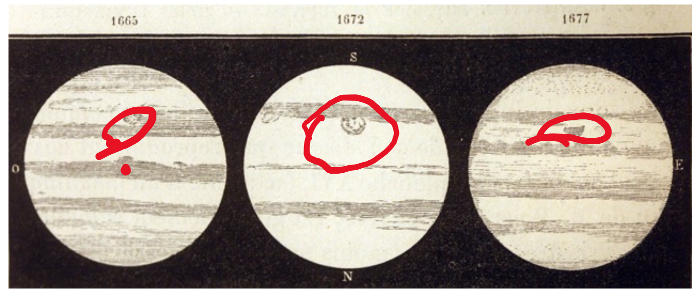
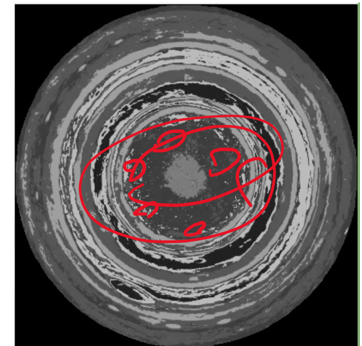
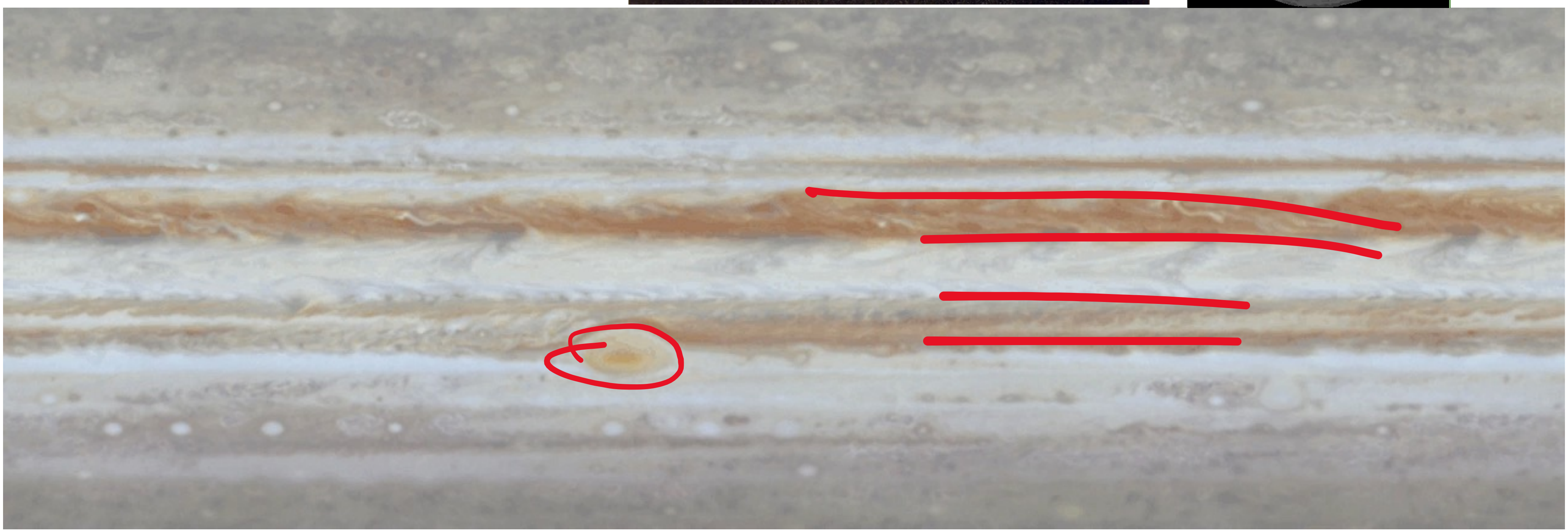
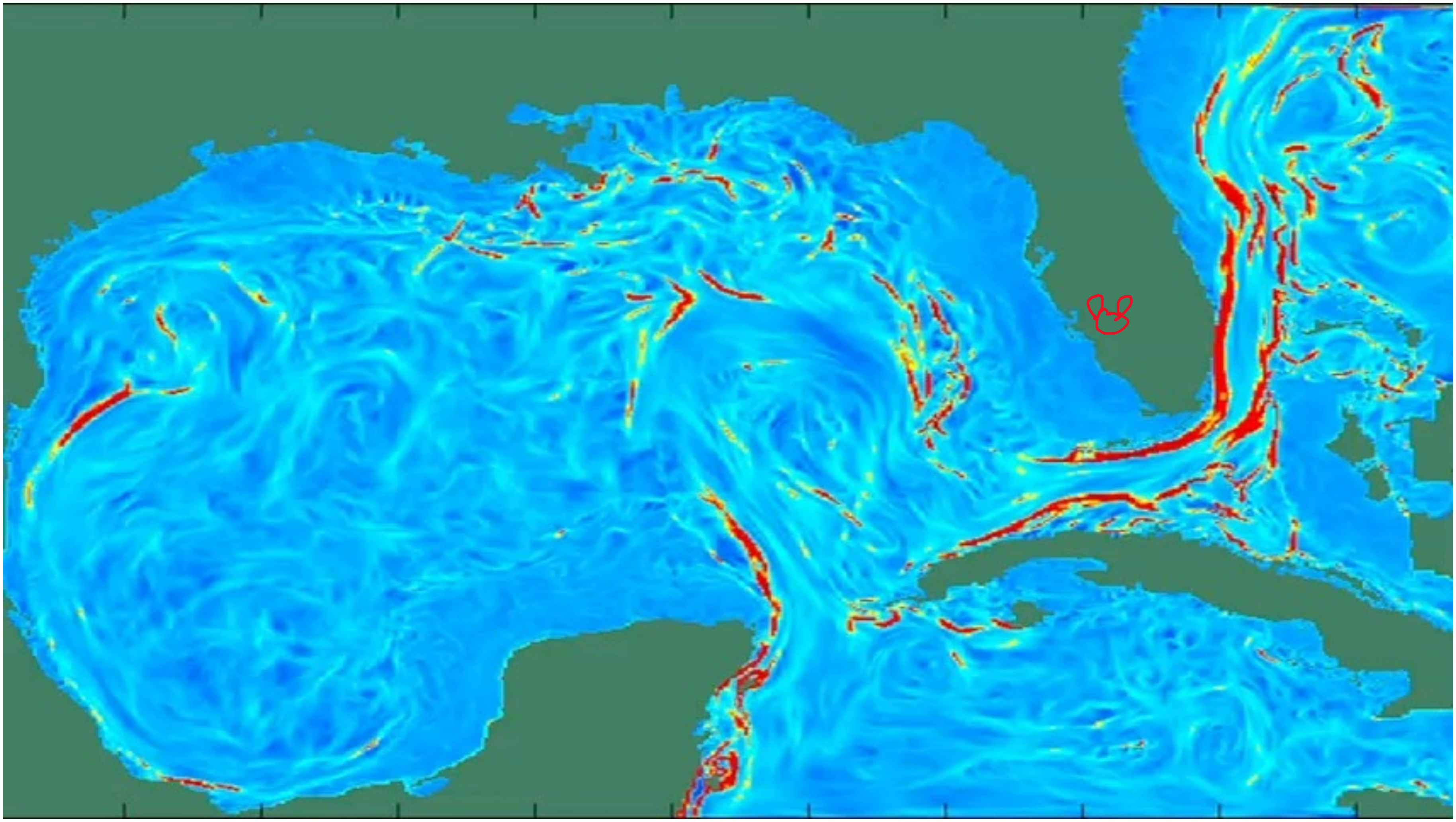
EE520 Data Driven Analysis of Complex Systems

Erik Bollt







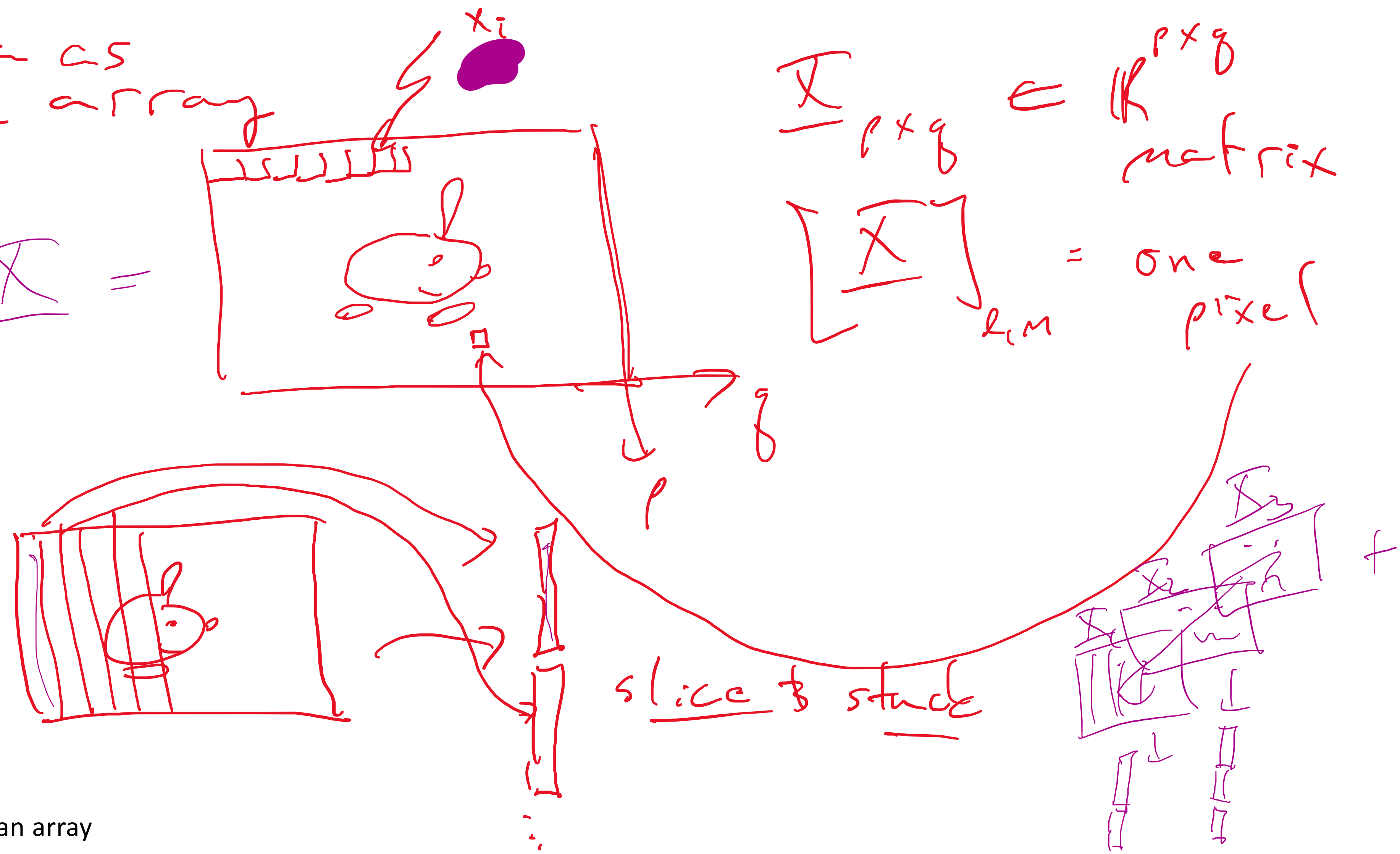


Data as an array

$\underline{X}_{p \times q} \in \mathbb{R}^{p \times q}$ matrix

$[\underline{X}]_{l,m}$ = one pixel

$\underline{X} =$



Data as an array

On Matrix Multiplication

$$A = \begin{pmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,n} \\ \vdots & & \ddots & \vdots \\ a_{m,1} & a_{m,2} & \cdots & a_{m,n} \end{pmatrix}, \text{ and each } a_{i,j} \in \mathbb{C}$$

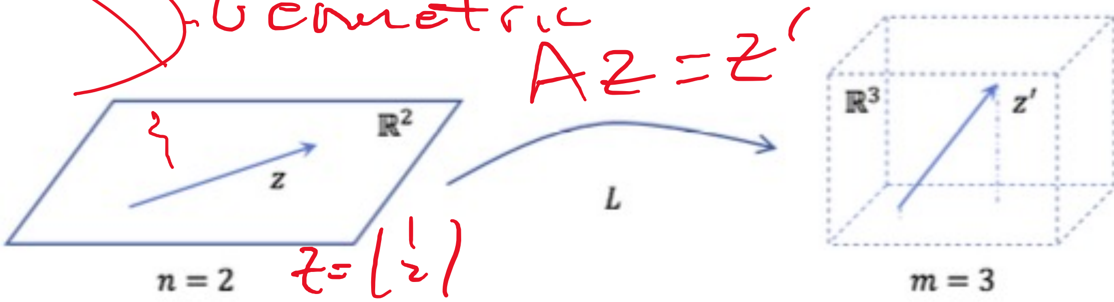
$$\begin{aligned} L(\mathbf{z}) : \mathbb{R}^n &\to \mathbb{R}^m \\ \mathbf{z} &\mapsto \mathbf{z}' = A\mathbf{z}, \end{aligned}$$

in terms of the usual matrix times vector multiplication,

$$[\mathbf{z}]'_i = \sum_{j=1}^{n} A_{i,j} [\mathbf{z}]_j, \text{ for each } i = 1, \cdots, m,$$

Geometric

$Az = z'$



$z = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$

• a vector has length & direction.

