmatrix} 2v_1 + 0v_2 + 0v_3 \\ 0v_1 + 5v_2 + 0v_3 \\ 0v_1 + 0v_2 + 1v_3 \end{bmatrix} = \begin{bmatrix} 2v_1 \\ 5v_2 \\ v_3 \end{bmatrix} = \begin{bmatrix} \lambda v_1 \\ \lambda v_2 \\ \lambda v_3 \end{bmatrix}$$

Since A is a 3x3 matrix, A has 3 eigenvalues and so there are 3 combinations of values for λ and v that will satisfy the above equation. The simple form of the equations suggests starting by checking each of the standard basis vectors* as v and then solving for λ. Doing so gives D as the correct answer.

*Each standard basis vector $e_i \in \mathbb{R}^n$ is the vector in which all components are zero except component i is 1.

Break & Quiz

Q 2.3: Suppose we are given a dataset with n=10000 samples with 100-dimensional binary feature vectors. Our storage device has a capacity of 50000 bits. What's the lower compression ratio we can use?

A. 20X
B. 100X
C. 5X
D. 1X

Break & Quiz

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D. 1X

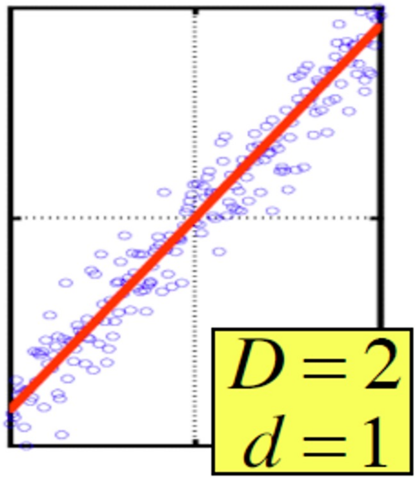
50,000 bits / 10,000 samples means compressed version must have 5 bits / sample.

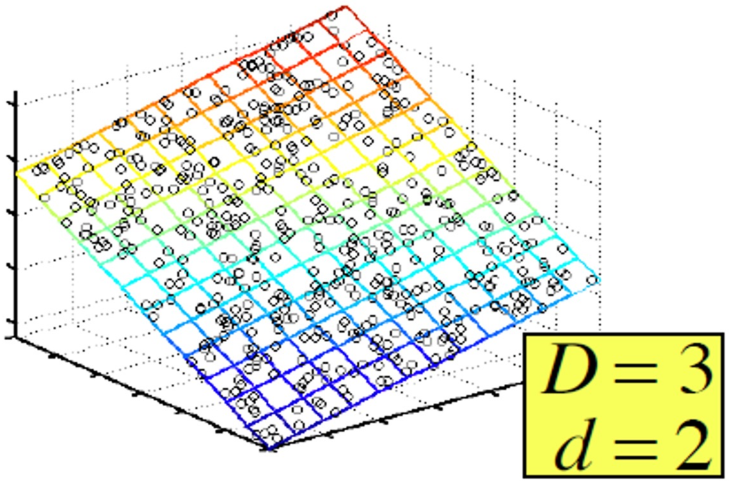
Dataset has 100 bits / sample.

Must compress 20x smaller to fit on device.

Principal Components Analysis (**PCA**)

