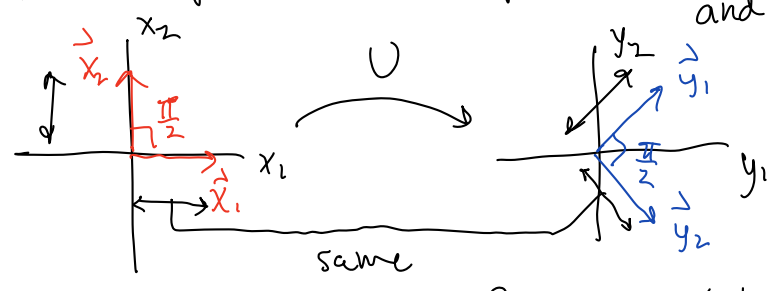


Q: non-square orthonormal matrices?

Learning objectives

- ① Tall orthonormal matrices, U , have $U^T U = I$
- ② Orthonormal transforms preserve inner products (and therefore lengths) and angles in \mathbb{R}^n



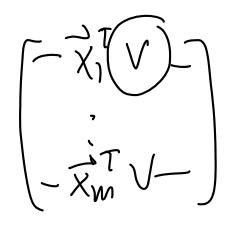
$\langle \vec{x}, \vec{y} \rangle = \|\vec{x}\| \|\vec{y}\| \cos \theta$

- ③ Least squares problem and solution from a particular perspective: If some factorization of a matrix, X , into $U \Sigma V^T$ exists, we can solve least squares really quickly. (U, V orthonormal, Σ diagonal)

★ This is a preview. You'll get more in lecture on Thursday and next week.

Some dependencies/reference sheet

- 1 • $\langle \vec{x}, \vec{y} \rangle = \vec{x}^T \vec{y} = \vec{y}^T \vec{x}$ (inner product) $\vec{x}, \vec{y} \in \mathbb{R}^n$
- 2 • $(AB)^T = B^T A^T$ (transpose of matrix product)
 - (to prove ↑ write columns of A , and rows of B and AB in terms of those vectors)
- 3 • $\|\vec{x}\|^2 = \langle \vec{x}, \vec{x} \rangle = \vec{x}^T \vec{x}$ (norm/magnitude/length in terms of inner product)
- 4 • $A \begin{bmatrix} \frac{1}{\|\vec{v}_1\|} \vec{v}_1 & \frac{1}{\|\vec{v}_2\|} \vec{v}_2 & \dots & \frac{1}{\|\vec{v}_n\|} \vec{v}_n \end{bmatrix} = \begin{bmatrix} A \frac{1}{\|\vec{v}_1\|} \vec{v}_1 & \dots & A \frac{1}{\|\vec{v}_n\|} \vec{v}_n \end{bmatrix}$
 - $\begin{bmatrix} -\vec{w}_1^T & - & - \\ -\vec{w}_2^T & - & - \\ \vdots & & \vdots \\ -\vec{w}_n^T & - & - \end{bmatrix} A = \begin{bmatrix} -\vec{w}_1^T A & - & - \\ -\vec{w}_2^T A & - & - \\ \vdots & & \vdots \\ -\vec{w}_n^T A & - & - \end{bmatrix}$
 - (How matrix multiplication affects columns and rows to the right and left respectively)
- 5 • $A \vec{x} \approx \vec{b} \rightarrow \hat{\vec{x}} = (A^T A)^{-1} A^T \vec{b}$ (least squares solution)
- $\hat{\vec{b}} = A (A^T A)^{-1} A^T \vec{b}$ (least squares projection)



EECS 16B Designing Information Devices and Systems II
 Fall 2021 Discussion Worksheet Discussion 9B

The following notes are useful for this discussion: **Note 14**

1. Orthonormality and Least Squares

(a) Let U be an $m \times n$ matrix with orthonormal columns, with $m \geq n$. Compute $U^T U$. How does this change if $m < n$?

$U = \begin{bmatrix} | & | & \dots & | \\ u_1 & u_2 & \dots & u_n \\ | & | & \dots & | \end{bmatrix}$
 $U^T U = I$
 $(U^T U)_{ij} = \vec{u}_i^T \vec{u}_j = \begin{cases} 1 & i=j \\ 0 & i \neq j \end{cases}$

$\vec{u}_i \in \mathbb{R}^m$
 U is tall or square ($m > n$) ($m = n$)

$U^T = \begin{bmatrix} - & \vec{u}_1^T & - \\ - & \vec{u}_2^T & - \\ - & \dots & - \\ - & \vec{u}_n^T & - \end{bmatrix}$

