

Class 10: 10/9

Reminder: Midterm I is one week from today! Details TBA.

Outline:

- I. Projection onto spaces
- II. Least Squares approximation.
- III. Orthogonal matrices + Gram Schmidt.

I. See yesterday's notes.

II. Say we can't solve $A\vec{x} = \vec{b}$ ($\vec{b}$ is not in the column space of A)

What do we do instead?

* Instead, solve $ATA\hat{x} = A^T\vec{b}$.

Why? We want to find $\hat{x}$ so that $A\hat{x}$ is as close to $\vec{b}$ as possible.

That is, if $\vec{e} = A\hat{x} - \vec{b}$, we want to minimize $\|\vec{e}\|$, and find the vector in the column space of A closest to $\vec{b}$.

* This is the projection of $\vec{b}$ onto the column space of A .

The solution $\hat{x}$ that minimizes $\|\vec{e}\|$ is called the least squares solution.

Applications

Fitting data:

Example: Find the best fit line for the points $(0, 8)$, $(1, 2)$ and $(2, 0)$.

We want to solve

$$\begin{aligned} C + D \cdot 0 &= 8 \\ C + D \cdot 1 &= 2 \\ C + D \cdot 2 &= 0 \end{aligned} \quad \leadsto \quad \underset{A}{\begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{bmatrix}} \underset{\vec{b}}{\begin{bmatrix} C \\ D \end{bmatrix}} = \begin{bmatrix} 8 \\ 2 \\ 0 \end{bmatrix}$$

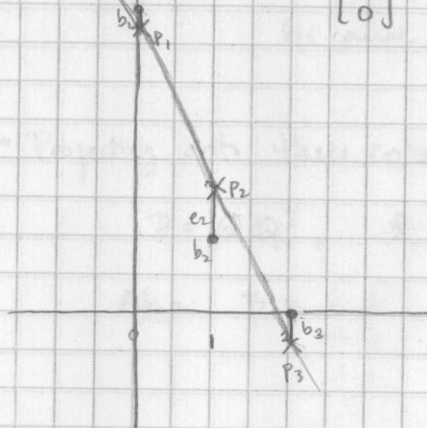
But there's no solution.

Solve $ATA\hat{x} = A^T\vec{b}$ instead: $\begin{bmatrix} 3 & 3 \\ 3 & 5 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 10 \\ 2 \end{bmatrix}$

$$\leadsto \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 22/3 \\ -4 \end{bmatrix}$$

So $\vec{p} = A\hat{x} = \begin{bmatrix} 22/3 \\ 10/3 \\ -2/3 \end{bmatrix}$

$\vec{e} = \vec{b} - \vec{p} = \vec{b} - A\hat{x} = \begin{bmatrix} 8 \\ 2 \\ 0 \end{bmatrix} - \begin{bmatrix} 22/3 \\ 10/3 \\ -2/3 \end{bmatrix} = \begin{bmatrix} 2/3 \\ -4/3 \\ 2/3 \end{bmatrix}$



Hypothetical question: Fitting a parabola?

III. Orthogonal matrices.

A projection matrix has the formula $P = A(A^T A)^{-1} A^T$.

Complicated! To simplify, would be nice if $A^T A = I$.

Definition: A set of vectors $\vec{v}_1, \vec{v}_2, \dots, \vec{v}_n$ is orthonormal if

- 1) $\vec{v}_i \cdot \vec{v}_j = 0$ if $i \neq j$
- 2) $\vec{v}_i \cdot \vec{v}_i = 1$

(vectors are unit vectors and orthogonal to each other).

A matrix Q with orthonormal columns satisfies $Q^T Q = I$.

If Q is square, this means $Q^T = Q^{-1}$ and we call such a matrix an orthogonal matrix.

Example: $Q = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$ (From prev. HW)

or $Q = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$ (permutation matrix)

Matrices with orthonormal columns are awesome:

- They preserve lengths: $\|Q\vec{x}\| = \|\vec{x}\|$ (like rotation matrix, permutation matrix)
- They preserve dot products: $(Q\vec{x}) \cdot (Q\vec{y}) = (\vec{x} \cdot \vec{y})$

$$\text{because } (Q\vec{x}) \cdot (Q\vec{y}) = (Q\vec{x})^T Q\vec{y} = \vec{x}^T Q^T Q \vec{y} = \vec{x}^T \vec{y}$$

- Projecting onto their column space is easy.

$$P = QQ^T, \quad \hat{x} = Q^T \vec{b}, \quad \vec{p} = Q \hat{x}$$

$$\text{Also: } \vec{p} = \begin{bmatrix} \vec{q}_1 & \dots & \vec{q}_n \end{bmatrix} \begin{bmatrix} \vec{q}_1^T \vec{b} \\ \vdots \\ \vec{q}_n^T \vec{b} \end{bmatrix} = \vec{q}_1 \vec{q}_1^T \vec{b} + \vec{q}_2 \vec{q}_2^T \vec{b} + \dots + \vec{q}_n \vec{q}_n^T \vec{b}$$

Note: $\vec{p}$ = sum of projections of $\vec{b}$ onto each line spanned by $\vec{q}_i$'s.