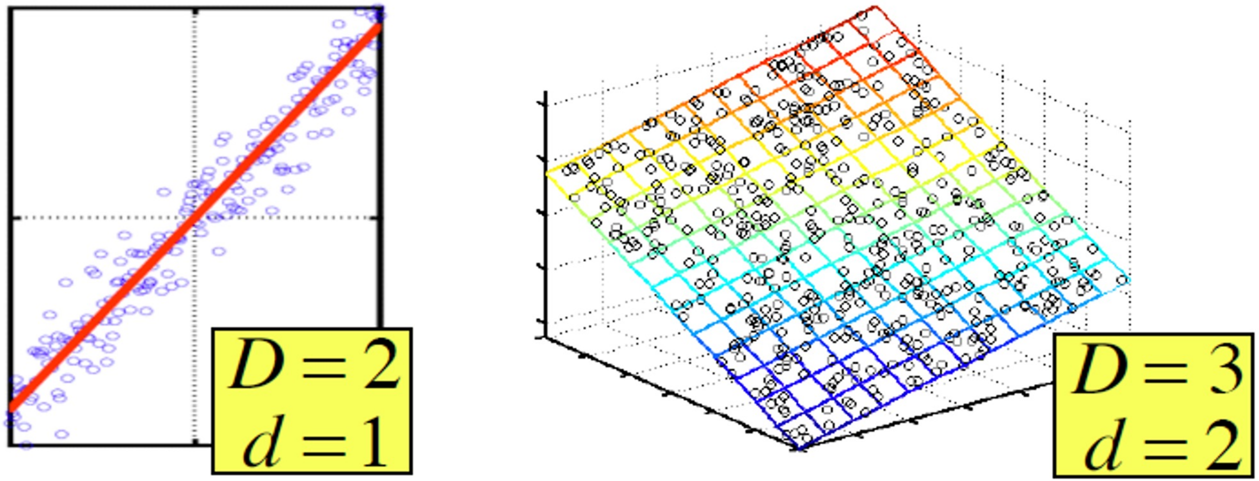
- A type of dimensionality reduction approach
  - For when data is **approximately lower dimensional**





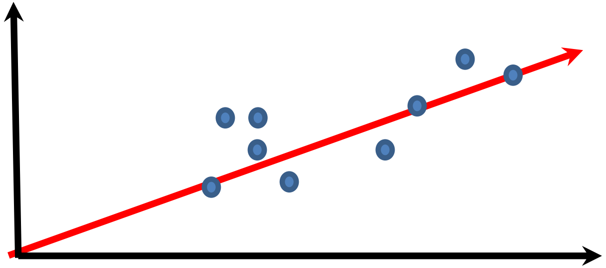
Principal Components Analysis (**PCA**)

- Goal: find **axes** of a subspace
  - Will project to this subspace; want to preserve data



Principal Components Analysis (**PCA**)

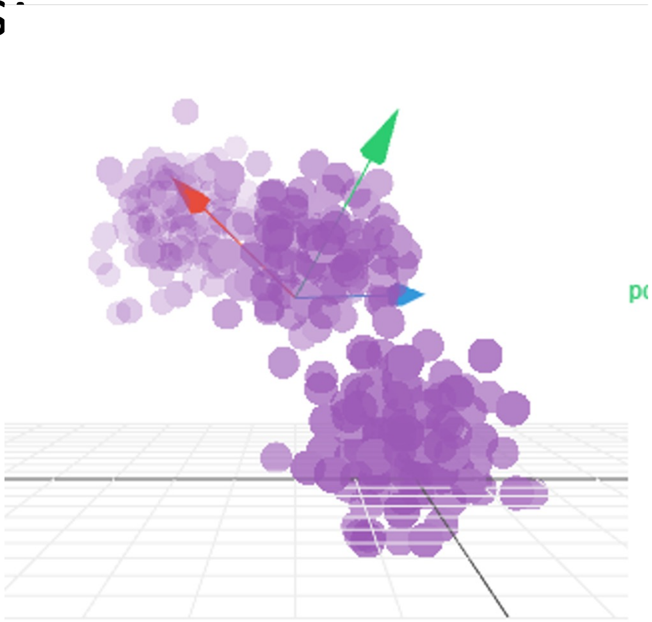
- From 2D to 1D:
  - Find a $v_1 \in \mathbb{R}^d$ so that we maximize "variability"
  - IE,



  - New representations are along this vector (1D!)