$U = \begin{bmatrix} \square & | \\ \square & | \end{bmatrix}$ $m < n$
 If we have m orthonormal columns \rightarrow forms a basis
 No other directions in \mathbb{R}^m
 $U^T U$ not identity ($m < n$)

these columns are repeats of first m or \vec{e}_i
 wide

square

(b) Suppose you have a real, square, $n \times n$ orthonormal matrix U (the columns of U are unit norm and mutually orthogonal). You also have real vectors $\vec{x}_1, \vec{x}_2, \vec{y}_1, \vec{y}_2$ such that

$U \vec{x} \rightarrow \vec{y}$
 $\vec{y}_1 = U \vec{x}_1$
 $\vec{y}_2 = U \vec{x}_2$
 $\vec{x}_1, \vec{x}_2, \vec{y}_1, \vec{y}_2 \in \mathbb{R}^n$

Calculate $\langle \vec{y}_1, \vec{y}_2 \rangle = \vec{y}_2^T \vec{y}_1 = \vec{y}_1^T \vec{y}_2$ in terms of $\langle \vec{x}_1, \vec{x}_2 \rangle = \vec{x}_2^T \vec{x}_1 = \vec{x}_1^T \vec{x}_2$.

$\langle \vec{x}_1, \vec{y}_2 \rangle = \vec{y}_2^T \vec{y}_1 = \left(U \vec{x}_2 \right)^T \left(U \vec{x}_1 \right)$

$= \vec{x}_2^T U^T U \vec{x}_1$

$= \vec{x}_2^T (I) \vec{x}_1$

$= \vec{x}_2^T \vec{x}_1 = \langle \vec{x}_2, \vec{x}_1 \rangle = \langle \vec{x}_1, \vec{x}_2 \rangle$

rotation

if inner products tell us about length $(\sqrt{\langle \vec{v}, \vec{v} \rangle}) = \|\vec{v}\|$

and angles between vectors \vec{v}

$\langle \vec{v}, \vec{w} \rangle = \|\vec{v}\| \|\vec{w}\| \cos \theta$ angle between \vec{v} & \vec{w}

Think: reflections or rotations

then orthonormal matrices/transformation preserve these quantities

(c) Following the previous question, express $\|\vec{y}_1\|_2^2$ and $\|\vec{y}_2\|_2^2$ in terms of $\|\vec{x}_1\|_2^2$ and $\|\vec{x}_2\|_2^2$.

$$\langle \vec{y}_1, \vec{y}_1 \rangle = \|\vec{y}_1\|_2^2$$

$$\langle \vec{x}_1, \vec{x}_1 \rangle = \|\vec{x}_1\|_2^2$$

$$\|\vec{y}_2\|_2^2 = \|\vec{x}_2\|_2^2$$

$$\|\vec{y}_2\|_2 = \|\vec{x}_2\|_2$$

$$\langle \vec{x}, \vec{x} \rangle = \sum_{i=1}^n x_i^2$$

(interpretation: U doesn't change lengths of vectors)

(d) Suppose you observe data coming from the model $y_i = \vec{a}^T \vec{x}_i$, and you want to find the linear scale-parameters (each a_i). We are trying to learn the model \vec{a} . You have m data points (\vec{x}_i, y_i) , with each $\vec{x}_i \in \mathbb{R}^n$. Note that \vec{x}_i refers to the i -th vector, not the i -th element of a single vector. Each \vec{x}_i is a different input vector that you take the inner product of with \vec{a} , giving a scalar y_i .

Set up a least squares formulation for estimating \vec{a} , and find the solution to the least squares problem.

want to find this

$$\vec{a} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}$$

$$\vec{a}^T = [a_1 \ a_2 \ \dots \ a_n]$$

$$\vec{x}_i \in \mathbb{R}^n$$

$y_1 = \vec{a}^T \vec{x}_1$
 $y_2 = \vec{a}^T \vec{x}_2$
 $y_3 = \vec{a}^T \vec{x}_3$
 $y_m = \vec{a}^T \vec{x}_m$

(\vec{x}_1, y_1) scalar
 $(\vec{x}_2, y_2) \dots (\vec{x}_m, y_m)$

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} = \begin{bmatrix} \vec{a}^T \vec{x}_1 \\ \vdots \\ \vec{a}^T \vec{x}_m \end{bmatrix} = \begin{bmatrix} \vec{x}_1^T \vec{a} \\ \vdots \\ \vec{x}_m^T \vec{a} \end{bmatrix}$$

$$\vec{a}^T \begin{bmatrix} \vec{x}_1 \\ \vec{x}_2 \\ \vdots \\ \vec{x}_m \end{bmatrix} = [\dots]$$

Least squares problem:
 Find \vec{a} that minimizes the error norm squared:
 $\|X\vec{a} - \vec{y}\|^2$

$$\vec{y} = X\vec{a}$$

$$\vec{a} = (X^T X)^{-1} X^T \vec{y}$$

Call this X (least square solution)

