CS 540 Introduction to Artificial Intelligence
Linear Algebra & PCA

Fred Sala
University of Wisconsin-Madison

Sep 15, 2022

Announcements

- **Homeworks:**
  - HW1 due 5 minutes ago; HW2 released today.
- Class roadmap:

Tuesday, Sep 13	Probability
Thursday, Sep 15	**Linear Algebra and PCA**
Tuesday, Sep 20	Statistics and Math Review
Thursday, Sep 22	Introduction to Logic
Tuesday, Sep 27	Natural Language Processing

Fundamentals

From Last Time

- Conditional Prob. & Bayes:

$$P(H|E_1, E_2, \ldots, E_n) = \frac{P(E_1, \ldots, E_n|H)P(H)}{P(E_1, E_2, \ldots, E_n)}$$

- Has more evidence.
  – Likelihood is hard---but **conditional independence assumption**

$$P(H|E_1, E_2, \ldots, E_n) = \frac{P(E_1|H)P(E_2|H)\cdots, P(E_n|H)P(H)}{P(E_1, E_2, \ldots, E_n)}$$

Classification

- Expression

$$P(H|E_1, E_2, \ldots, E_n) = \frac{P(E_1|H)P(E_2|H)\cdots, P(E_n|H)P(H)}{P(E_1, E_2, \ldots, E_n)}$$

- *H*: some class we'd like to infer from evidence
  - We know prior *P(H)*
  - Estimate $P(E_i|H)$ from data! ("training")
  - Very similar to envelopes problem. **Part of HW2**

Linear Algebra: What is it good for?

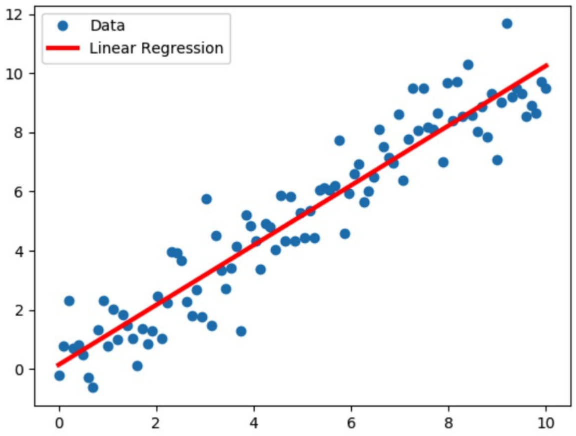
- Everything is a **function**
  - Multiple inputs and outputs