Principal Components Analysis (**PCA**)

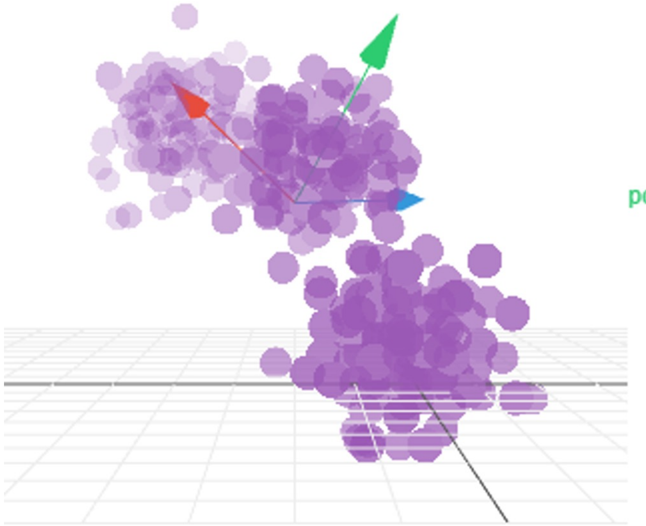
- From *d* dimensions to *r* dimensions
  - Sequentially get $v_1, v_2, \ldots, v_r \in \mathbb{R}^d$
  - Orthogonal!
  - Still minimize the projection error
    - Equivalent to **"maximizing variability"**
  - The vectors are the **principal components**



Victor Powell

PCA Setup

- **Inputs**
  - Data: $x_1, x_2, \ldots, x_n, \; x_i \in \mathbb{R}^d$
  - Can arrange into $X \in \mathbb{R}^{n \times d}$
  - **Centered**! $\frac{1}{n}\sum_{i=1}^{n} x_i = 0$
- **Outputs**
  - Principal components $v_1, v_2, \ldots, v_r \in \mathbb{R}^d$
  - Orthogonal!