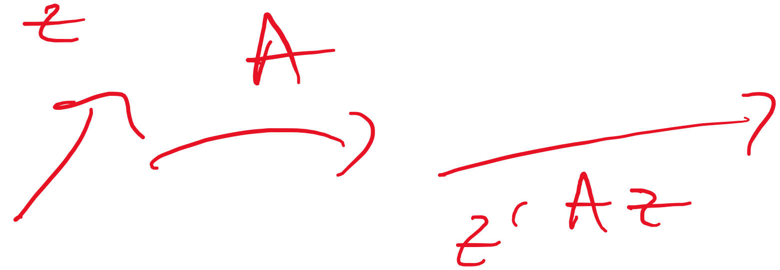
But as linear algebra

i.e. Matrices × vectors

$$A_{2\times 2} = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}$$

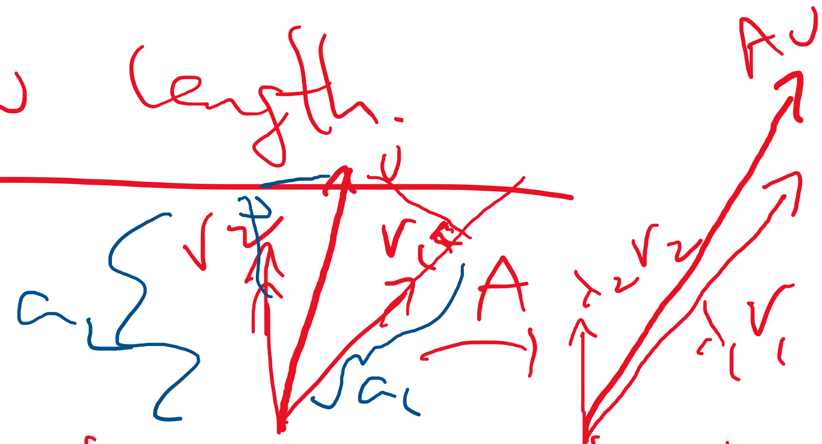
$$A\begin{pmatrix} 3 \\ 4 \end{pmatrix} = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}\begin{pmatrix} 3 \\ 4 \end{pmatrix} = \begin{pmatrix} 1\cdot 3 + 2\cdot 4 \\ 3\cdot 3 + 4\cdot 4 \end{pmatrix} = \begin{pmatrix} 11 \\ 25 \end{pmatrix}$$

$z' = Az$



new direction, new length.

Eig for square.



① $\underset{2\times 2}{A}v = \lambda v$

Characterize matrices by knowing just these

② eig. special directions

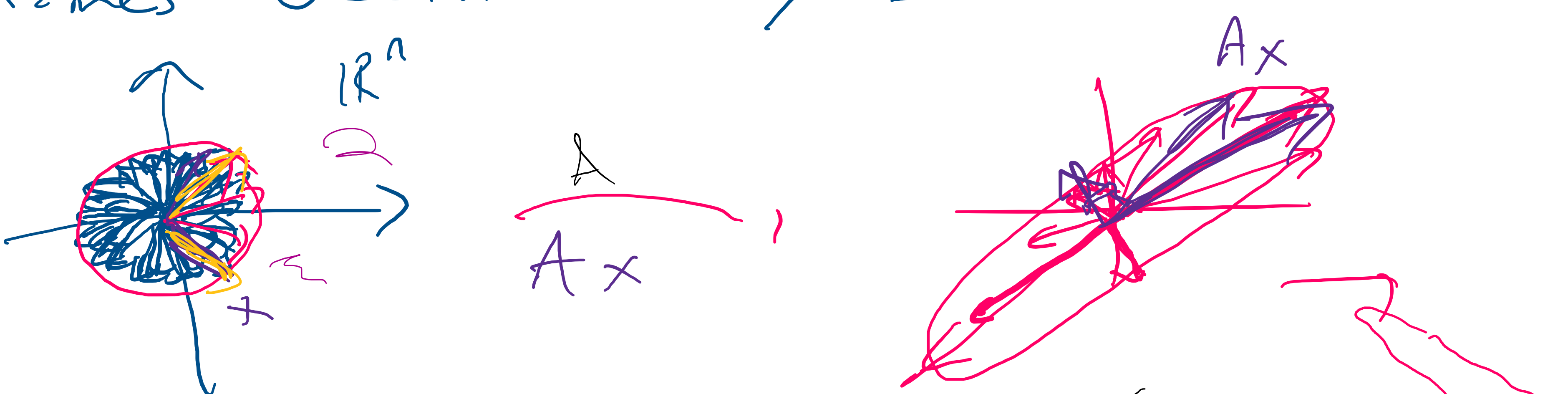
• $Au = A(a_1v_1 + a_2v_2) = a_1Av_1 + a_2Av_2$ $\det(A - \lambda I) = 0$

$= a_1\lambda_1 v_1 + a_2\lambda_2 v_2$ $(A - \lambda I)v = 0$

Matrix time circle =

all vectors of length 1.

? Matrix x circle ?! But matrix times vector. $\nearrow$ =



$S = \{x \mid \|x\|_2 = 1, x \in E \cong \mathbb{R}^2\}$; $A \cdot S = \{y : y = Ax, x \in S\}$

Theorem 2.1.1 — Singular Value Decomposition. Let A be an $m \times n$ matrix whose entries come from the field $\mathcal{K}$, which is either the field of real numbers or the field of complex numbers. Then the singular value decomposition of A exists, and it takes the form of a product of matrices:

$$A_{m\times n} = U_{m\times m}\Sigma_{m\times n}V^*_{n\times n}, \tag{2.5}$$

where

- U is an $m \times m$ unitary matrix.
- Σ is a diagonal $m \times n$ matrix with non-negative real numbers on the diagonal.
- V is an $n \times n$ unitary matrix, and V^* is the conjugate transpose of V.

$$\Sigma := diag(\sigma_1, \sigma_2, \cdots, \sigma_p), p = min(m, n),$$

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p \geq 0.$$

$$\Sigma = \begin{pmatrix} \sigma_1 & & 0 \\ & \sigma_2 & \\ 0 & & \ddots \end{pmatrix}$$

$$A = U \Sigma V^T$$

$$u_1^T u_1 = u_1 \cdot u_1 = 1$$

$$\begin{pmatrix} u_1^T u_1 & u_1^T u_2 & u_1^T u_3 & \cdots \\ u_2^T u_1 & u_2^T u_2 & \cdots & \end{pmatrix}$$

$$u_i^T u_j = \delta_{ij} = 1 \text{ or } 0$$

The singular values are the nonegative values: $\sigma_i \geq 0, i = 1, \cdots, n$,

The left singular vectors: u_i are the columns of $U = [u_1, u_2, ..., u_m]$.

The right singular vectors: v_i are the columns of $V = [v_1, v_2, ..., v_n]$.

$$\|u\|^2 \cos\theta = \vec{u_1} \cdot \vec{u_1} = 1 \qquad u_1^T u_2 = 0$$

$\cdot$ U unitary $\Leftrightarrow U^* U = U U^* = I$

$$U^T U = \begin{pmatrix} u_1 & u_2 & \cdots & u_m \end{pmatrix}^T \begin{pmatrix} u_1 & u_2 & \cdots & u_m \end{pmatrix} = I = \begin{pmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{pmatrix}$$

Definition 2.1.1 — Singular values and singular vectors. The singular values of A are the scalar values, σ_i, and the columns of U and V have columns that are the corresponding i^{th} left and right singular vectors, u_i and v_i:

The singular values are the nonegative values: $\sigma_i \geq 0, i = 1, \cdots, n$,

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The right singular vectors: v_i are the columns of $V = [v_1, v_2, ..., v_n]$.

Since V is orthogonal, then right multiplying Eq. (2.5) by V,

$$AV = U\Sigma V^* V = U\Sigma, \tag{2.8}$$

Fri 08/21/20

$Ax = b$

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 4 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

if

A is square

$AV = U\Sigma$

$$[A]\,[v_1 v_2 \cdots v_n] = [u_1 u_2 \cdots u_n]\, diag(\sigma_1, \sigma_2, \cdots, \sigma_n).$$

■ **Example 2.1** Let $A = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 4 & 6 \end{pmatrix}_{2\times 3}$. By SVD of the matrix A we have:

$$\begin{aligned} A &= U\Sigma V^T \\ &= \begin{pmatrix} \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\ \frac{-2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \end{pmatrix} \begin{pmatrix} \sqrt{70} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{14}} & \sqrt{\frac{2}{7}} & \frac{3}{\sqrt{14}} \\ \frac{-3}{\sqrt{10}} & 0 & \frac{1}{\sqrt{10}} \\ \frac{-1}{\sqrt{35}} & \sqrt{\frac{5}{7}} & \frac{-3}{\sqrt{35}} \end{pmatrix}. \end{aligned} \tag{2.28}$$

We see that the second singular value, $\sigma_2 = 2$, meaning that number of non-zero singular values $r < \min\{m, n\}$. Such matrix is called rank deficient matrix. If we take the economy version (with $r = 1$) of the SVD we will have:

$$\begin{aligned} u_1\sigma_1 v_1^T &= \begin{pmatrix} \frac{1}{\sqrt{5}} \\ \frac{-2}{\sqrt{5}} \end{pmatrix} \left(\sqrt{70}\right) \begin{pmatrix} \frac{1}{\sqrt{14}} & \sqrt{\frac{2}{7}} & \frac{3}{\sqrt{14}} \end{pmatrix} \\ &\approx \begin{pmatrix} 1 & 2 & 3 \\ 2 & 4 & 6 \end{pmatrix} \end{aligned} \tag{2.29}$$

■

$A^TA = V\Sigma^T\Sigma V^T \cdot V$

$A^TAV = \Sigma^T\Sigma V$

$V = (v_1\ v_2 \cdots v_n)$

$$[A]\,[v_1 v_2 \cdots v_n] = [u_1 u_2 \cdots u_n]\, diag(\sigma_1, \sigma_2, \cdots, \sigma_n).$$

Full ☆

The Economy SVD, and Reduced Rank SVD

The general SVD, Eq. (2.5) may be written in terms of submatrices.

Definition 2.1.3 — The Economy SVD. For any matrix $A \in \mathbb{R}^{m\times n}$, the general SVD Eq. (2.5) can be written in terms of smaller matrices,

$$A_{m\times n} = \hat{U}_{m\times n}\hat{\Sigma}_{n\times n}V^*_{n\times n}, \tag{2.21}$$

and $U = [\hat{U}_{m\times n}|\hat{U}_{(n-m)\times n}]$, written in terms of an orthogonal "buffer" matrix

$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > \sigma_{r+1} = 0$

$= 0 \dots$

Definition 2.1.4 — Rank Deficient SVD. For a matrix $A \in \mathbb{R}^{m\times n}$ such that the SVD results in singular values

$$\sigma_r > \sigma_{r+1} = 0, \text{ for some } r < n. \tag{2.22}$$

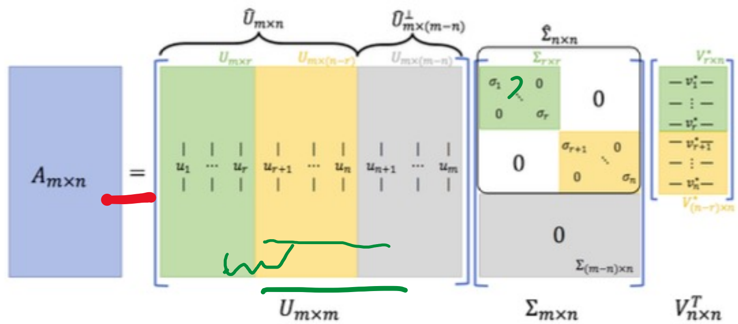
then the SVD can be written in terms of an economy form as smaller matrices,

$$A_{m\times n} = \hat{U}_{m\times r}\hat{\Sigma}_{n\times n}V^*_{n\times r}, \tag{2.23}$$

and related to the general SVD Eq. (2.5) by $U = [\hat{U}_{m\times r}|\hat{U}_{(n-r)\times n}]$, but $r < n$.