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

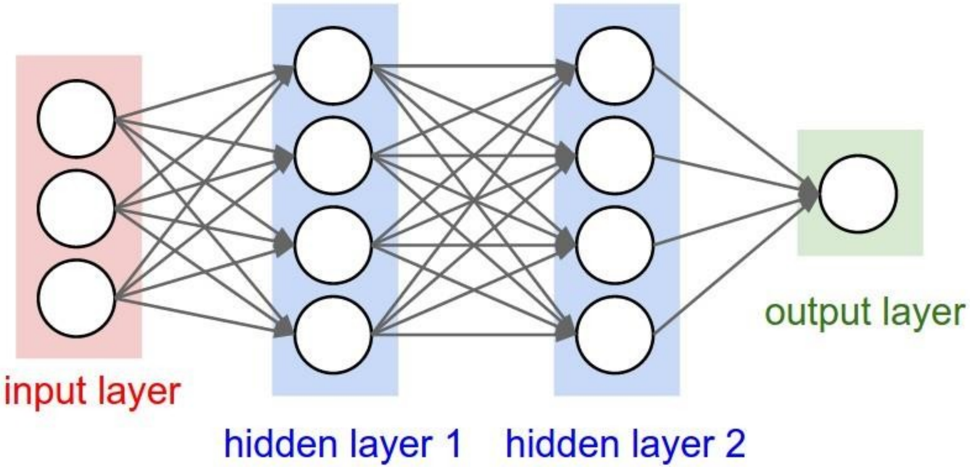
In AI/ML Context

Building blocks for **all models**

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



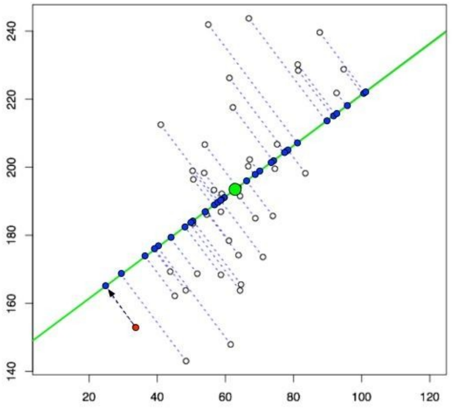
Hieu Tran



Stanford CS231n

Outline

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

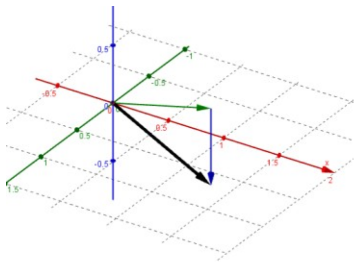


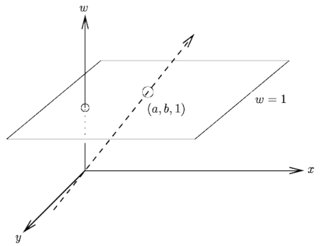
Lior Pachter

Basics: Vectors

Vectors

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

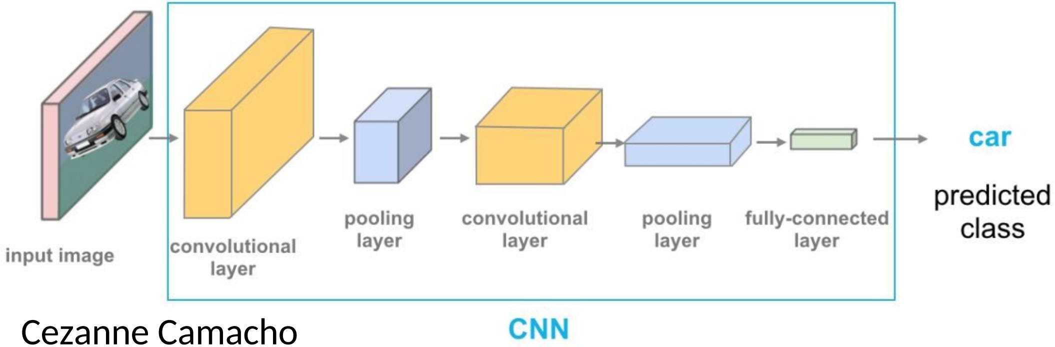




$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix}$$

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!



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

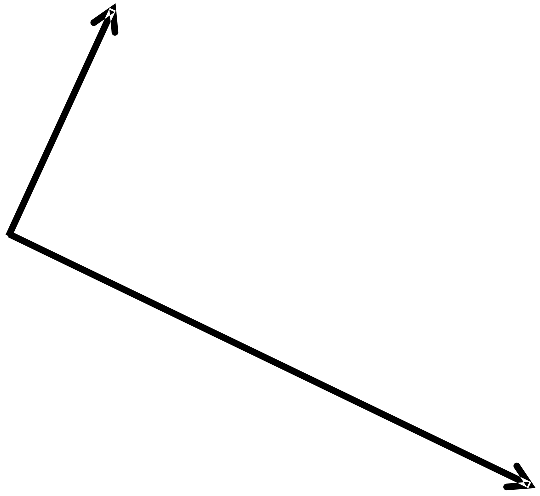
$$xy^T = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \begin{bmatrix} y_1 & y_2 & y_3 \end{bmatrix} = \begin{bmatrix} x_1 y_1 & x_1 y_2 & x_1 y_3 \\ x_2 y_1 & x_2 y_2 & x_2 y_3 \\ x_3 y_1 & x_3 y_2 & x_3 y_3 \end{bmatrix}$$