Victor Powell

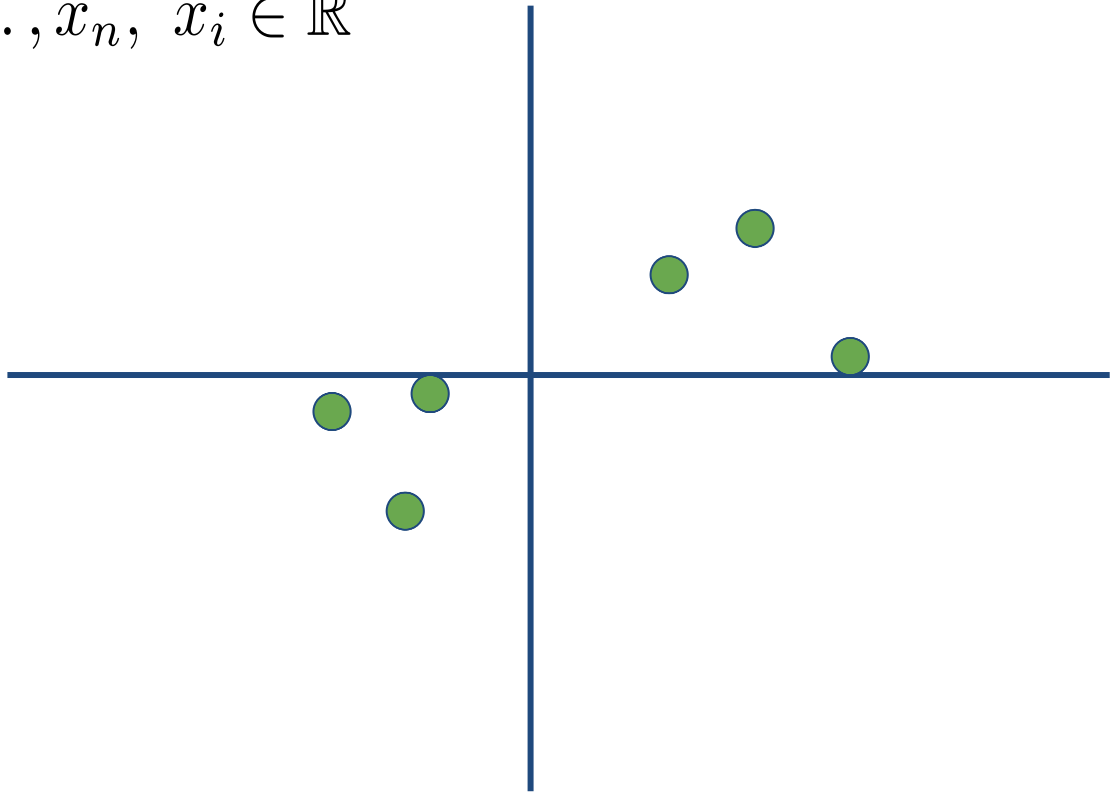
PCA Goals

- Want directions/components (unit vectors) so that
  - Projecting data maximizes variance $$\sum_{i=1}^{n} \langle x_i, v \rangle^2 = \|Xv\|^2$$
  - What's projection?

Let's look at an example!

Projection: An Example

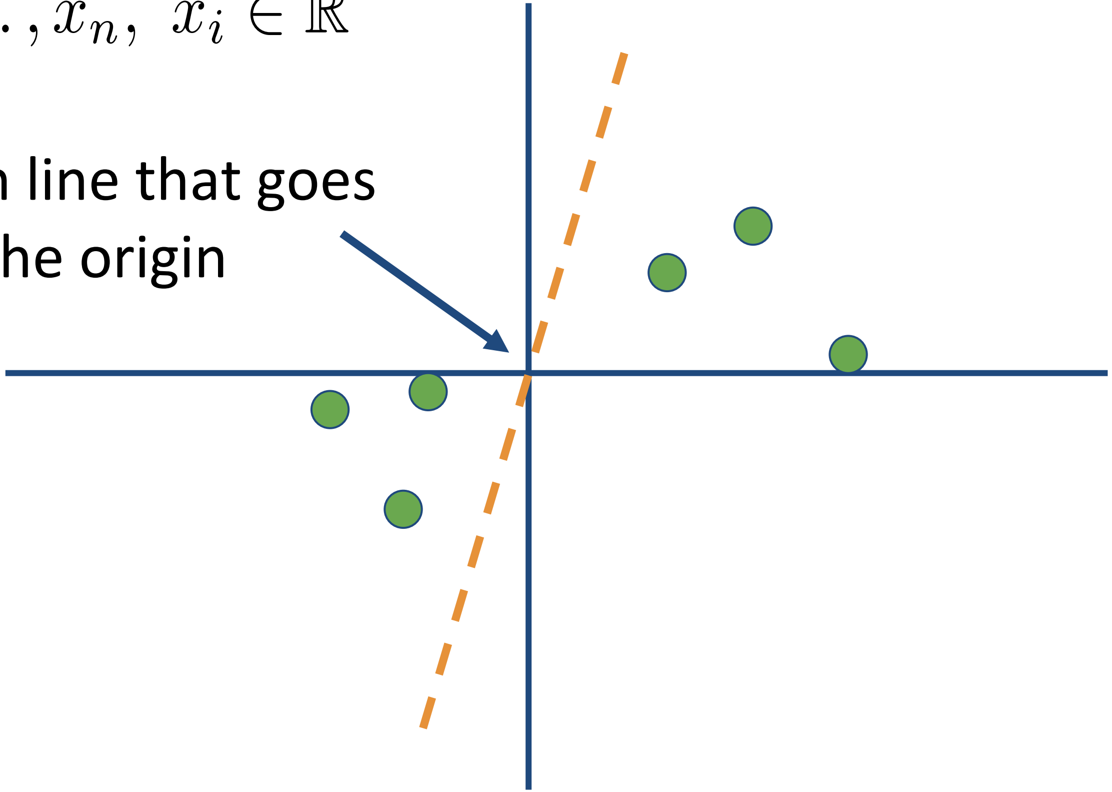
$x_1, x_2, \ldots, x_n,\ x_i \in \mathbb{R}^2$