(e) Now suppose V is an orthonormal square matrix, and rather than observing $\vec{a}^T \vec{x}$ directly, we actually observe data points that result from our inputs being transformed by V^T as follows:

$$\vec{\tilde{x}} = V^T \vec{x} \rightarrow \vec{\tilde{x}}^T = \vec{x}^T (V^T)^T = \vec{x}^T V \quad (1)$$

That is, our model acts on the modified input data $\vec{\tilde{x}}_i$, so the data points we collected are now $(\vec{\tilde{x}}_i, y_i)$. We must now consider the new model:

$$y_i = \vec{a}^T \vec{\tilde{x}}_i \quad (2)$$

$$= \tilde{a}^T V^T \tilde{x}_i \tag{3}$$

Set up a least-squares formulation for \tilde{a} . How is \tilde{a} related to \hat{a} ?

$$\begin{aligned} \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix} &= \begin{bmatrix} \tilde{x}_1^T \tilde{a} \\ \vdots \\ \tilde{x}_m^T \tilde{a} \end{bmatrix} = \begin{bmatrix} \tilde{x}_1^T \\ \vdots \\ \tilde{x}_m^T \\ X \end{bmatrix} \tilde{a} = \begin{bmatrix} -\tilde{x}_1^T V \\ -\tilde{x}_2^T V \\ \vdots \\ -\tilde{x}_m^T V \end{bmatrix} \tilde{a} \\ &= \underbrace{\begin{bmatrix} -\tilde{x}_1^T \\ \vdots \\ -\tilde{x}_m^T \end{bmatrix}}_{X \text{ in } \mathcal{d}} V \tilde{a} \end{aligned}$$

$$\tilde{X} = X V \leftarrow$$

\tilde{a} (solution, minimizes $\|\tilde{X}\tilde{a} - \tilde{y}\|^2$)

$$\tilde{a} = (X^T X)^{-1} X^T \tilde{y}$$

V is a orthonormal square matrix
then V is invertible

$$\begin{aligned} \tilde{a} &= ((XV)^T (XV))^{-1} (XV)^T \tilde{y} \\ &= (V^T X^T X V)^{-1} V^T X^T \tilde{y} \\ &= V^{-1} (X^T X)^{-1} (V^T)^{-1} V^T X^T \tilde{y} \end{aligned}$$

can compute when X 's nullspace is only $\{0\}$ or alt. X has linear independent columns

$$\begin{aligned} &= V^{-1} (X^T X)^{-1} X^T \tilde{y} \\ &= V^T (X^T X)^{-1} X^T \tilde{y} = V^T \hat{a} \end{aligned}$$

$$(AB)^{-1} = B^{-1}A^{-1}$$

square, invertible

$$AB(B^{-1}A^{-1}) = A \underbrace{BB^{-1}}_I A^{-1} = I$$

$$V^T V = I \text{ (orthonormal } V \text{ matrix)}$$

$$V^T = V^{-1}$$

Compare \tilde{x}_i 's and \tilde{a} 's

$$\begin{aligned} \tilde{x}_i &= V^T x_i \\ \tilde{a} &= V^T \hat{a} \leftarrow \end{aligned}$$

Big picture!
When we transform our data (\tilde{x} vectors) \rightarrow least squares solution also ends up being transformed the same way

$$V = \begin{bmatrix} | & & | \\ \vec{v}_1 & \dots & \vec{v}_n \\ | & & | \end{bmatrix} \quad \Sigma = \begin{bmatrix} \sigma_1 & & \\ & \sigma_2 & \\ & & \dots \\ & & & \sigma_n \\ \hline & & & & 0_{m-n \times n} \end{bmatrix}$$

(f) Now suppose that we have the matrix

$$U = \begin{bmatrix} | & | & | \\ u_1 & u_2 & \dots & u_m \\ | & | & | \end{bmatrix}$$

$$\vec{u}_i \in \mathbb{R}^m \quad \begin{bmatrix} \vec{x}_1^T \\ \vec{x}_2^T \\ \vdots \\ \vec{x}_m^T \end{bmatrix} \triangleq X = U \Sigma V^T$$

$\vec{v}_i \in \mathbb{R}^n$
 $m \times m \quad m \times n \quad n \times n \approx m \times n$

where U is an $m \times m$ matrix, and V is an $n \times n$ matrix. Here, $\Sigma = \begin{bmatrix} \sigma_1 & 0 & \dots & 0 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_n & 0 & \dots & 0 \end{bmatrix}$.

Here we assume that we have more data points than the dimension of our space (that is, $m > n$). Also, the transformation V in part e) is the same V in this factorized representation.