Matrix & Vector **Operations**

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

- Vector norms: “size”

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



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*

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

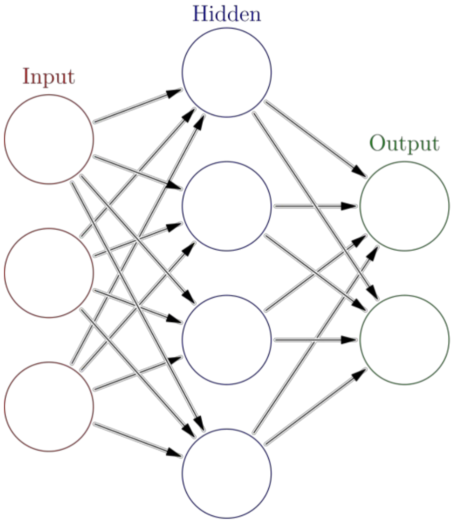
Matrix & Vector **Operations**

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**

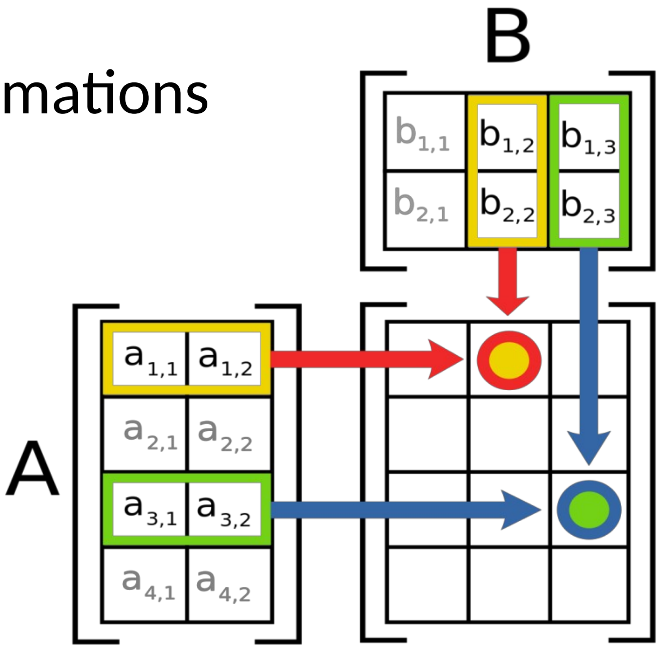
Wikipedia

Output of layer k: vector

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

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

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

More on Matrices: Inverses

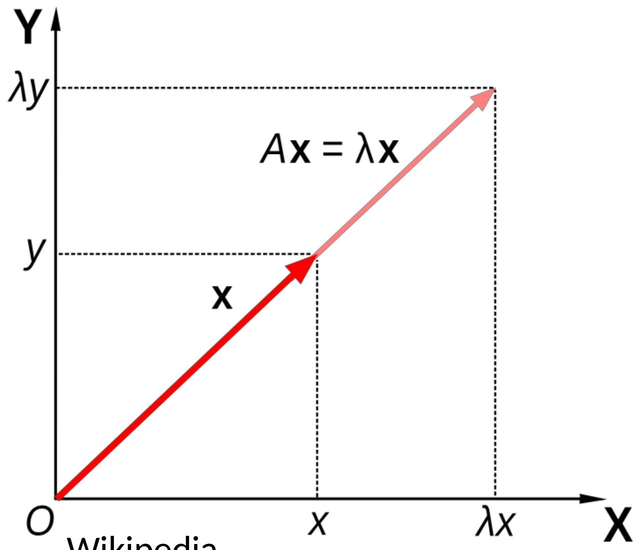
- If for *A* there is a *B* such that $AB = BA = I$
  - Then *A* is invertible/nonsingular, B is its inverse
  - Some matrices are **not** invertible!
  - Usual notation: A^{-1}