Projection: An Example

$x_1, x_2, \ldots, x_n, \ x_i \in \mathbb{R}^2$

A random line that goes through the origin



Projection: An Example

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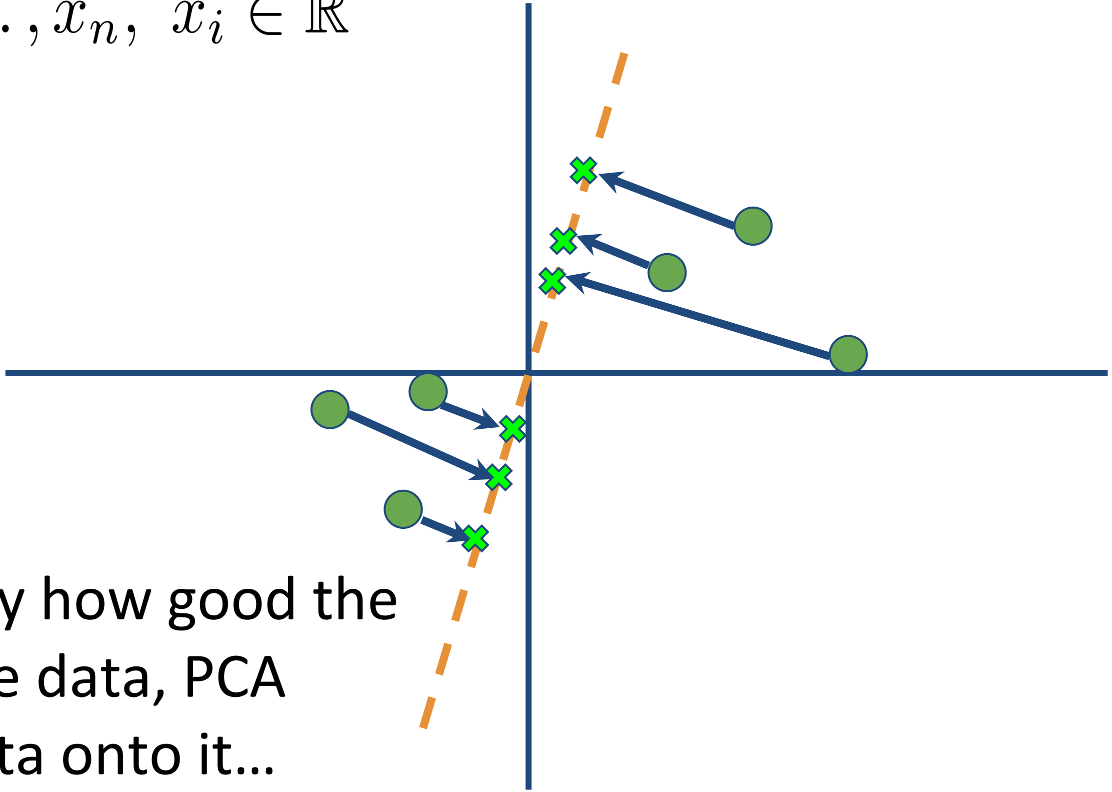
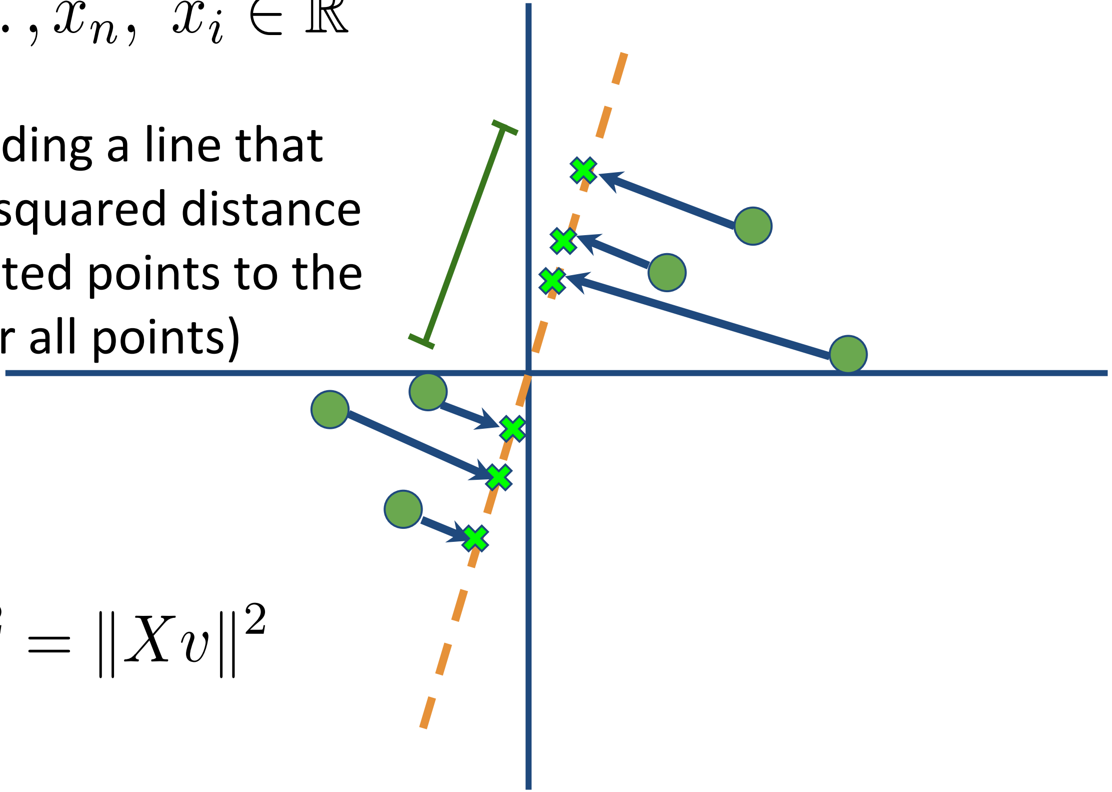


