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Applications of the SVD

(1) Rank-k approximation

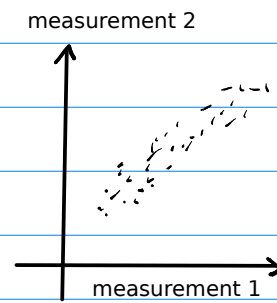
$$A = \begin{pmatrix} | & | & | \\ \hline & & \\ \hline | & | & | \end{pmatrix} \begin{pmatrix} \sigma_1 & & \\ & \sigma_2 & \\ & & \ddots \end{pmatrix} \begin{pmatrix} \hline \hline \hline \\ \hline \hline \hline \end{pmatrix}$$

$U \quad \Sigma \quad V^T$

$$\approx \sigma_1 \underbrace{\vec{u}_1 \vec{v}_1^T} + \sigma_2 \underbrace{\vec{u}_2 \vec{v}_2^T} + \dots +$$

(4) Principal Component Analysis ("PCA")

Have: a pile of "data"
 More precisely: m 'measurements' from n 'trials'
 each resulting in a real number
 $x_{ij} \quad i=1 \dots m \quad j=1 \dots n$



Data matrix: $X = (x_{ij}) = \begin{pmatrix} | & | & | & | & | \\ | & | & | & | & | \\ | & | & | & | & | \end{pmatrix}$
 \downarrow i : measurements
 \rightarrow j : trials

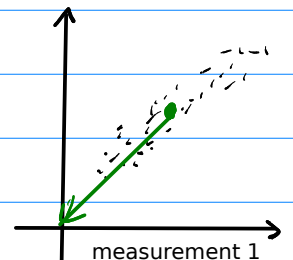
Want: Underlying relationships between measurements
 "If measurement i changes by amount x , then I want to be able to predict that measurement i' will change by an amount I can compute from x ."

How do I compute a PCA?

(1) Compute an estimate of the mean: $u_i = \frac{1}{n} \sum_{j=1}^n x_{ij}$
 measurement 2

(2) "Remove" the means: $y_{ij} = x_{ij} - u_i$

$\rightarrow Y[i,j]$ have mean zero



(3) Compute (an estimate of) the covariance matrix:

$$C_{i_1 i_2} = \frac{1}{n-1} \sum_{j=1}^n y_{i_1 j} y_{i_2 j} \quad C = Y \cdot Y^T$$

$$(AB)_{ij} = \sum_k A_{ik} B_{kj}$$

\uparrow unbiased estimate of the cov. matrix

How do I compute a PCA? (cont'd)

(4) Diagonalize the covariance matrix (sym.pos.def.)

$$C = U \overset{\text{diagonal}}{\Sigma^2} U^T$$

$$\Sigma^2 = U^T C U \quad \text{orthogonal}$$

$$C = \frac{1}{n-1} Y Y^T = U \Sigma^2 U^T$$

$$C = \frac{1}{n-1} Y Y^T = U \Sigma V^T V \Sigma U^T$$

(5) Transform the data into their "principal components"

Find a V so that

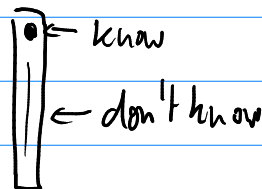
$$\frac{1}{\sqrt{n-1}} Y = U \underbrace{\Sigma V^T}_{\text{determines a linear combination of the columns of } U}$$

-> PCA can be computed by taking the SVD of

$$\frac{1}{\sqrt{n-1}} Y$$

columns of U are the "principal components"

$$\frac{1}{\sqrt{n-1}} Y \approx \sigma_1 u_1 v_1^T$$



(6) "Total" least squares

For a given matrix A , find the vector x so that

- $\|Ax\|_2$ is minimal

- $\|x\|_2 = 1$

$$A = \begin{pmatrix} u_1 & u_2 \\ | & | \\ | & | \\ | & | \\ | & | \end{pmatrix} \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_{n-1} \\ & & & 0 \end{pmatrix} \begin{pmatrix} -v_1 \\ \vdots \\ -v_n \end{pmatrix}$$