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

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

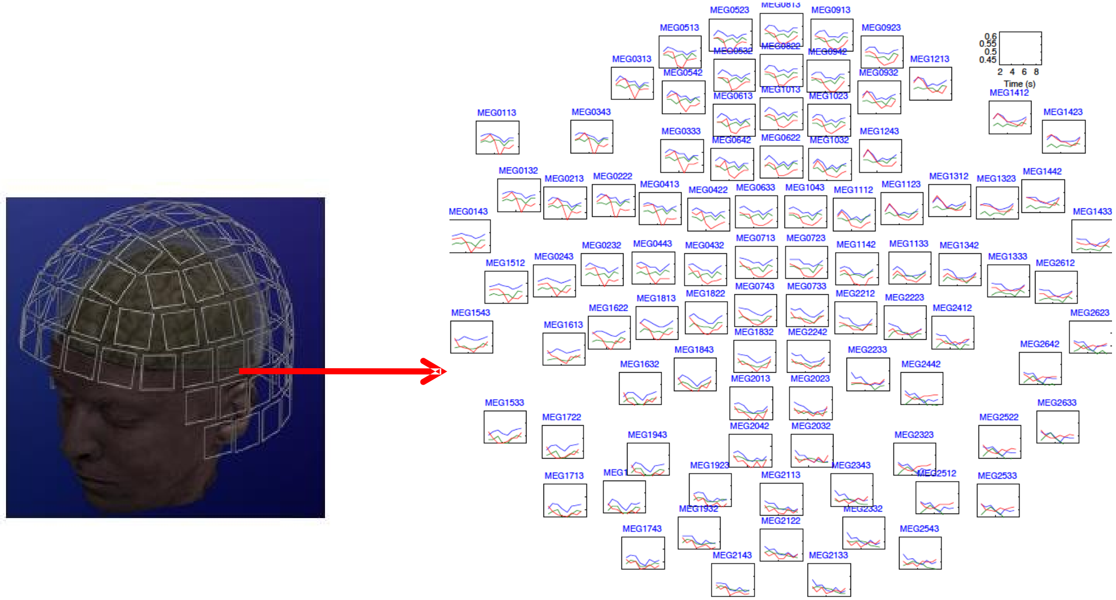
- Vectors used to store features
  - Lots of data -> lots of features!
- Document classification
  - Each doc: thousands of words/millions of bigrams, etc
- Netflix surveys: 480189 users x 17770 movies