To quantify how good the line fits the data, PCA project data onto it…

Projection: An Example

$x_1, x_2, \ldots, x_n, \; x_i \in \mathbb{R}^2$

Goal of PCA: finding a line that **maximizes** the squared distance from the projected points to the origin (sum over all points)



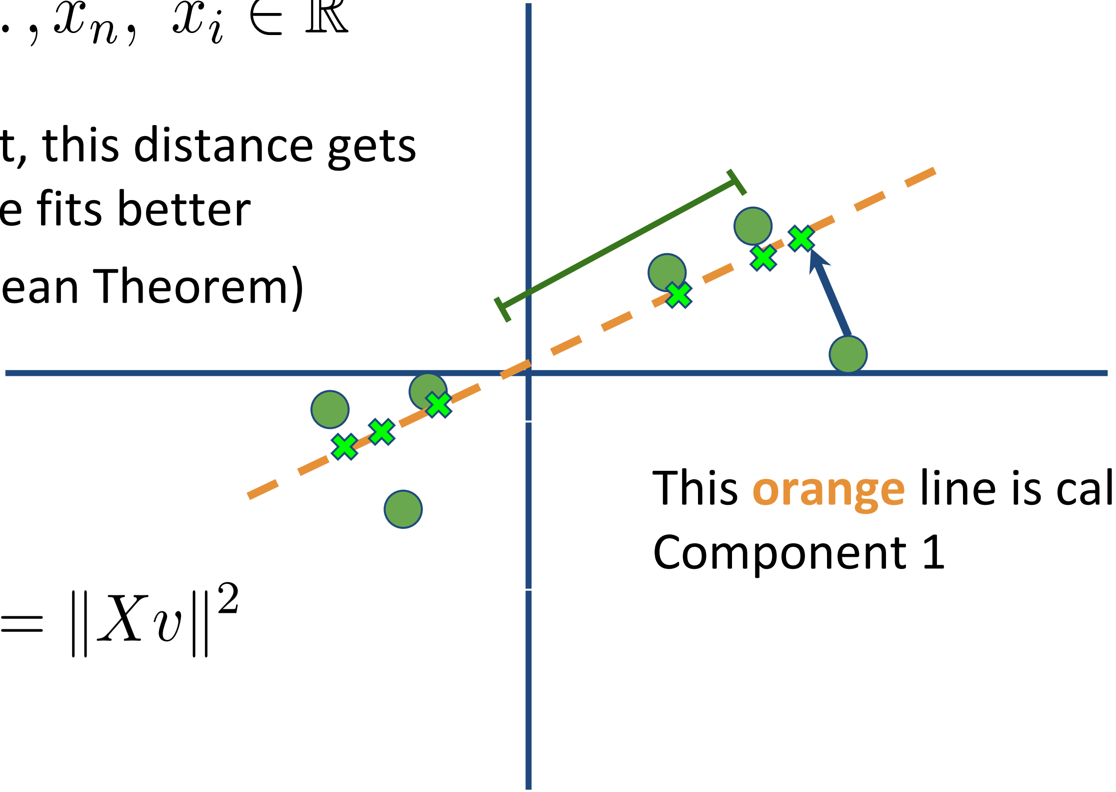
$$\sum_{i=1}^{n} \langle x_i, v \rangle^2 = \|Xv\|^2$$