Set up a least squares formulation for estimating \vec{a} and find the solution to the least squares. Is there anything interesting going on?

Note: Don't worry about how we would find U, Σ, V^T for now; assume that X has the given form and that U and V are orthonormal.

Hint: Start by substituting the factorized representation of X into the answer of the previous part.

$$\begin{aligned} \vec{\hat{a}} &\approx V^T \vec{\hat{a}} = V^T (X^T X)^{-1} X^T \vec{y} \quad X = U \Sigma V^T \\ &\approx V^T \left[(U \Sigma V^T)^T (U \Sigma V^T) \right]^{-1} (U \Sigma V^T)^T \vec{y} \\ &= V^T \left[V \Sigma^T U^T U \Sigma V^T \right]^{-1} V \Sigma^T U^T \vec{y} \\ &\approx V^T (V \Sigma^T \Sigma V^T)^{-1} V \Sigma^T U^T \vec{y} \\ &\approx \underbrace{V^T (V^T)^{-1}}_{(orthonormal) \text{ square matrix}} (\Sigma^T \Sigma)^{-1} \underbrace{V^{-1} V}_{I} \Sigma^T U^T \vec{y} \\ &= (\Sigma^T \Sigma)^{-1} \Sigma^T U^T \vec{y} \end{aligned}$$

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$$\begin{aligned}
 (\Sigma^T \Sigma)^{-1} &= \left(\left[\begin{array}{ccc|c} \sigma_1 & \sigma_2 & \dots & \sigma_n \\ \hline & & & 0_{n \times m-n} \end{array} \right] \left[\begin{array}{c} \sigma_1 \\ \sigma_2 \\ \dots \\ \sigma_n \\ \hline 0 \end{array} \right] \right)^{-1} \\
 &= \left(\left[\begin{array}{ccc} \sigma_1^2 & & \\ & \sigma_2^2 & \\ & & \dots \\ & & & \sigma_n^2 \end{array} \right] \right)^{-1} = \left[\begin{array}{ccc} \frac{1}{\sigma_1^2} & & \\ & \frac{1}{\sigma_2^2} & \\ & & \dots \\ & & & \frac{1}{\sigma_n^2} \end{array} \right]
 \end{aligned}$$

assume $\sigma_i \neq 0$ all i 's

$$\begin{aligned}
 \text{RSS} &= \left[\begin{array}{ccc} \frac{1}{\sigma_1^2} & & \\ & \dots & \\ & & \frac{1}{\sigma_n^2} \end{array} \right] \left[\begin{array}{ccc|c} \sigma_1 & \sigma_2 & \dots & 0 \\ \hline & & & \sigma_n \end{array} \right] U^T y
 \end{aligned}$$

$$= \left[\begin{array}{ccc|c} \frac{1}{\sigma_1} & & & 0 \\ & \dots & & \\ & & \frac{1}{\sigma_n} & \end{array} \right] U^T y \rightarrow \begin{bmatrix} \vec{u}_1^T y \\ \vdots \\ \vec{u}_m^T y \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1}{\sigma_1} \vec{u}_1^T y \\ \vdots \\ \frac{1}{\sigma_n} \vec{u}_n^T y \end{bmatrix}$$

Note! only inner products!

has the vibe of least squares with an orthonormal matrix $A!$ ($A^T A = I$)
 But didn't assume X was orthonormal ($A^T x \approx b$)
 $x = A^T b$

If we have some factorization for X that gives us orthonormal matrices

least squares is not computationally heavy

Q: $(\Sigma^T \Sigma)^{-1} \stackrel{?}{=} (\Sigma^{-1})(\Sigma^T)^{-1}$ A: No! Σ is not square!

Q: What is the name of the factorization?

$$X = U \Sigma V^T \quad \text{SVD}$$

$m \times n$ matrix U, V : orthonormal Σ : singular value decomposition

Q: $X^T X \rightarrow$ if X or $X^T X$ has lin. dep. cols
is $(X^T X)^{-1}$ computable?

A: No, need linearly independent columns of X .

$$X^T X \vec{a} = X^T \vec{y} \Leftrightarrow \text{always has a solution.}$$

BUT solution may not be unique. If so,

① To solve, find nullspace of $X^T X$

$$\vec{a}_N \in N(X^T X) \rightarrow X^T X (\vec{a}_s + \vec{a}_N) = X^T X \vec{a}_s = \vec{y}$$

(\vec{a}_s is a solution)

\uparrow find one solution

② Alternatively: Take X , run GS on its columns / delete lin. dep. columns \rightarrow get $\tilde{X} \rightarrow$ Do least squares: $\tilde{\vec{a}}$

$\tilde{\vec{a}} \rightarrow \vec{a}$ by adding appropriate zeroes / transformation