	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

CreativeBloq

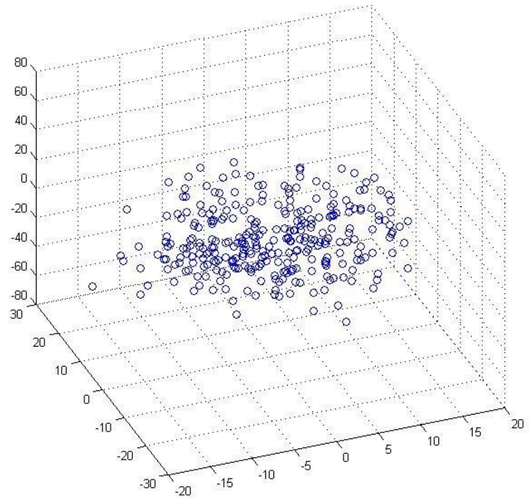
Reduce dimensions

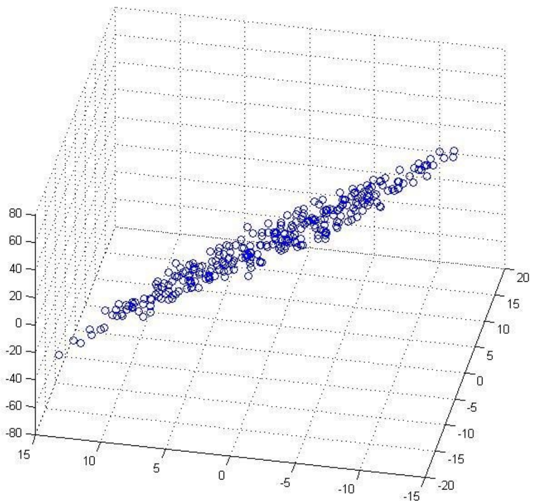
- Why?
  - Lots of features redundant
  - Storage & computation costs

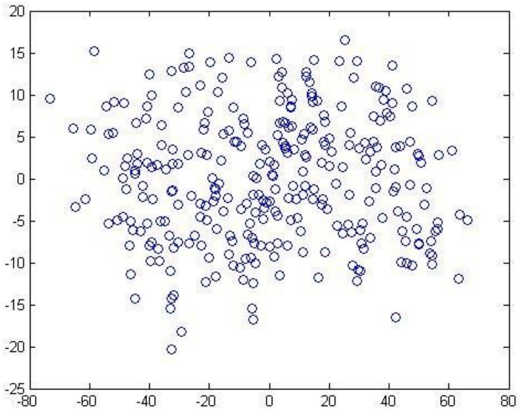
- Goal: take $x \in \mathbb{R}^d \rightarrow x \in \mathbb{R}^r$ for $r << d$
  - But, minimize information loss

Compression

Examples: 3D to 2D



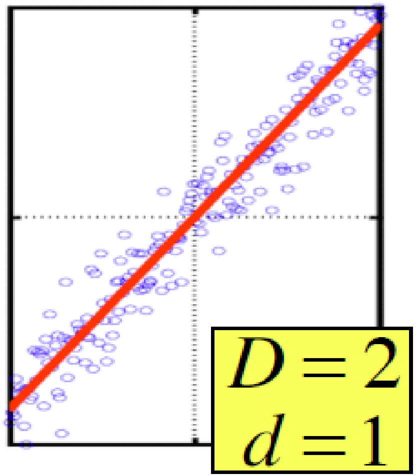


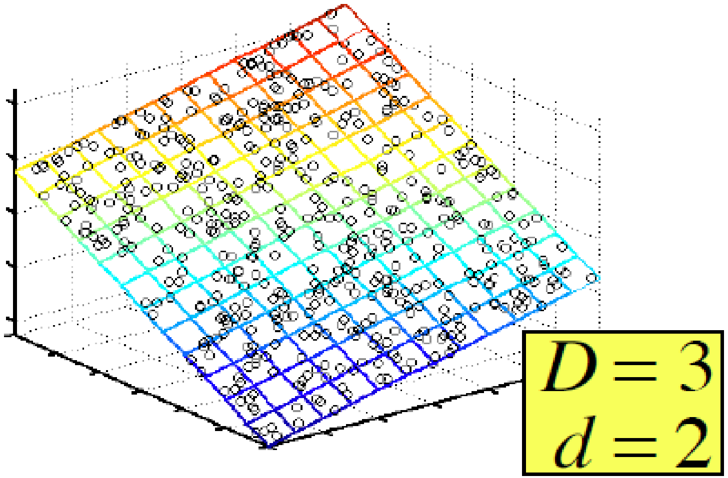


Andrew Ng

Principal Components Analysis (**PCA**)