Projection: An Example

$x_1, x_2, \ldots, x_n, \; x_i \in \mathbb{R}^2$

For a fixed point, this distance gets larger as the line fits better

(why? Pythagorean Theorem)



This **orange** line is called Principal Component 1

$$\sum_{i=1}^{n} \langle x_i, v \rangle^2 = \|Xv\|^2$$

PCA First Step

- First component,

$$v_1 = \arg\max_{\|v\|=1} \sum_{i=1}^{n} \langle v, x_i \rangle^2$$

- Same as getting

$$v_1 = \arg\max_{\|v\|=1} \|Xv\|^2$$

PCA Goals

- Want directions/components (unit vectors) so that
  - Projecting data maximizes variance $\sum_{i=1}^{n} \langle x_i, v \rangle = \|Xv\|^2$
  - What's projection?

- Do this **recursively**
  - Get orthogonal directions $v_1, v_2, \ldots, v_r \in \mathbb{R}^d$

PCA Recursion

- Once we have *k-1* components, next?

$$\hat{X}_k = X - \sum_{i=1}^{k-1} X v_i v_i^T$$

Deflation

- Then do the same thing

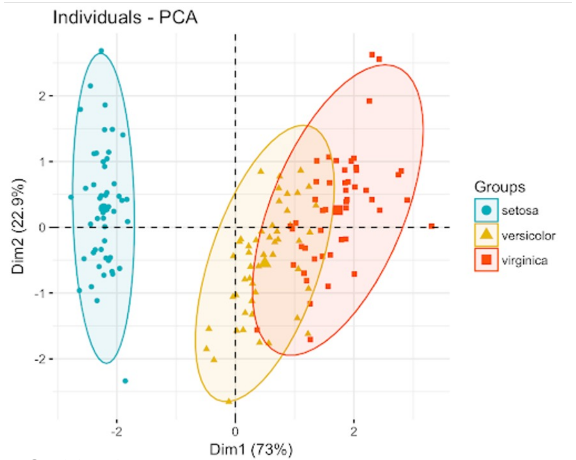
$$v_k = \underset{||v||=1}{\operatorname{argmax}} \left|\left|\hat{X}_k v\right|\right|^2$$

PCA Interpretations

- The v's are eigenvectors of $X^T X$ **(Gram matrix)**
  - Show via Rayleigh quotient
- $X^T X$ (proportional to) sample covariance matrix
  - When data is 0 mean!
  - I.e., PCA is eigendecomposition of sample covariance
- Nested subspaces *span(v1), span(v1,v2),…,*

Lots of Variations

- PCA, Kernel PCA, ICA, CCA
  - Unsupervised techniques to extract structure from high dimensional dataset
- Uses:
  - **Visualization**
  - Efficiency
  - Noise removal
  - Downstream machine learning use