Rank ill conditioned

Full,
Economy,
Truncated
SVD



$m>n$

Figure 2.3: $m>n$ tall skinny

$\sigma_{r+1}=0$

$\sigma_r=10^{-6}$

$\sigma_{r+1}\approx 10^{-13}$

$<\varepsilon$

$A=[\ \ ]$ $m<n$

Recall that,

$$
\begin{aligned}
A_{m\times n} &= \hat{U}_{m\times n}\hat{\Sigma}_{n\times n}\hat{V}^T_{n\times n} \\
&= \begin{bmatrix} | & | & & | \\ u_1 & u_2 & \dots & u_n \\ | & | & & | \end{bmatrix}
\begin{bmatrix} \sigma_1 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_n \end{bmatrix}
\begin{bmatrix} - & v_1^T & - \\ - & v_2^T & - \\ - & \vdots & - \\ - & v_n^T & - \end{bmatrix}
\end{aligned}
\tag{2.24}
$$

but $V^TV=I$, orthogonality allows:

$$A_{m\times n}\hat{V}_{n\times n}=\hat{U}_{m\times n}\hat{\Sigma}_{n\times n} \tag{2.25}$$

so,

$$
A_{m\times n}\begin{bmatrix} | & | & & | \\ v_1 & v_2 & \dots & v_n \\ | & | & & | \end{bmatrix}
= \begin{bmatrix} | & | & & | \\ u_1 & u_2 & \dots & u_n \\ | & | & & | \end{bmatrix}
\begin{bmatrix} \sigma_1 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_n \end{bmatrix}
\tag{2.26}
$$

but this just states n-matrix times vector statements:

$$
\begin{aligned}
Av_1 &= \sigma_1 u_1 \\
Av_2 &= \sigma_2 u_2 \\
&\vdots \\
Av_n &= \sigma_n u_n
\end{aligned}
\tag{2.27}
$$

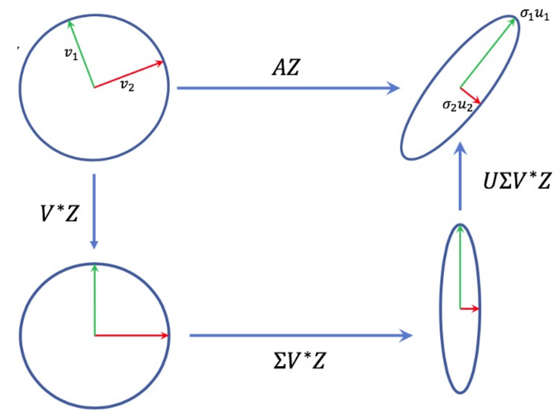
$A = U \Sigma V^T$

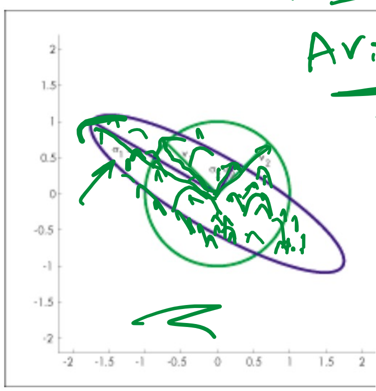
$A V = U \Sigma$

$A v_i = \sigma_i u_i$

Geometry:.

1. V^* rotates to a standard configuration.
2. Σ stretches each orthogonal axis to the major covariance axis of the corresponding ellipsoid, and
3. U rotates results back to the configuration that associates with A.





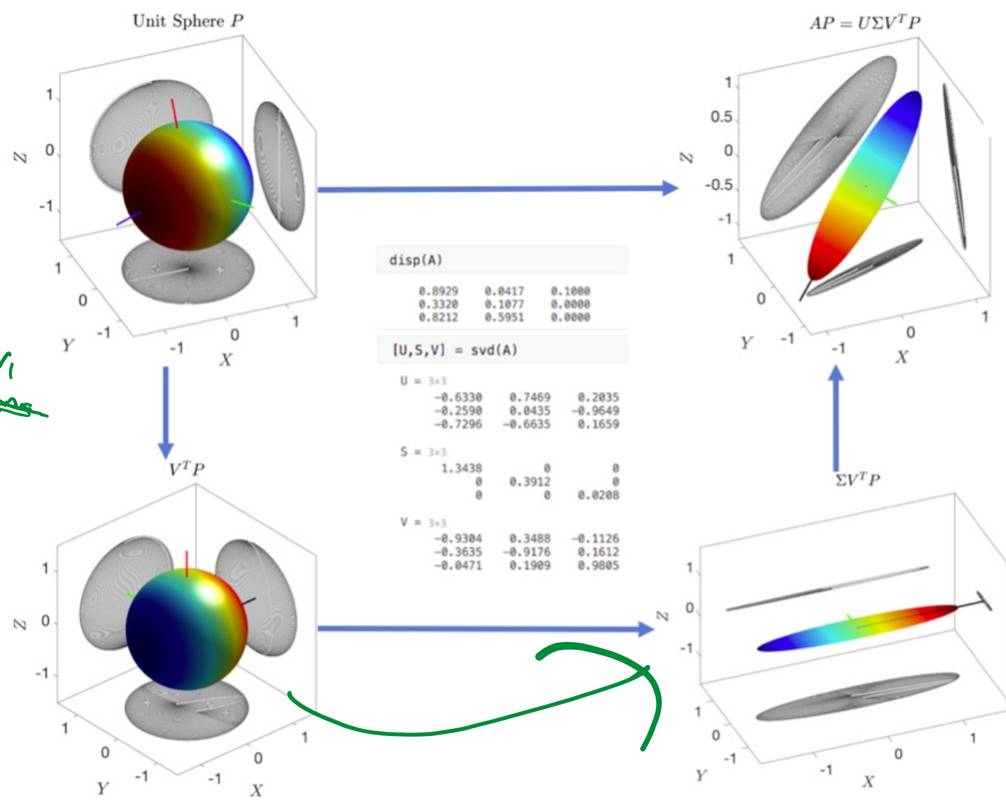
$\sigma_1 \sim 1.5$

$\sigma_2 \sim 0.5$

what if

$\sigma_1 = 2$

$\sigma_2 = 0.0003$




```
disp(A)

    0.8929    0.0417    0.1000
    0.3320    0.1077    0.0000
    0.8212    0.5951    0.0000

[U,S,V] = svd(A)

U = 3×3
   -0.6330    0.7469    0.2035
   -0.2590    0.0435   -0.9649
   -0.7296   -0.6635    0.1659

S = 3×3
    1.3438         0         0
         0    0.3912         0
         0         0    0.0208

V = 3×3
   -0.9304    0.3488   -0.1126
   -0.3635   -0.9176    0.1612
   -0.0471    0.1909    0.9805
```

$\sigma_1 u_1$ v_1

A

$A w = U \Sigma V^T w$

$v_i^T w$

$= v_i \cdot w$

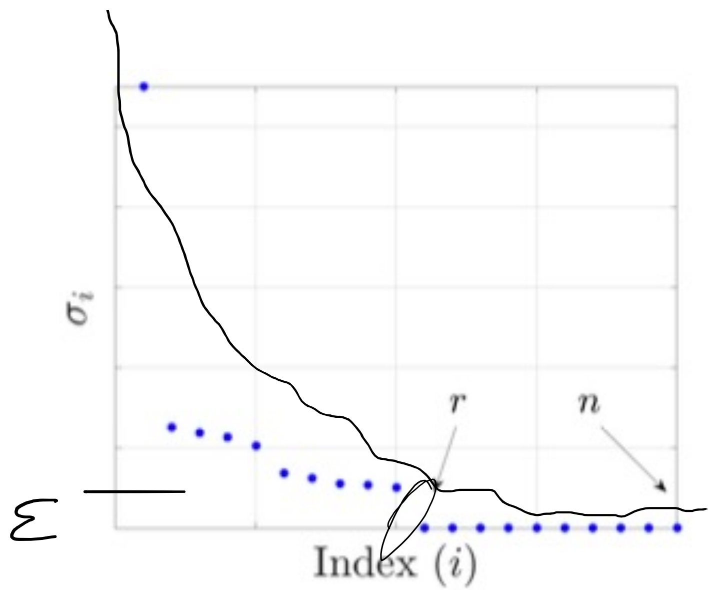
1 2 3 4

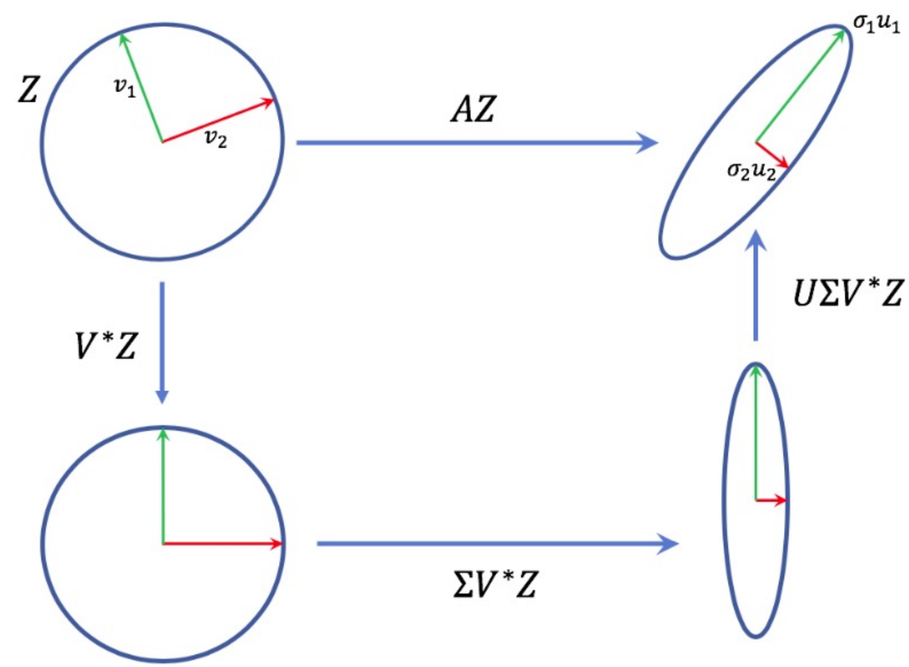
$X = [\, h \;\; \varphi \;\; f \;\; \ldots \,]$