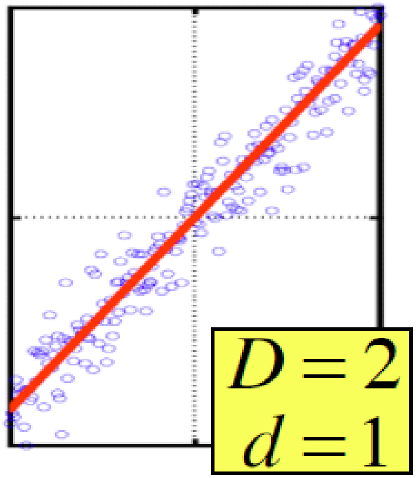
- A type of dimensionality reduction approach
  - For when data is **approximately lower dimensional**

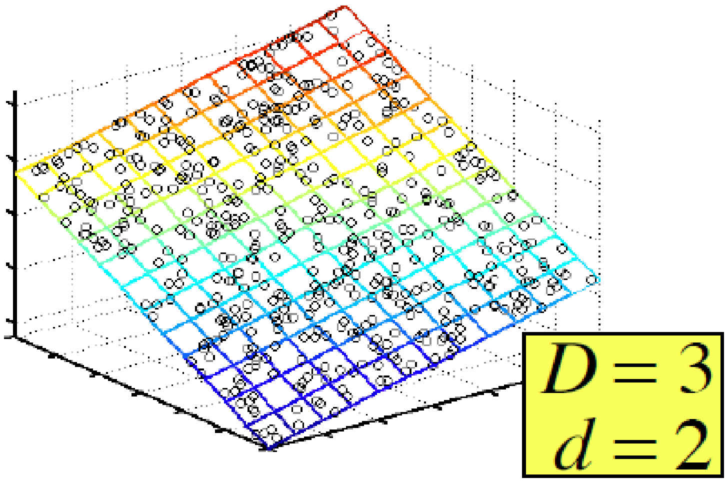




Principal Components Analysis (**PCA**)

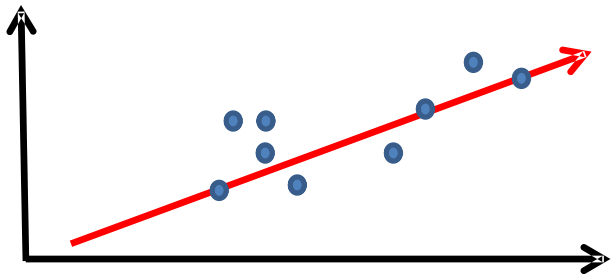
- Goal: find **axes** of a subspace
  - Will project to this subspace; want to preserve data





Principal Components Analysis (**PCA**)

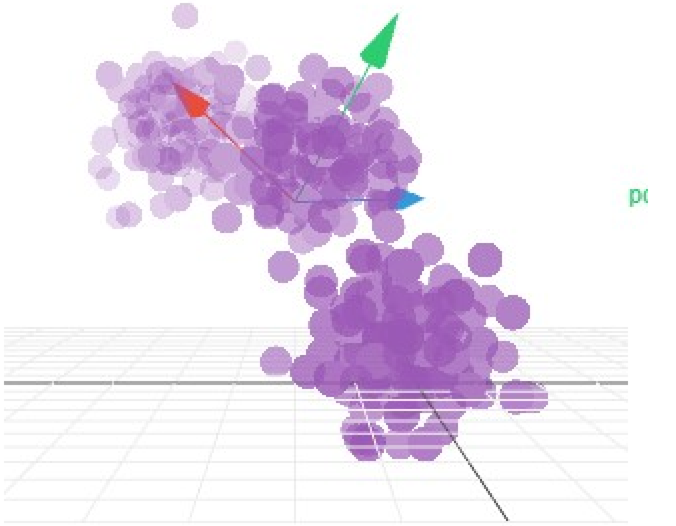
- From 2D to 1D:
  - Find a $v_1 \in \mathbb{R}^d$ so that we maximize "variability"
  - IE,



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

Principal Components Analysis (**PCA**)