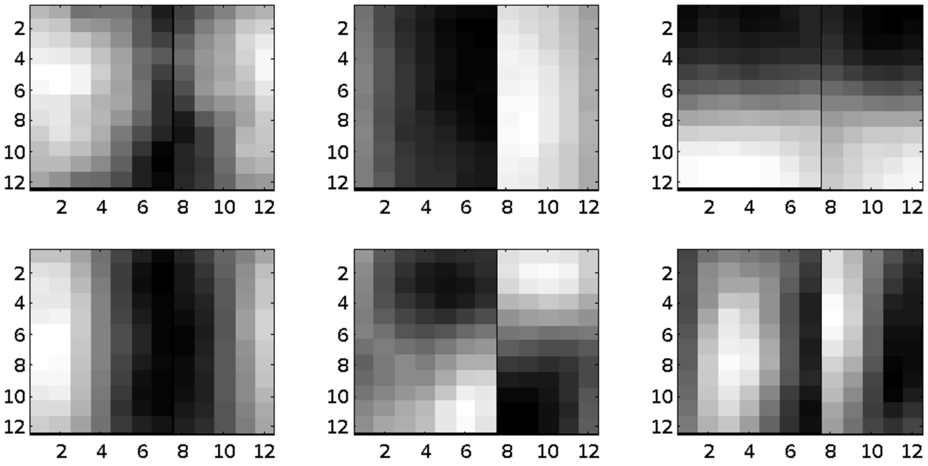
STHDA

Application: Image Compression

- Start with image; divide into 12x12 patches
  - I.E., 144-D vector
  - **Original image:**

Application: Image Compression

- 6 most important components (as an image)



Application: Image Compression

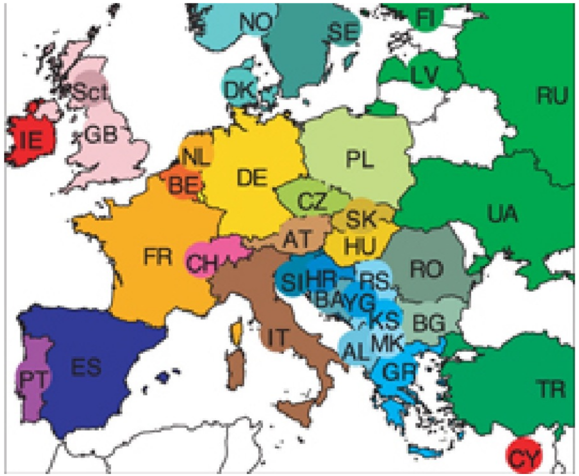
- Project to 6D,

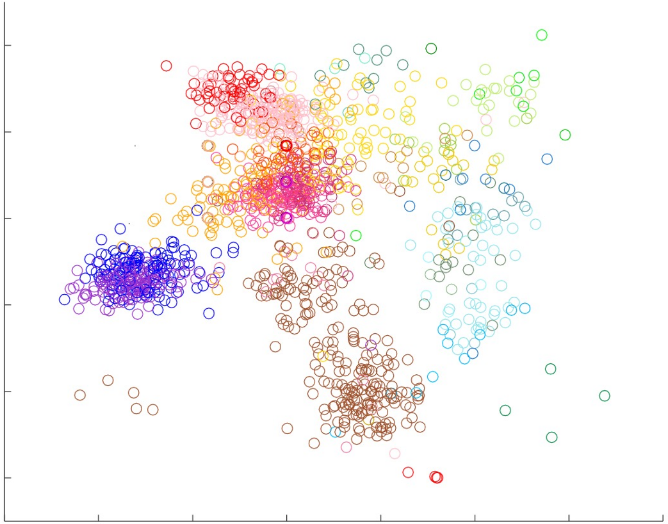
Compressed

Original

Application: Exploratory Data Analysis

- [**Novembre et al. ’08**]: Take top two singular vectors of people x SNP matrix (POPRES)





“Genes Mirror Geography in Europe”

Readings

- Vast literature on linear algebra.
- Local class: **Math 341**.

- **Suggested reading:**
  - Lecture notes on PCA by Roughgarden and Valiant
    https://web.stanford.edu/class/cs168/l/l7.pdf
  - 760 notes by Zhu https://pages.cs.wisc.edu/~jerryzhu/cs760/PCA.pdf