w

redundant if $\sigma_{r+1} \sim 0$

And ROM





$\sigma_r > \varepsilon > \sigma_{r+1}$

~ 0

Bunny Compression

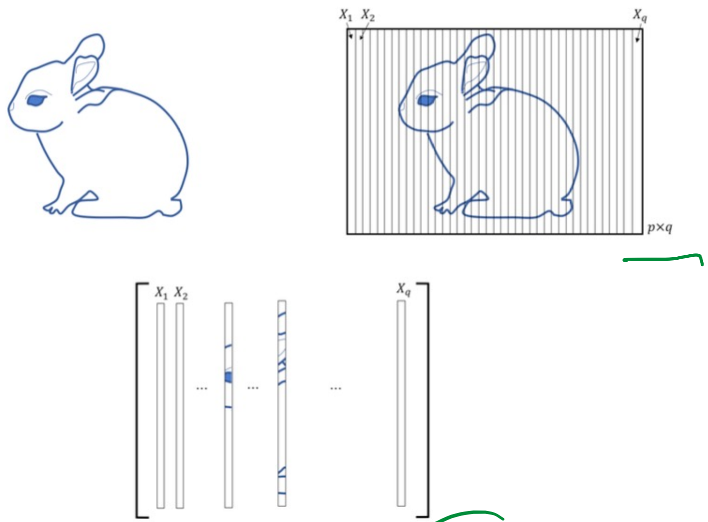


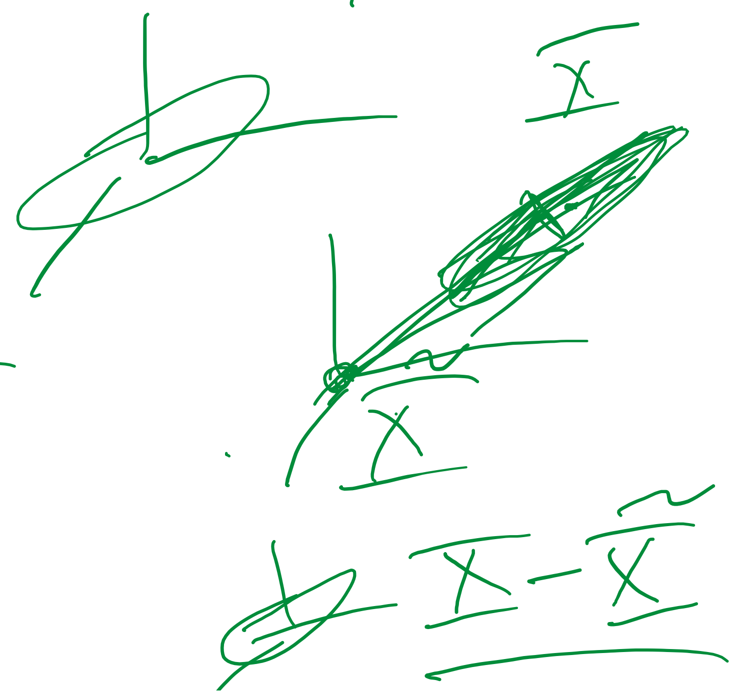
Figure 2.6: Caption

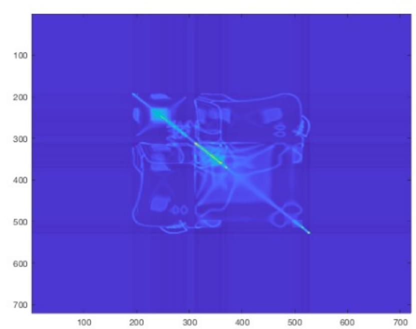
$\underline{X}$

Covariance – notice the demean step

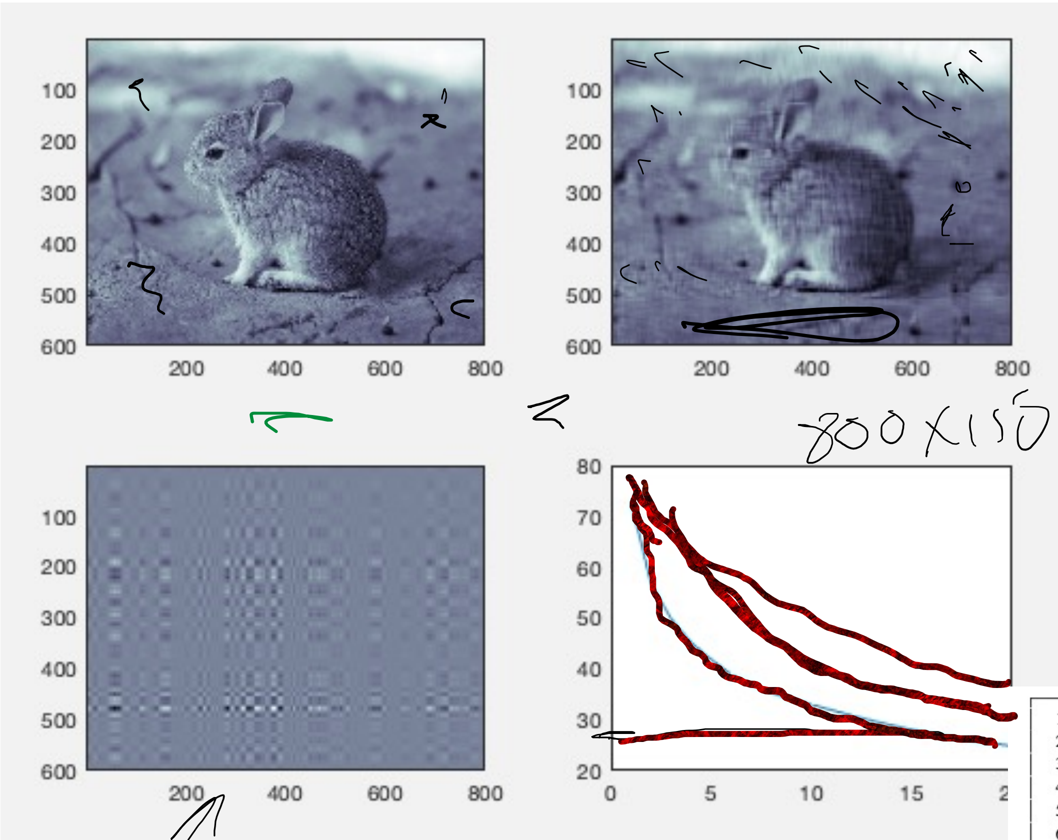
$$C_I = \frac{1}{n-1}\left(X - \tilde{X}\right)^T\left(X - \tilde{X}\right)$$

$A^T \quad A$





$\underline{X}^T \underline{X}$



$$u(x,t) = \sum a_i(t)\phi_i(x)$$

$$|a_i(t)| \xrightarrow{i\to\infty} 0$$

as fast as possible.

$$I = U\Sigma V^T$$

800x150

$$\approx \hat{U}\hat{\Sigma}\hat{V}^T$$

800x10

$$D \approx \tilde{D}$$

```
I = imread('Bunny.jpg');

figure
subplot(1,2,1)
imshow(I)
xticks({}); yticks({});
pbaspect([1 1 1])
title('RGB Image')

I = rgb2gray(I);  %Convert the 3D RGB color to 1D grayscale
I = im2double(I); %Convert integer value to double (scaled ...
    from 0 to 1)

subplot(1,2,2)
imshow(I)
xticks({}); yticks({});
pbaspect([1 1 1])
title('Grayscale Image')
```

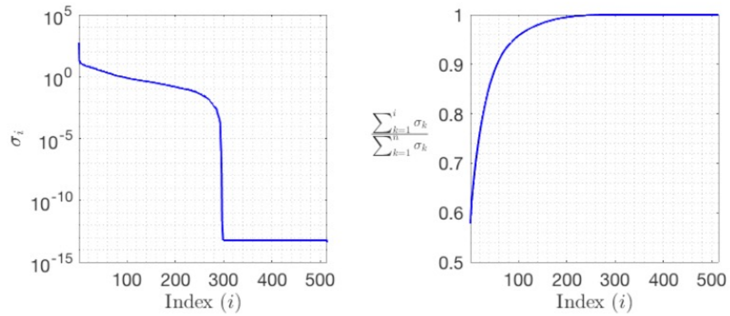
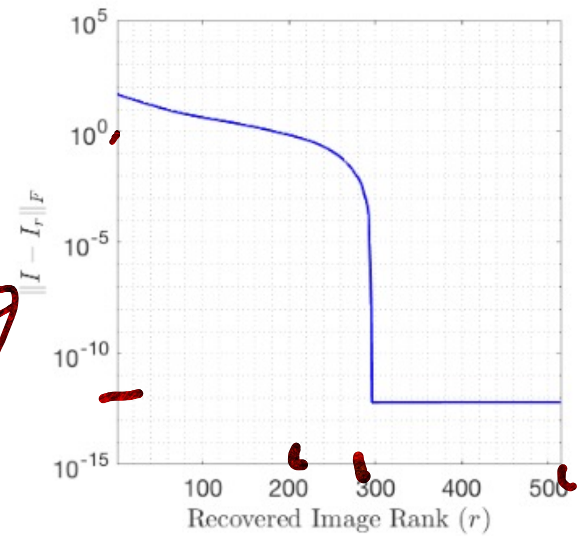
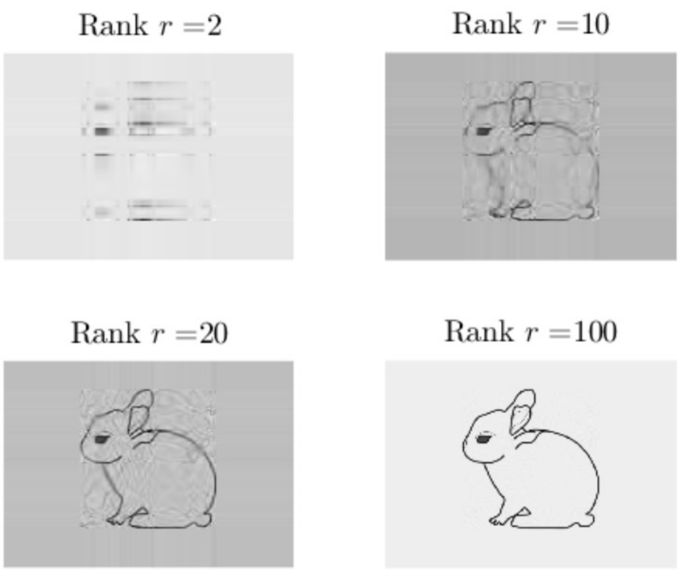