$$\|v_n\|_2 = 1 \quad \checkmark$$

$$\begin{aligned} \|Av_n\|_2 &= \left\| \begin{pmatrix} u_1 & u_2 \\ | & | \\ | & | \\ | & | \\ | & | \end{pmatrix} \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_{n-1} \\ & & & 0 \end{pmatrix} \begin{pmatrix} -v_1 \\ \vdots \\ -v_n \end{pmatrix} \right\|_2 \\ &= \left\| \begin{pmatrix} u_1 & u_2 \\ | & | \\ | & | \\ | & | \\ | & | \end{pmatrix} \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_{n-1} \\ & & & 0 \end{pmatrix} \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix} \right\|_2 \\ &= \left\| \begin{pmatrix} u_1 & u_2 \\ | & | \\ | & | \\ | & | \\ | & | \end{pmatrix} \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix} \right\|_2 = 0 \end{aligned}$$

In this case, but also in general: v_n is the solution to TLS

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Function Spaces

What is interpolation?

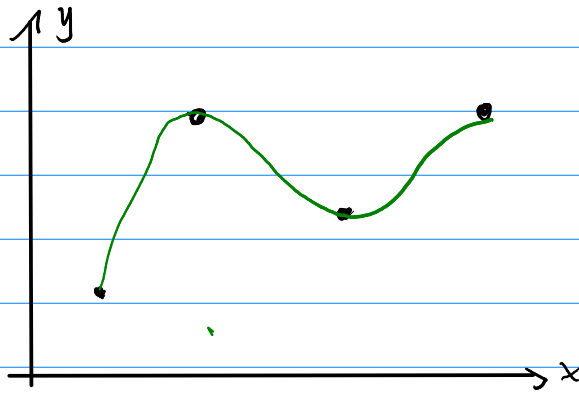
$1 \quad x \quad x^2 \quad \dots \quad x^{n-1}$

$\downarrow \quad \downarrow \quad \downarrow \quad \swarrow$

Given a basis of functions

$\varphi_1, \dots, \varphi_n$

match the data points



given

x	y
x_1	y_1
x_2	y_2
\vdots	\vdots
x_m	y_m

But there are lots of possible functions through those points. Be more precise.

$$V = \begin{pmatrix} \overset{x_1}{\varphi_1(x_1)} & \dots & \overset{x_n}{\varphi_n(x_1)} \\ \vdots & & \vdots \\ \varphi_1(x_n) & & \varphi_n(x_n) \end{pmatrix}$$

$$V \vec{\alpha} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

$$\rightarrow \alpha_1 \varphi_1(x) + \dots + \alpha_n \varphi_n(x) = f(x)$$

$$\alpha_1 \varphi_1'(x) + \dots + \alpha_n \varphi_n'(x) = f'(x)$$

$$V \cdot \begin{pmatrix} \text{basis} \\ \text{coeffs} \end{pmatrix} = \begin{pmatrix} \text{function} \\ \text{values} \end{pmatrix} \rightsquigarrow V^{-1} \begin{pmatrix} \text{function} \\ \text{values} \end{pmatrix} = \begin{pmatrix} \text{basis} \\ \text{coeffs} \end{pmatrix}$$

$$V' = \begin{pmatrix} \overset{x_1}{\varphi'_1(x_1)} & \dots & \varphi'_n(\tilde{y}_1) \\ \vdots & & \vdots \\ \varphi'_1(x_n) & & \varphi'_n(x_n) \end{pmatrix}$$

$$V' \begin{pmatrix} \text{coeffs} \end{pmatrix} = \begin{pmatrix} \text{function values of the derivative} \end{pmatrix}$$

$$\underbrace{V' \quad V^{-1}}_{\text{coeffs}} \begin{pmatrix} \text{point values} \end{pmatrix}$$

function values of the derivative

in class:

$$\varphi_0(x) = 1$$

$$\varphi_1(x) = x$$

$$\varphi_2(x) = x^2$$

$$\varphi_3(x) = x^3$$

$$V = \begin{pmatrix} \varphi_1(x_1) & \dots & \varphi_n(x_1) \\ \vdots & & \vdots \\ \varphi_1(x_n) & & \varphi_n(x_n) \end{pmatrix}$$

$$V \vec{x} = \vec{y}$$