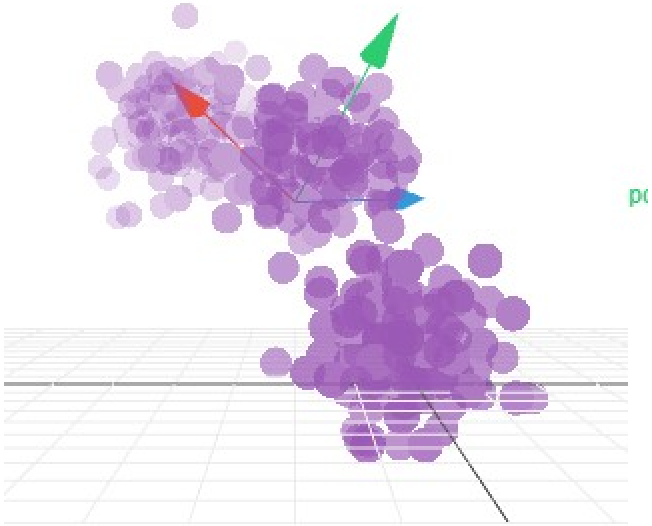
- From *d* dimensions to *r* dimensions
  - Sequentially get $v_1, v_2, \ldots, v_r \in \mathbb{R}^d$
  - Orthogonal!
  - Still minimize the projection error
    - Equivalent to **"maximizing variability"**
  - The vectors are the **principal components**



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
  - What's projection?

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

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

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 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

$$v_k = \arg\max_{\|v\|=1} \|\hat{X}_k w\|^2$$

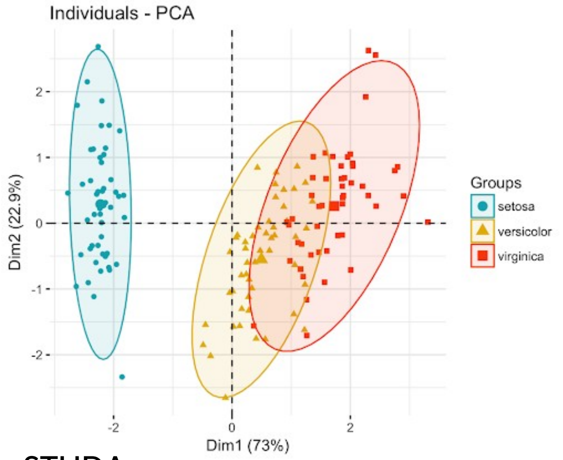
PCA Interpretations

- 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



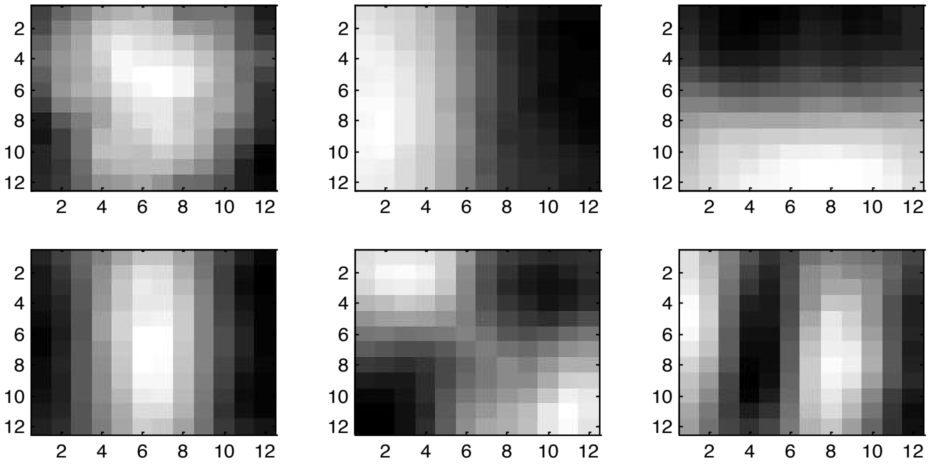
STHDA

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