Figure 2.8: (Left) Singular Values. (Right) Energy



$$e_{rel} = \frac{\|I - I_i\|_F}{\|I\|_F}$$



: Distance $\|I - I_r\|_F$, where I_r is the recovered image using the reduced

Code 2.1: Read, convert, and display images.

```
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```

History

Gene Golub's license plate, photographed by Professor P. M. Kroonenberg of Leiden University.Gene Howard Golub (February 29, 1932 – November 16, 2007), Fletcher Jones Professor of Computer Science at Stanford University. His work made fundamental contributions that have made the singular value decomposition practical as one of the most powerful and widely used tools in modern matrix computation.

Lot's of Machine Learning

& Data Analysis

is solving an ill-posed

- optimize a cost function.

$$AA^T = U\Sigma \underbrace{V^T (V}\Sigma^T U^T)$$

$$= U\Sigma\Sigma^T U^T$$

$$(AA^T)\,\bar{U} = U(\Sigma\Sigma^T) = (\Sigma\Sigma^T)\,\bar{U}$$

$$\bar{U} = \left(u_1 \;\; u_2 \; \dots \; u_m \right)$$

Definition 2.1.2 — Induced Norm. Suppose a vector norm $\|\cdot\|$ on $\mathcal{K}^m$ is given. Any matrix $A_{m\times n}$ induces a linear operator from $\mathcal{K}^n$ to $\mathcal{K}^m$ with respect to the standard basis, and one defines the corresponding induced norm or operator norm on the space $\mathcal{K}^{m\times n}$ of all $m\times n$ matrices as follows:

$$\|A\|_p = \sup_{x\neq 0}\frac{\|Ax\|_p}{\|x\|_p} \tag{2.14}$$

or, taking a vector x such that $\|x\|_p = 1$, then we have

$$\|A\|_p = \sup_{\|x\|_p=1}\|Ax\|_p \tag{2.15}$$

Some Special (Simple) Matrix Norms

The first 3 of these are induced norms, but the 4th is not.

- For $p = 1$:

$$\|A\|_1 = \max_{1\le j\le n}\sum_{i=1}^{m}|a_{ij}| \tag{2.16}$$

- For $p = \infty$:

$$\|A\|_\infty = \max_{1\le i\le m}\sum_{j=1}^{n}|a_{ij}| \tag{2.17}$$

- A special case is the spectral norm when $p = 2$, in which we have:

$$\|A\|_2 = \sqrt{\lambda_{max}(A^TA)} = \sigma_{max} \tag{2.18}$$

where σ_{max} is the maximum singular value of the matrix A.

- The Frobenius norm is given by:

$$\|A\|_F = \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n}|a_{ij}|^2} = \sqrt{\sum_{i=1}^{\min\{m,n\}}\sigma_i^2} \tag{2.19}$$

Theorem 2.1.2 For a matrix A, the product of the singular values of A, equals the absolute value of its determinant:

$$|det(A)| = \prod_{i=1}^{n}\sigma_i \tag{2.20}$$

$Ax = x'$

$p=1$: $\|(x_1,x_2)\|_1 = |x_1| + |x_2|$

$p=\infty$: $\|(x_1,x_2)\|_\infty = \max_i |x_i|$

$p=2$: $\|(x_1,x_2)\|_2 = \sqrt{x_1^2+x_2^2}$

$\vec{x} = \begin{pmatrix}1\\3\end{pmatrix}$; $\|x\|_1 = 1+3 = 4$

$\|x\|_\infty = 3$

$\|x\|_2 = \sqrt{1^2+3^2} = \sqrt{10}$

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Fun facts about matrix estimation (data estimation)

If A, $\sigma_1 \geq \dots \geq \sigma_r > \sigma_{r+1} = 0$

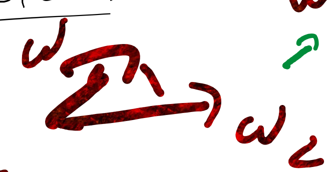
- $\text{range}(A) = \text{span}(u_1, u_2, \dots, u_r)$
- $\text{null}(A) = \text{span}(v_{r+1}, v_{r+2}, \dots, v_n)$ $\Big\} \; 0 \xrightarrow{A}$

$\sigma_2 = 0$

$r = 1$

- $\|A\|_2 = \sigma_1$; $\|A\|_F = \sqrt{\sigma_1^2 + \sigma_2^2 + \dots + \sigma_r^2}$
- $A = \sum_{i=1}^{r} \sigma_i u_i v_i^* = \sigma_1 u_1 v_1^* + \sigma_2 u_2 v_2^* + \dots + \sigma_r v_r^*$

rank-1 outer products.



$w_1^T w_2 = w_1 \cdot w_2 = \|w_1\| \|w_2\| \cos\theta$

$A = U \Sigma V^T$

$$\begin{pmatrix} u_1 & u_2 & \cdots & u_n \end{pmatrix}_{m \times ?} \begin{pmatrix} \sigma_1 & \sigma_2 & \cdots & \sigma_r \end{pmatrix} \begin{pmatrix} - v_1^T - \\ - v_2^T - \\ \vdots \end{pmatrix} \quad 1 \times n$$

$$\begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix}$$

Matrix Estimation / Data Estimation. $A_{m \times n}$

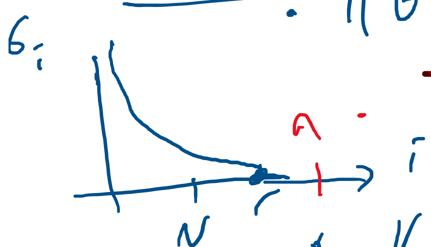
A

- let $0 \le N \le r$ and $A_N = \sum_{i=1}^{N} \sigma_i u_i v_i^*$

(so we may be skipping some of them ... $\sum_{i=N+1}^{r}$

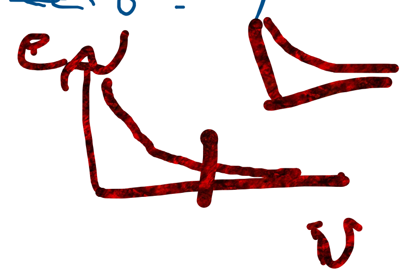
Then: $\|A - A_N\|_2 = \sigma_{N+1}$ (first one skipped))

(what if it zero?)



e_N

$$\|A - A_N\|_F = \sqrt{\sigma_{N+1}^2 + \sigma_{N+2}^2 + \dots + \sigma_r^2}$$

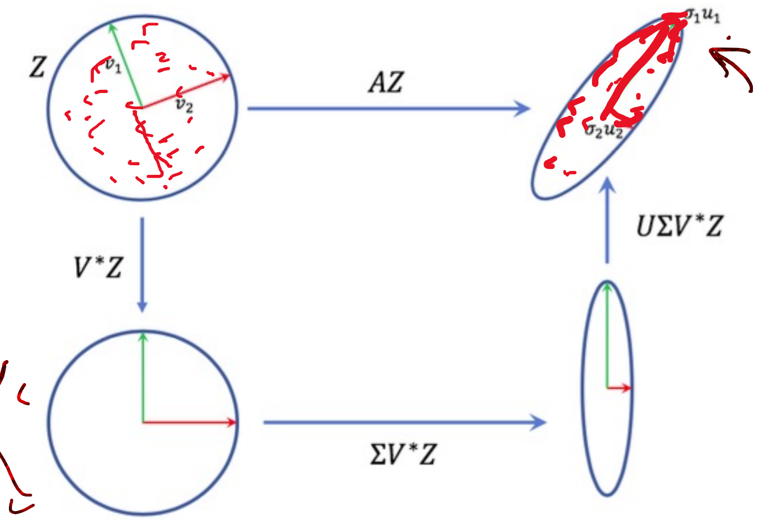


On PCA Principal Component Analysis, Eigenface

-On Raleigh Ritz Quotient

-On Spectral Decomposition Theorem

-On Data Clouds



$$X = [x_1 \mid x_2 \mid \dots \mid x_n] \qquad \vec{x}_i = a_1^i \vec{v}_1 + a_2^i \vec{v}_2 + \dots + a_r^i \vec{v}_r$$

v's as basis set.

x_i — PCA gives basis set where $\langle a_j^i \rangle_i \downarrow$ as fast as possible vs any other basis set.

$$\langle a_1^i \rangle_i = \frac{1}{n} \sum_{i=1}^{n} a_1^i$$

$\langle a_j^i \rangle^2$

Data for PCA - "Pretend data looks like an ellipsoid"

Ex: $X_i \sim 4500 \times 1$ gene expression table for each i.

$i = 1 \ldots 216$ patients

$$X_i = \begin{pmatrix} x_i^1 \\ x_i^2 \\ \vdots \\ x_{4500} \end{pmatrix}$$

$y_i = 0$ or 1 "0" if not cancer "1" if cancer.

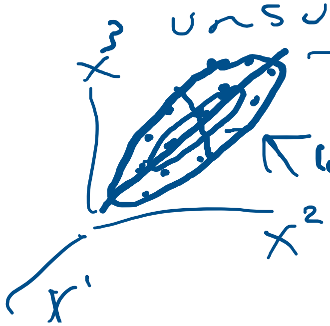
$$f : \mathbb{R}^{4500} \to \mathbb{Z}_2 \qquad \mathbb{Z}_2 = \{0, 1\}.$$

$x \in \mathbb{R}^{4500}$

- Supervised vs. unsupervised.

unsupervised - just input - just structural geometry.

just x



"Data Cloud" ~ distribution $\rho(x) : \mathbb{R}^{4500} \to \mathbb{R}^+$ of R.V. $x \sim \underline{X}$

level sets of ρ

- supervised learning is descriptive $f : x \to y$ labels

The spectral decomposition

Let A be a $n \times n$ symmetric matrix. From the spectral theorem, we know that there is an orthonormal basis $u_1, \cdots, u_n$ of $\mathbb{R}^n$ such that each u_j is an eigenvector of A. Let λ_j be the eigenvalue corresponding to u_j, that is,

$$Au_j = \lambda_j u_j.$$

real

Then

$$A = PDP^{-1} = PDP^T$$

where P is the orthogonal matrix $P = [u_1 \ \cdots \ u_n]$ and D is the diagonal matrix with diagonal entries $\lambda_1, \cdots, \lambda_n$. The equation $A = PDP^T$ can be rewritten as:

$$\begin{aligned} A &= [u_1 \ \cdots \ u_n] \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} \begin{bmatrix} u_1^T \\ \vdots \\ u_n^T \end{bmatrix} \\ &= [\lambda_1 u_1 \ \cdots \ \lambda_n u_n] \begin{bmatrix} u_1^T \\ \vdots \\ u_n^T \end{bmatrix} \\ &= \lambda_1 u_1 u_1^T + \cdots + \lambda_n u_n u_n^T. \end{aligned}$$

outer

$n \times 1 \cdot 1 \times n$
$n \times n$

The expression

$$A = \lambda_1 u_1 u_1^T + \cdots + \lambda_n u_n u_n^T.$$

is called the spectral decomposition of A. Note that each matrix $u_j u_j^T$ has rank 1 and is the matrix of projection onto the one dimensional subspace spanned by u_j. In other words, the linear map P defined by $P(x) = u_j u_j^T x$ is the orthogonal projection onto the subspace spanned by u_j.

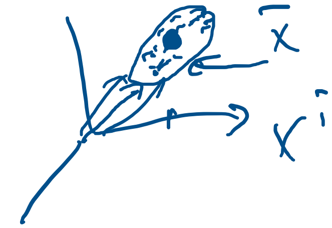
- $A = B^T B$ is symmetric
  $\Rightarrow$ spectral Decomp. theorem
  i.e. also covariance matrices.
- A is pos. definite if
  $\lambda_i > 0$ all i.

$\|v_i\|^2 = v_i \cdot v_i = v_i^T v_i$ scalar - inner product

PCA as algorithm

(say $m = 4000$, $n = 216$)

- Data $\underline{\overline{X}} = \begin{pmatrix} \vert & \vert & & \vert \\ x_1 & x_2 & \cdots & x_n \\ \vert & \vert & & \vert \end{pmatrix}_{m \times n}$ ith



- what if $x_i \sim \underline{\mathcal{N}(\bar{x}, \Sigma)}$ — covariance matrix.

$B = \underline{X} - \bar{B}$; $\bar{B} = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}_{n \times 1} \bar{x}^T_{1 \times n} = \underline{1}\,\bar{x}^T$. $\bar{x} = \begin{pmatrix} \bar{x}_1 \\ \bar{x}_2 \\ \vdots \\ \bar{x}_n \end{pmatrix}$

$\bar{x}_i = \frac{1}{n} \sum_{i=1}^{n} \underline{\overline{X}}_{ij}$

$B = U \Sigma V^T$; $U = [u_1\ u_2 \ldots u_n]$

and u_1 is major axis — most energetic — feature that most explains data.

u_2 is first minor axis

Side Note:

$\frac{1}{i}$ is slowest converging to zero σ_i^2

i.e. $\frac{1}{i}$ is slowest converging σ_i

$\sigma_i \le \frac{1}{i}$

$\sum_{i=1}^{\infty} \frac{1}{i^p} < \infty$ if ~~p~~ bad.

$p \le 1$, $p = 1$ harmonic

σ_i^2 the power spectrum

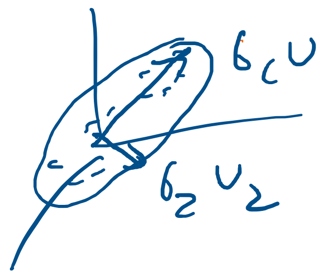
$= 1 + \frac{1}{2^p} + \frac{1}{3^p} + \frac{1}{4^p} + \dots$ $p = 1$

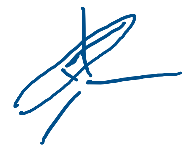
$B = I\bar{X}^T$; let $C = \frac{1}{n-1} B^T B$ everywhere

is covariance matrix.

$B = U \Sigma V^T$

$U = [u_1 | u_2 \ldots | u_n]$





- $u_1 = \underset{\|u\|=1}{\arg\max}\ u^T B^T B u = \underset{u}{\arg\max} \dfrac{(u^T B^T)(B u)}{u^T u}$

$\|Bu\|_2^2$

Rayleigh-Ritz quotient.

$Bu \cdot Bu = \|Bu\|_2^2$

- $u_2 = \underset{\substack{\|u\|=1 \\ u \perp u_1}}{\arg\max}\ u^T B^T B u$

The Eigs of C=B'B give optimal projection – thus PCA and…. KL

- $CV = VD$ eigenvectors of C all stacked.

Ax optimize $x^T A x$, maximize. ($A = B^T B$, $x = 0$)

$$x = \begin{pmatrix} x^1 \\ \vdots \\ x^n \end{pmatrix} \leftarrow j \qquad r(x) = \frac{x^T A x}{x^T x}$$

$$\frac{\partial r}{\partial x^j} = \frac{\partial}{\partial x^j}\left(r(x)\right) = \frac{\frac{\partial}{\partial x^j}(x^T A x) - x^T A x \frac{\partial}{\partial x^j}(x^T x)}{(x^T x)^2}$$

$$= \frac{2(Ax)_j}{x^T x} - \frac{(x^T A x)\, 2x_j}{(x^T x)^2} = \frac{2}{x^T x}\left(Ax - r(x)x\right)_j$$

$$\nabla r(x) = \frac{2}{x^T x}\left(Ax - r(x)x\right) = \frac{2}{x^T x}\left(A - r(x)\right)x = 0$$

$$A x = \underbrace{r(x)}_{\lambda}\, x \quad \Rightarrow \quad A x = \lambda x$$

Conclude

The x that optimes $r(x) = \dfrac{x^T A x}{x^T x}$

is an eigenvector and $r(x)$ is its

eigenvalue.

S.D.T. for $A = B^T B = \sum_{i=1}^{n} \lambda_i u_i u_i^T$

are the v's

let $B = U \Sigma V^T$ svd.

$$B^T B = V \Sigma^T \cancel{U^T U} \Sigma V^T = V \underbrace{\Sigma^T \Sigma} V^T$$

$$D = \begin{pmatrix} \sigma_1 & & & \\ & \ddots & & \\ & & \sigma_r & \\ & & & \ddots \\ & & & & 0 \end{pmatrix} \left(\begin{array}{ccccc|c} \sigma_1 & & & & & \\ & \ddots & & & & \\ & & \sigma_r & & & 0 \\ & & & \ddots & & \\ & & & & 0 & \end{array} \right) = \begin{pmatrix} \sigma_1^2 & & & & \\ & \sigma_2^2 & & & \\ & & \ddots & & \\ & & & \sigma_r^2 & \\ & & & & \ddots \\ & & & & & 0 \end{pmatrix}$$

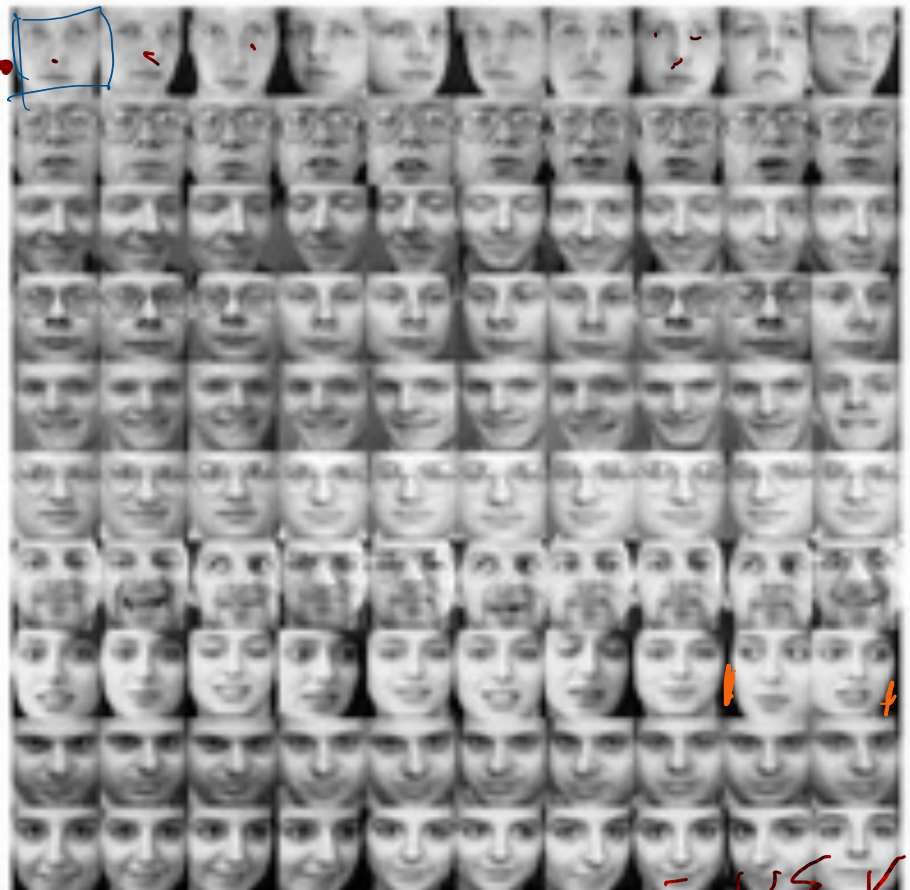
$$= V D V^T = \sum_{i=1}^{r} \sigma_i^2 v_i v_i^T$$

Eigenface

08/31/20

$p = 6000, q = 2000$

i^{th} picture



i — $p \times q$ array

reshape as vector

$$\begin{bmatrix} \\ x_i \\ \\ \end{bmatrix}_{M \times 1} \qquad e_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$M = pq$

$$X = [x_1 | x_2 | \cdots | x_n]_{M \times n} = U \Sigma V^T$$

- remove variance

Register

$\mathbb{R}^{pq} = \mathbb{R}^M$

E_1, E_2, E_3, σ_i^2

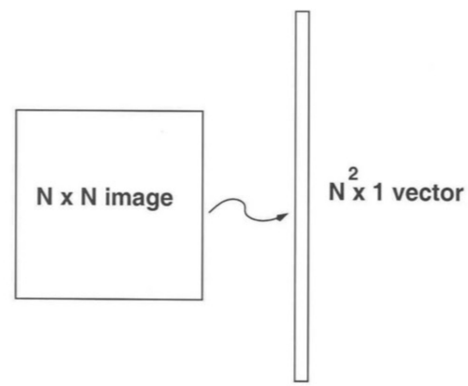
$x_i \cdot e_1 = x_i^T e_1 = E$

Eigenfaces for Face Detection/Recognition

(M. Turk and A. Pentland, "Eigenfaces for Recognition", *Journal of Cognitive Neuroscience*, vol. 3, no. 1, pp. 71-86, 1991, hard copy)

• Face Recognition

- The simplest approach is to think of it as a template matching problem:



- Problems arise when performing recognition in a high-dimensional space.

- Significant improvements can be achieved by first mapping the data into a *lower-dimensionality* space.

- How to find this lower-dimensional space?

• Main idea behind eigenfaces

- Suppose Γ is an N^2x1 vector, corresponding to an NxN face image I.

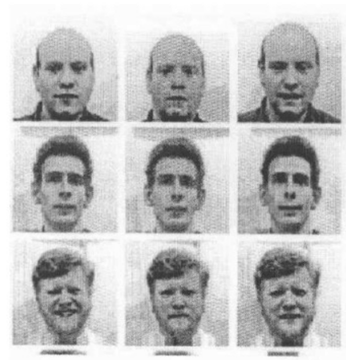
- The idea is to represent Γ (Φ=Γ - mean face) into a low-dimensional space:

$$\hat{\Phi} - mean = w_1 u_1 + w_2 u_2 + \cdots w_K u_K \ (K << N^2)$$

Computation of the eigenfaces

Step 1: obtain face images $I_1, I_2, \ldots, I_M$ (training faces)

(**very important:** the face images must be *centered* and of the same *size*)



Step 2: represent every image I_i as a vector Γ_i

Step 3: compute the average face vector Ψ:

$$\Psi = \frac{1}{M} \sum_{i=1}^{M} \Gamma_i$$

Step 4: subtract the mean face:

$$\Phi_i = \Gamma_i - \Psi$$

Step 5: compute the covariance matrix C:

$$C = \frac{1}{M} \sum_{n=1}^{M} \Phi_n \Phi_n^T = AA^T \quad (N^2 \text{x} N^2 \text{ matrix})$$

where $A = [\Phi_1 \; \Phi_2 \cdots \Phi_M]$ $\quad (N^2 \text{x} M \text{ matrix})$

$C = X^T X$

Step 6: compute the eigenvectors u_i of AA^T

The matrix AA^T is very large --> not practical !!

Step 6.1: consider the matrix $A^T A$ (M x M matrix)

Step 6.2: compute the eigenvectors v_i of $A^T A$

$$A^T A v_i = \mu_i v_i$$

What is the relationship between us_i and v_i?

$A^T A v_i = \mu_i v_i \Rightarrow AA^T A v_i = \mu_i A v_i \Rightarrow$

$CAv_i = \mu_i A v_i$ or $Cu_i = \mu_i u_i$ where $u_i = Av_i$

Thus, AA^T and $A^T A$ have the same eigenvalues and their eigenvectors are related as follows: $u_i = Av_i$!!

Note 1: AA^T can have up to N^2 eigenvalues and eigenvectors.

Note 2: $A^T A$ can have up to M eigenvalues and eigenvectors.

Note 3: The M eigenvalues of $A^T A$ (along with their corresponding eigenvectors) correspond to the M *largest* eigenvalues of AA^T (along with their corresponding eigenvectors).

Step 6.3: compute the M best eigenvectors of AA^T: $u_i = Av_i$

(**important:** normalize u_i such that $\|u_i\| = 1$)

Step 7: keep only K eigenvectors (corresponding to the K largest eigenvalues)

Representing faces onto this basis

- Each face (minus the mean) Φ_i in the training set can be represented as a linear combination of the best K eigenvectors:

$$\hat{\Phi}_i - mean = \sum_{j=1}^{K} w_j u_j, \quad (w_j = u_j^T \Phi_i)$$

(we call the u_j's *eigenfaces*)

- Each normalized training face Φ_i is represented in this basis by a vector:

$$\Omega_i = \begin{bmatrix} w_1^i \\ w_2^i \\ \dots \\ w_K^i \end{bmatrix}, \quad i = 1, 2, \dots, M$$

$X = U \Sigma V^T$

$U = [u_1 | u_2 | \dots | u_s | u_{s+1} | \dots | u_r | u_{r+1} \dots u_n]$

• imagesc(g)

• g = reshape(U(:, i), p, q)

$\|\vec{a}\|_2^2 = \sum a_i^2$

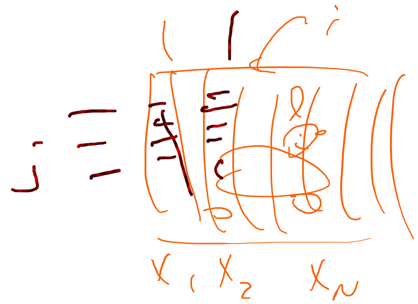
Parseval ineq.

$\|\vec{a}_i\|_2^2 = \|f\|_2^2 = \int |f(x)|^2 dx$

Fourier

Taylor

Bunny



$\rightarrow \bar{X} = [\vec{x}_1 | \vec{x}_2 | \dots | \vec{x}_N]$ one column

$= U \Sigma V^T$

PCA of the bunny

$\vec{x}_i = a_1^i \vec{u}_1 + a_2^i \vec{u}_2 + \dots + a_N^i \vec{u}_N$

basis

a_i^2

full of as possible for the data set

$a_1^i = x_i^T u_1 = \text{comp}_{u_1} x_i = \frac{u_1 \cdot x_i}{\cancel{\|u_1\|}} = \|u_1\| \|x_i\| \cos\theta$

On basis, functions, and Hilbert space.
Fourier, Taylor, Wavelet, POD-KL

lead in

3B ② – in 5 min. Signals analysis, Harmonic

- Historically favorite basis set. $B = \{\omega_1, \omega_2, \ldots\}$

(vs. energy favorite basis set comes from PCA)

- Taylor Polynomials. $f(x) = a_0 + a_1 x + a_2 x^2 + \ldots + a x^i$

  $B = \{x^0, x^1, x^2, \ldots\}$

  $a_i = \dfrac{f^{(i)}(0)(x-0)^i}{i!}$

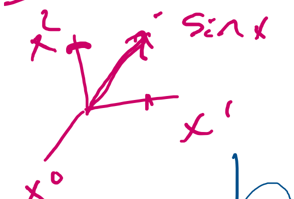
- Fourier modes.

  $f(x) = a_1 \sin x + a_2 \sin 2x + a_3 \sin 3x + \ldots$

  $B = \{\sin x, \sin 2x, \ldots\}$

  ~~where~~ $a_1 = (f(x), \sin x) = \dfrac{1}{2\pi}\int_0 f(x)\sin x \, dx$

$\mathcal{H}$: Hilbert space

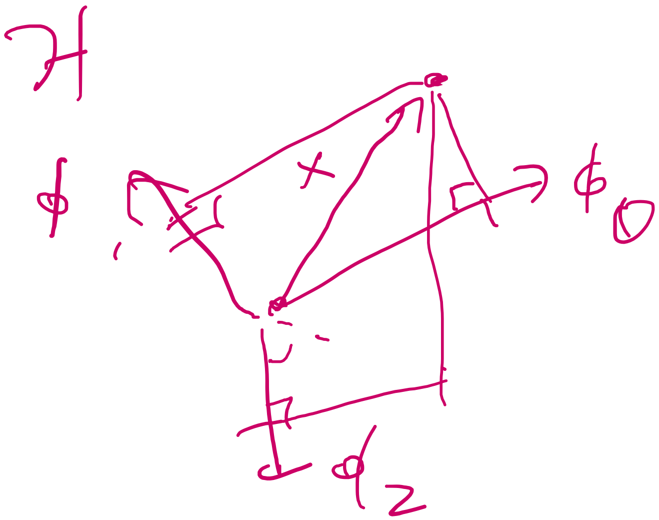


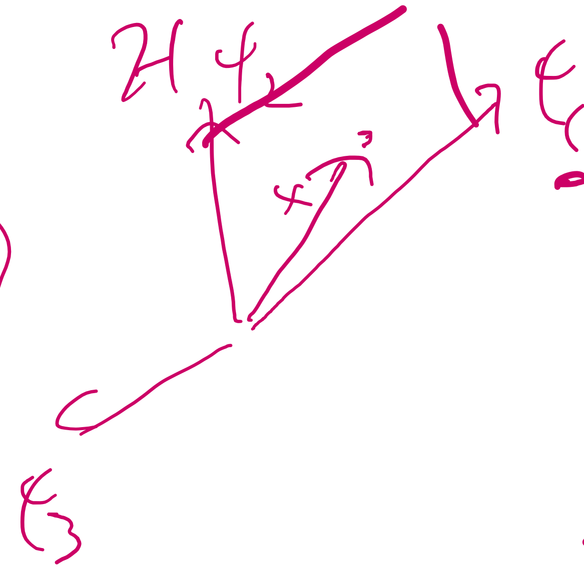
- Wavelet basis.
- Chebychev polys, Legendre ...

$\sin x = 1x - \frac{x^3}{3!} + \frac{x^5}{5!} + \ldots$

$\text{comp}_x \sin x = 1$

Changing basis is a sort of coord. rot.





$\phi_0(y) = y^0$

$\phi_1(y) = y^1$

$\phi_2(y) = y^2$

$\vdots$

$\to \varphi_1(y) = \sin(y)$

$\varphi_2(y) = \sin(2y)$

$\varphi_3(y) = \sin(3y)$

On basis, functions, and Hilbert space. Fourier, Taylor, Wavelet, POD-KL

vs. 2.1

Hilbert Space – a complete inner product space.

- An inner product space is a "vector space" E (with limits) together with a function called "inner product" $\langle\cdot,\cdot\rangle : E\times E \to \mathbb{C}$ ($\mathbb{R}$.) with properties.
  - conjugate (symm.) $\langle u,v\rangle = \overline{\langle v,u\rangle}$ $\forall u,v\in E$
  - linear $\langle au_1+bu_2, v\rangle = a\langle u_1,v\rangle + b\langle u_2,v\rangle$ $\forall a,b\in\mathbb{C}$ field. $u_1,u_2,v\in E$
  - pos. defn: $\langle u,u\rangle > 0$ $\forall u\in E, u\neq 0$.

Gift: you set geometry in E as an angle $\angle(u,v) := \operatorname{acos}\frac{\langle u,v\rangle}{\|u\|\,\|v\|}$ and projection.

- vector space.

set of objects "like vectors" that have a + and scalar multiplication – including communative, associative, add. ident, inverse, distributive vs scalar and vectors. identity for scalar.

Ex: arrays of real numbers that are 2x1. $3\begin{bmatrix}2\\1\end{bmatrix} + 6\begin{bmatrix}4\\2\end{bmatrix} = \begin{bmatrix}30\\15\end{bmatrix}$ vs.

Norm: $\|x\|^2 = \langle x,x\rangle^{1/2}$

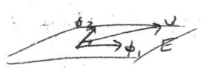
Ex functions in $C([0,1])$ e.g. $\underset{\phi_1(x)}{3\cdot x^2} + \underset{\phi_2(x)}{4x^3} + \underset{\phi_3(x)}{7\sin x} = f(x) \in C([0,1])$

Ex: Name an inner product space (vector space of functions) $E = L^2([0,1]) = \{ f \mid \int_0^1 |f(x)|^2 dx < \infty \}$

$(L^2([0,1]) \subset C([0,1]))$

let $\langle f,g\rangle_{L^2([0,1])} = \int_0^1 f(x)\,\overline{g(x)}\,dx$ & btw $\|f\|_{L^2([0,1])} = \left(\int_0^1 |f(x)|^2 dx\right)^{1/2}$

Basis of unit vectors. • orthogonal $B = \{\phi_i \mid \phi_i \in B \subset E$ and $\langle\phi_i,\phi_j\rangle = \delta_{ij}$ and $\|\phi_i\| = 1\}$

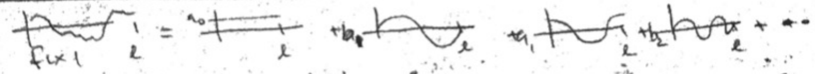


$u = \sum_i a_i\phi_i$

projection!

Ex: $L([0,\ell))$; $B = \{\cos\frac{2\pi kx}{\ell}, \sin\frac{2\pi kx}{\ell}, 1 \mid k\in\mathbb{N}\} = \{-, \sim, \backsim, \ldots\}$

if $\ell = 1$; $f(x) = \frac{a_0}{2} + \sum_{k=1}^{\infty} a_k\cos kx + b_k\sin kx$; $a_k = \frac{\langle f(x), \cos kx\rangle}{\|\cos kx\|} = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\cos kx\,dx$; $b_k =$ … $\sin kx$

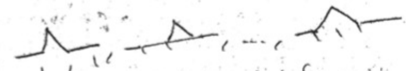


$\phi_k(x) = \frac{2}{\ell}\cos\frac{kx}{\ell}$ or $\frac{2}{\ell}\sin\frac{kx}{\ell}$

finite if a "trig. poly".

- similar if $\phi_k(x) = c\,e^{ikx}$

or maybe $B' = \{x^k\}$ Taylor poly

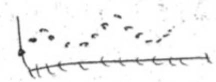
or maybe $B'' = \{$  $, \ldots \}$ wavelets.

"Hat" functions 2.13

Finite dimensional inner product space & functions.

$x_1 < x_2 < \ldots < x_n$ a grid on $[0,\ell]$
$G = \{x_i\}_{i=1}^{n}$

and "function values." $f: G \to \mathbb{R}$.
let $f_i := f(x_i) \Rightarrow \vec{f}$

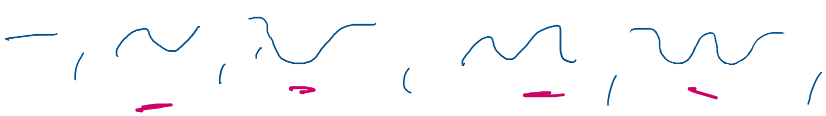


- connect dots if you like.

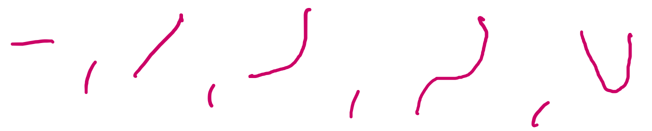
Ex: let $\langle\vec{f},\vec{g}\rangle = \sum_{k=1}^{n} f_k\,\overline{g_k}$

- this inner product space is "isomorphic" to vectors in $\mathbb{C}^n$.

- separable. there exists a ~~fin~~ countable basis B.
  Ex: $L^2([0,1])$ vs. $L^2(\mathbb{R})$

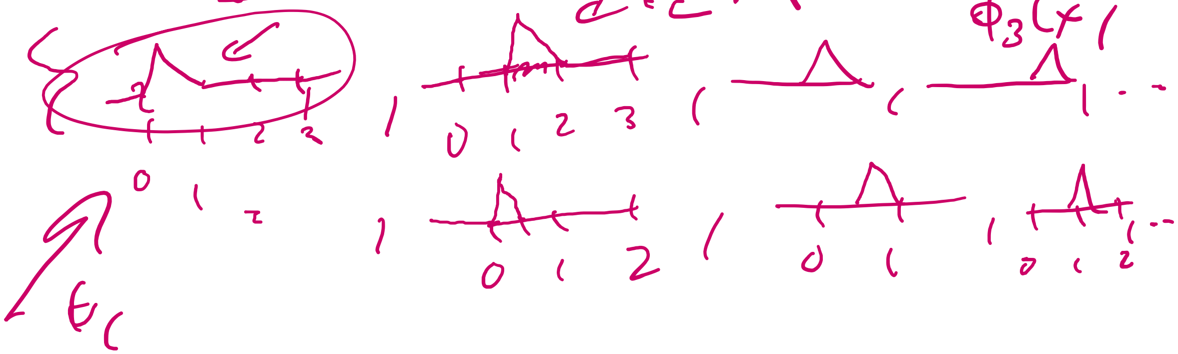
∘ $B = \{$  $\}$ $[0,1]$ Fourier $\Rightarrow$

Fourier $\{1, \sin x, \cos x, \sin 2x, \cos 2x, \ldots\}$

∘ $B' = \{$  $, \ldots\} = \{1, x, x^2, x^3, \ldots\}$

Taylor ... Legendre, Taylor.

$\phi_1(x)$ $\phi_3(x)$

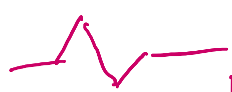
∘ $B'' = \{$  $, \ldots\}$

Wavelet.

ϕ_1

$f(x) \in L^2(\mathbb{R})$,

$f(x) = \sum a_i \phi_i(x)$; $a_i = \dfrac{\langle f, \phi_i(x)\rangle}{\|\phi_i(x)\|}$

∘  Haar....

On Compressed Sensing and on to Sparsity

$$f(x) = \sin x + 3\sin 3x + 4\sin 7x \in L^2[0,\pi]$$

$$= \sum_{n=1}^{\infty} a_n \sin nx \qquad \frac{\sin kx}{k}$$

$$\hat{f}(x) = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 3 \\ 0 \\ 0 \\ 0 \\ 4 \\ 0 \\ \vdots \end{pmatrix}$$

$$; f(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \cdots$$

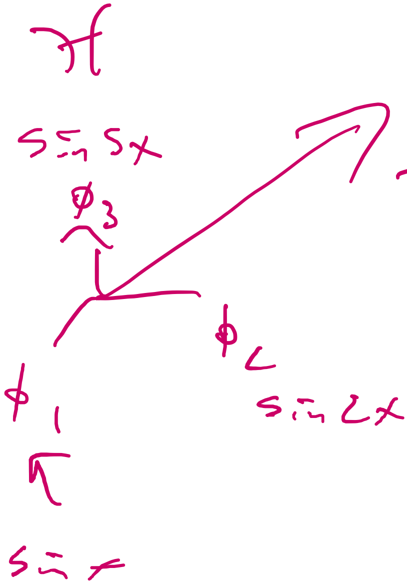
$$+ 3\left(3x - \frac{(3x)^3}{3!} + \frac{(3x)^5}{5!} - \cdots\right)$$

$$+ 4\left(7x - \frac{(7x)^3}{3!} + \frac{(7x)^5}{5!} + \cdots\right)$$

$$\hat{f}_T = \begin{pmatrix} 38 \\ 0 \\ c_3 \\ 0 \\ c_5 \\ \vdots \end{pmatrix}$$

$$= 38x - \left(\frac{1}{3!} + \frac{3^3}{3!} + \frac{4 \cdot 7^3}{3!}\right)x^3 + \cdots$$

c_3



$$f = \underline{\sin} x + 3 \underline{\sin} 3x + 4 \sin \underline{7x}$$

- a vector $v \in E$ is k-sparse if $[v]$ has exactly k-nonzero values, and $k < \dim(E)$

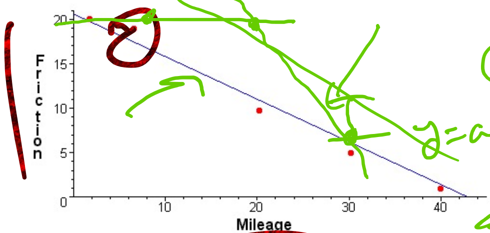
On Moore Penrose Pseudo Inverse, Matrix Least Squares, Geometric Least Squares.

Example

An engineer is tracking the friction index over mileage of a breaking system of a vehicle. She expects that the mileage-friction relationship is approximately linear. She collects five data points that are show in the table below.

Mileage	2000	6000	20,000	30,000	40,000
Friction Index	20	18	10	6	2

The graph below shows these points



We are interested in the line that best fits the data. More specifically, if **b** is the vector of friction index data values and **y** is the vector consisting of y values when we plug in the mileage data for x and find y by the equation of the line, then we want the line that minimizes the distance between **b** and **y**. If the equation of the line is

$$ax + b = y$$

then we get the five equations

$$\begin{aligned} 2a + b &= 20 \\ 6a + b &= 18 \\ 20a + b &= 10 \\ 30a + b &= 6 \\ 40a + b &= 2 \end{aligned}$$

The corresponding matrix equation is

$$Ax = y$$

or

$$\begin{pmatrix} 2 & 1 \\ 6 & 1 \\ 20 & 1 \\ 30 & 1 \\ 40 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 20 \\ 18 \\ 10 \\ 6 \\ 2 \end{pmatrix}$$

Although this does not have an exact solution, it does have a closest solution. We have

$$\begin{pmatrix} a \\ b \end{pmatrix} = (A^T A)^{-1} A^T \mathbf{b} = \begin{pmatrix} -0.48 \\ 20.6 \end{pmatrix}$$

We can conclude that the equation of the regression line is

$$y = -0.48x + 20.6$$

$$J(a,b) = \sum_{i=1} \| y_i - (ax_i + b) \|_2^2$$

$(2000, 20)$

$y = ax + b$

$= (x_i, y_i)$

$y_i = ax_i + b$

$y = ax + b = ax + b \cdot 1$

$2 \cdot a + 1 \cdot b = 20$

$6 \cdot a + 1 \cdot b = 18$

$Ax = y$

$x = \begin{pmatrix} a \\ b \end{pmatrix}$

wish

$x = A^{-1} y$

$x = A^{+} y$ vs A^T

Least Squares

Definition and Derivations

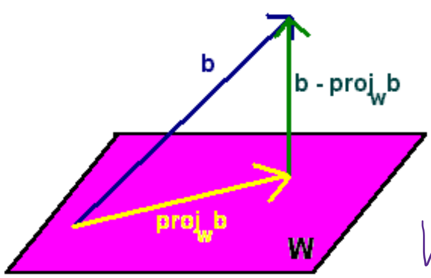
We have already spent much time finding solutions to

$$\mathbf{Ax} = \mathbf{b}$$

If there isn't a solution, we attempt to seek the $\mathbf{x}$ that gets closest to being a solution. The closest such vector will be the $\mathbf{x}$ such that

$$\mathbf{Ax} = \mathrm{proj}_W \mathbf{b}$$

where W is the column space of A.



$W = \mathrm{col}(A)$

Notice that $\mathbf{b} - \mathrm{proj}_W\mathbf{b}$ is in the orthogonal complement of W hence in the null space of A^T. Hence if $\mathbf{x}$ is a this closest vector, then

$$A^T(\mathbf{b} - A\mathbf{x}) = 0 \qquad A^TA\mathbf{x} = A^T\mathbf{b}$$

Now we need to show that A^TA nonsingular so that we can solve for $\mathbf{x}$.

Lemma

If A is an m x n matrix of rank n, then A^TA is nonsingular.

$$\underbrace{\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & & \\ a_{31} & & & \\ \vdots & & & \\ a_{m1} & \cdots & \cdots & a_{mn} \end{pmatrix}}_{m \times n} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{pmatrix}$$

m - eqns

n - unknowns

x

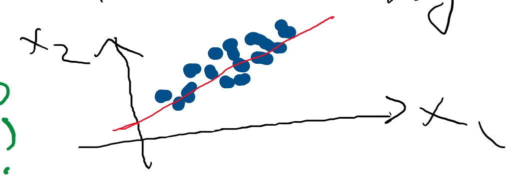
$\Longleftrightarrow$ $a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n = b_1$

$\vdots$

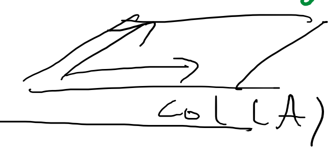
$a_{m1}x_1 + a_{m2}x_2 + \dots + a_{mn}x_n = b_n$

$m > n$ tall skinny, $n = 2$

How many?



How many?



$$x_1 \begin{pmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{m1} \end{pmatrix} + x_2 \begin{pmatrix} a_{12} \\ \vdots \\ a_{m2} \end{pmatrix} + \dots + x_n \begin{pmatrix} a_{1n} \\ \vdots \\ a_{mn} \end{pmatrix} = \begin{pmatrix} b_1 \\ \vdots \\ b_m \end{pmatrix}$$

Theorem

Let A be an m x n matrix or rank n, then the system

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

has the unique *least squares* solution

$$\hat{\mathbf{x}} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{b}$$

$(A^TA)^{-1}$ - never form that

$\underset{m\times n}{Ax=b}$

• Square & nonsing.

$x = A^{-1}b$ uniquely.

A^{-1} d.n.e.

• Not, $m > n$

$\underset{n\times n}{A^TA}\,x = \underset{n\times m}{A^T}b$ "normal equations"

Covariance matrix (if demeaned.)

Example

Find the least squares solution to

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

with

$$A = \begin{pmatrix} 1 & 3 \\ 2 & 4 \\ 1 & 6 \end{pmatrix} \qquad \mathbf{b} = \begin{pmatrix} 4 \\ 1 \\ 3 \end{pmatrix}$$

Solution

$m > n$ - tall skinny

We can quickly check that A has rank 2 (the first two rows are not multiples of each other). Hence we can compute

$$\mathbf{x} = (A^TA)^{-1}A^T\mathbf{b} = \begin{pmatrix} -0.377 \\ .662 \end{pmatrix}$$

$$\left(\begin{pmatrix} 1 & 2 & 1 \\ 3 & 4 & 6 \end{pmatrix}^T \begin{pmatrix} 1 & 3 \\ 2 & 4 \\ 1 & 6 \end{pmatrix}\right)^{-1} \begin{pmatrix} 1 & 2 & 1 \\ 3 & 4 & 6 \end{pmatrix} \begin{pmatrix} 4 \\ 1 \\ 3 \end{pmatrix}$$

Notice that

$$A\mathbf{x} = \begin{pmatrix} 1.61 \\ 1.90 \\ 3.60 \end{pmatrix}$$

not exactly **b**, but as close as we are going to get.

Matrix Formulation of LS slick for general Models

Best Fitting Curves

Often, a line is not the best model for the data. Fortunately the same technique works if we want to use other nonlinear curves to fit the data. Here we will explain how to find the least squares cubic. The process for other polynomials is similar.

Example

A bioengineer is studying the growth of a genetically engineered bacteria culture and suspects that is it approximately follows a cubic model. He collects six data points listed below

Time in Days	1	2	3	4	5	6
Grams	2.1	3.5	4.2	3.1	4.4	6.8

He assumes the equation has the form

$$ax^3 + bx^2 + cx + d = y$$

Grams = f(time)

y = f(x)

This gives six equations with four unknowns

$$\begin{aligned} a + b + c + d &= 2.1 \\ 8a + 4b + 2c + d &= 3.5 \\ 27a + 9b + 3c + d &= 4.2 \\ 64a + 16b + 4c + d &= 3.1 \\ 125a + 25b + 5c + d &= 4.4 \\ 216a + 36b + 6c + d &= 6.8 \end{aligned}$$

$$2.1 = a\cdot 1^3 + b\cdot 1^2 + c\cdot 1 + d \qquad i = 1$$

$$3.5 = a\cdot 2^3 + b\cdot 2^2 + c\cdot 2 + d \qquad i = 2$$

The corresponding matrix equation is

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 8 & 4 & 2 & 1 \\ 27 & 9 & 3 & 1 \\ 64 & 16 & 4 & 1 \\ 125 & 25 & 5 & 1 \\ 216 & 36 & 6 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} 2.1 \\ 3.5 \\ 4.2 \\ 3.1 \\ 4.4 \\ 6.8 \end{pmatrix}$$

$$\begin{pmatrix} x_1^3 & x_1^2 & x_1 & 1 \\ x_2^3 & x_2^2 & x_2 & 1 \\ \vdots & \vdots & \vdots & \vdots \\ x_n^3 & x_n^2 & x_n & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

$$\underbrace{X}_{A}\ \underbrace{\beta}_{x} = \underbrace{y}_{b}$$

$$Ax = b \qquad X\beta = y$$

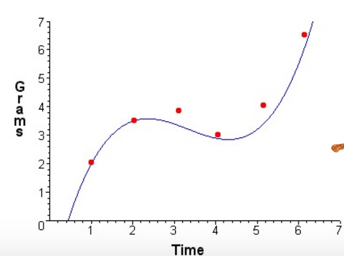
We can use the least squares equation to find the best solution

$$\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = (A^T A)^{-1} A^T \mathbf{b} = \begin{pmatrix} 0.2 \\ -2.0 \\ 6.1 \\ -2.3 \end{pmatrix}$$

So that the best fitting cubic is

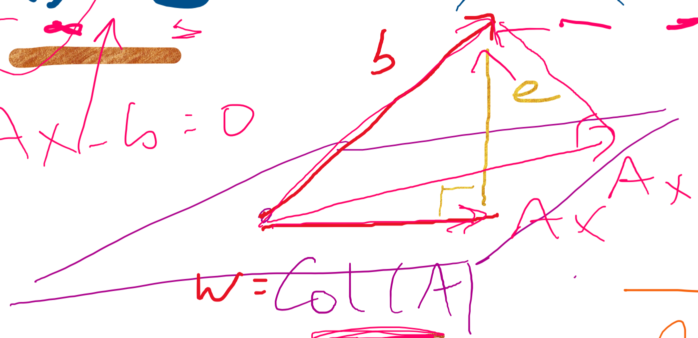
$$y = 0.2x^3 - 2.0x^2 + 6.1x - 2.3$$

The graph is shown below



$Ax = b$ $\Rightarrow$ $x_1 \vec{a}_1 + x_2 \vec{a}_2 + \dots + x_n \vec{a}_n = \vec{b}$

$Ax - b = 0$



$A\tilde{x} = \text{proj}_W b$; $\tilde{x} = \underset{x}{\text{argmin}} \|Ax - b\|_2^2$ (e over $Ax-b$)

$\Rightarrow$ LS solution

$W = \text{Col}(A)$

Recall $u \perp v$ iff $u \cdot v = u^T v = 0$

v vs. v

$u \cdot v = \|u\|\|v\| \cos\theta$

$\vec{e} = A\tilde{x} - b$

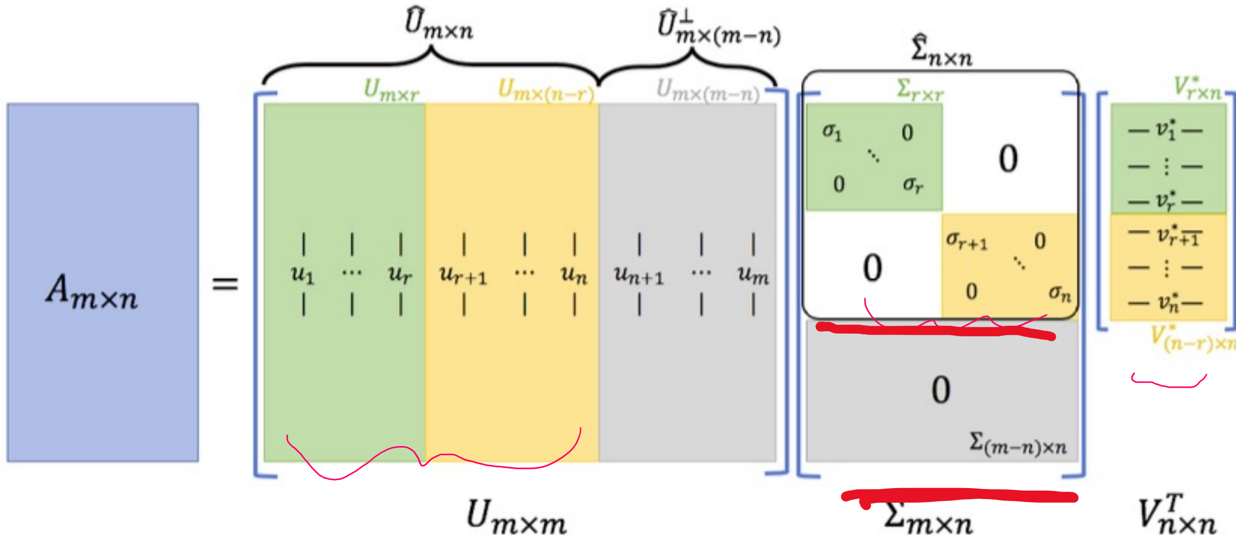
$\Rightarrow$ $A^T(A\tilde{x} - b) = 0 \Longleftrightarrow$

$$\begin{pmatrix} -a_1' - \\ -a_2' - \\ \vdots \\ -a_n' - \end{pmatrix}(Ax - b) = 0 \text{ "} \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \text{"}$$

$A^T(Ax - b) = 0$

$\Rightarrow \vec{a}_i \perp (A\tilde{x} - b) \ \forall i$

$\Rightarrow (A\tilde{x} - b) \perp$ every vector in $\text{Col}(A) \Longleftrightarrow$ Solve "normal eqns" $A^T A \tilde{x}$ $A^T b$



$$(\hat V\hat\Sigma^T\cancel{\hat U^T})(\hat U\hat\Sigma\hat V^T)\tilde x$$

$$\hat V\hat\Sigma^T\hat\Sigma\hat V^T\tilde x = \hat V\hat\Sigma^T\hat U^T b$$

$$(\hat\Sigma^T\hat\Sigma)V^T\tilde x = \hat\Sigma^T U^T b$$

$$\cancel{V V^T}\tilde x = V(\hat\Sigma^T\hat\Sigma)^{-1}\hat\Sigma^T U^T b$$

$$\boxed{\tilde x = V\underbrace{(\hat\Sigma^T\hat\Sigma)^{-1}\hat\Sigma^T U^T}_{A^+} b}$$

$$A^T A x = A^T b$$

$$A_{m\times n} = \hat U_{m\times n}\hat\Sigma_{n\times n}\hat V^T_{n\times n}$$

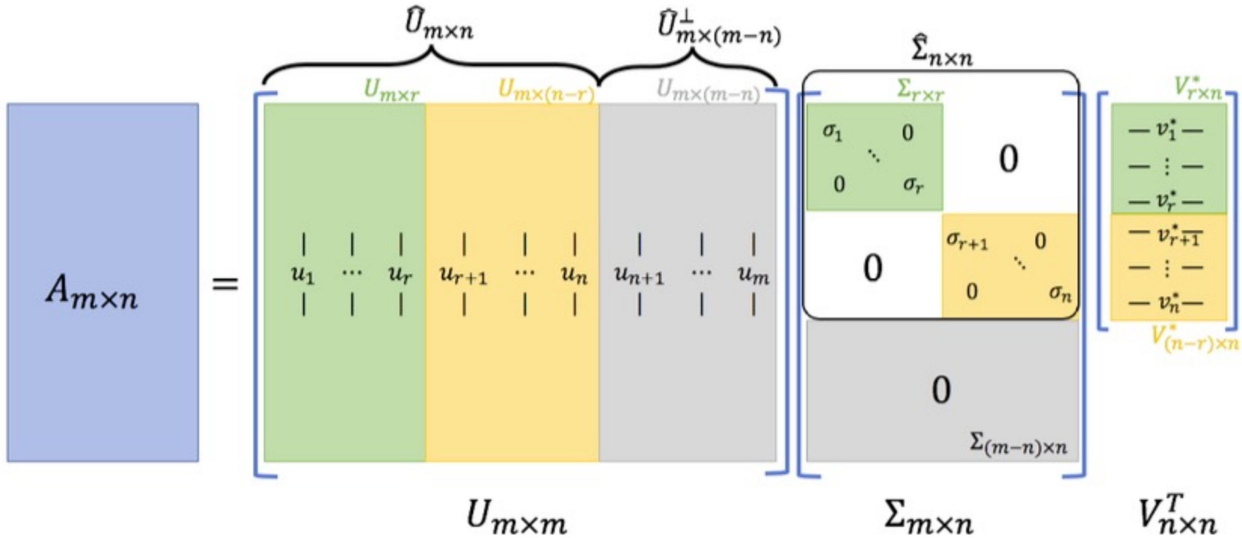
$$= \begin{bmatrix} | & | & & | \\ u_1 & u_2 & \dots & u_n \\ | & | & & | \end{bmatrix} \underbrace{\begin{bmatrix} \sigma_1 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_n \end{bmatrix}}_{\hat\Sigma} \begin{bmatrix} - & v_1^T & - \\ - & v_2^T & - \\ & \vdots & \\ - & v_n^T & - \end{bmatrix}$$

$\hat\Sigma^T\hat\Sigma$:

σ_1^2 … σ_{r+1}^2 … σ_n

when exist

>0 $=0$



$$
\begin{aligned}
A_{m\times n} &= \hat{U}_{m\times n}\hat{\Sigma}_{n\times n}\hat{V}^T_{n\times n} \\
&= \begin{bmatrix} | & | & & | \\ u_1 & u_2 & \dots & u_n \\ | & | & & | \end{bmatrix}
\begin{bmatrix} \sigma_1 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_n \end{bmatrix}
\begin{bmatrix} - & v_1^T & - \\ - & v_2^T & - \\ - & \vdots & - \\ - & v_n^T & - \end{bmatrix}
\end{aligned}
$$

$\hat{\Sigma}^+ = (\hat{\Sigma}^T\hat{\Sigma})^{-1}\hat{\Sigma}$

if $\hat{\Sigma}$ is invertible

- if $r = n$

if $\sigma_i > 0$ $1 \le i \le n$

- But if $r < n$

$\sigma_r > 0,\ \sigma_{r+1} = 0$

$(\hat{\Sigma}^T\hat{\Sigma}) = \begin{pmatrix} 1/\sigma_1^2 & & & 0 \\ & \ddots & & \\ & & 1/\sigma_r^2 & \\ 0 & & & \ddots \end{pmatrix}$

" $= \frac{1}{0}$ "

$\boxed{\text{" } \frac{1}{0} \text{ " } := 0}$

" $= 1/\sigma$ "

LS soln = solve normal equations

$$A^T A \tilde{x} = A^T b$$

When inverse exists

$$\tilde{x} = (A^T A)^{-1} A^T b$$

$$= A^+ b$$

Moore-Penrose ; Pseudo-Inverse

A^+

$Ax = b$

- In terms of SVD?
- and what if inverse doesn't exist.

$$A = U\Sigma V^T \qquad \Sigma^+ := (\Sigma^T\Sigma)^{-1}\Sigma$$

$$Ax = b$$

$$U^T \cancel{U} \Sigma V^T x = U^T b$$

$$(\Sigma^T \Sigma) V^T x = \Sigma^T V^T b$$

$$V^T x = (\Sigma^T \Sigma)^{-1} \Sigma^T U^T b$$

$$= \Sigma^{-1} \cancel{\Sigma^{T-1}} \cancel{\Sigma^T} U^T b$$

$$= \Sigma^{-1} U^T b$$

$$x = \underbrace{V \Sigma^{-1}}_{A^{-1}} U^T b := \underbrace{V \Sigma^+ U^T}_{A^+} b \quad \text{if exists}$$

$$= \begin{pmatrix} 1/\sigma_1 & & & \\ & \ddots & & \\ & & 1/\sigma_r & \\ & & & 0 \\ & & & & \ddots \\ & & & & & 0 \end{pmatrix}$$

$\sigma_r \neq 0$

$\sigma_{r+1} = 0 \Rightarrow$ "$\frac{1}{0} = 0$"

..

n

if