If you wanted to, you could project separately onto each column, then sum

Example: Project $\begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$ onto the column space of $Q = \begin{bmatrix} \frac{1}{\sqrt{3}} & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} \end{bmatrix}$

$$\text{Method 1: } QQ^T = \begin{bmatrix} \frac{1}{\sqrt{3}} & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{1}{3} & \frac{1}{3} & -\frac{1}{3} \\ \frac{1}{3} & \frac{5}{6} & \frac{1}{6} \\ -\frac{1}{3} & \frac{1}{6} & \frac{5}{6} \end{bmatrix}$$

$$\text{So } \vec{p} = QQ^T \vec{b} = \begin{bmatrix} \frac{1}{3} \\ \frac{7}{3} \\ \frac{5}{3} \end{bmatrix}$$

$$\text{Method 2: } \vec{q}_1 \vec{q}_1^T = \begin{bmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{3}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \end{bmatrix} = \begin{bmatrix} \frac{1}{3} & \frac{1}{3} & -\frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{1}{3} & \frac{1}{3} \end{bmatrix}$$

$$\text{So } \vec{q}_1 \vec{q}_1^T \vec{b} = \begin{bmatrix} \frac{1}{3} \\ \frac{1}{3} \\ -\frac{1}{3} \end{bmatrix}$$

$$\vec{q}_2 \vec{q}_2^T \vec{b} = \begin{bmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \vec{b} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} = \begin{bmatrix} 0 \\ 2 \\ 2 \end{bmatrix}$$

Q: How do we make matrices with orthonormal columns?

A: Gram-Schmidt.

Explanation by example:

Say you start with 3 independent vectors, $\vec{a}, \vec{b}, \vec{c}$, and you want 3 orthonormal vectors that span the same space.

1) Choose $\vec{A} = \vec{a}$. To make $\vec{B} \perp \vec{A}$, subtract off the projection of $\vec{b}$ onto $\vec{A}$.

$$\vec{B} = \vec{b} - \frac{\vec{A}^T \vec{b}}{\vec{A}^T \vec{A}} \vec{A} = \vec{b} - \frac{\vec{a}^T \vec{b}}{\vec{a}^T \vec{a}} \vec{a}$$

2) How do we choose $\vec{C}$? It needs to be perpendicular to the space spanned by $\vec{A}$ and $\vec{B}$. Subtract off the projection of $\vec{C}$ onto this space, which is the sum of the projections onto $\vec{A}$ and $\vec{B}$.

$$\vec{C} = \vec{c} - \frac{\vec{A}^T \vec{c}}{\vec{A}^T \vec{A}} \vec{A} - \frac{\vec{B}^T \vec{c}}{\vec{B}^T \vec{B}} \vec{B}$$

3) If there were more vectors, continue

4) Normalize.

$$\vec{q}_1 = \frac{\vec{A}}{\|\vec{A}\|}, \quad \vec{q}_2 = \frac{\vec{B}}{\|\vec{B}\|}, \quad \vec{q}_3 = \frac{\vec{C}}{\|\vec{C}\|}$$

Fact This gives a factorization of A .

$$A = QR = (\text{orthonormal columns}) \cdot (\text{triangular}).$$

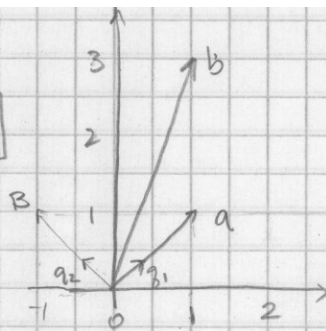
$$\begin{bmatrix} | & | & | \\ \vec{a} & \vec{b} & \vec{c} \\ | & | & | \end{bmatrix} = \begin{bmatrix} | & | & | \\ \vec{q}_1 & \vec{q}_2 & \vec{q}_3 \\ | & | & | \end{bmatrix} \begin{bmatrix} \vec{q}_1^T \vec{a} & \vec{q}_1^T \vec{b} & \vec{q}_1^T \vec{c} \\ 0 & \vec{q}_2^T \vec{b} & \vec{q}_2^T \vec{c} \\ 0 & 0 & \vec{q}_3^T \vec{c} \end{bmatrix}$$

$$R = Q^T A \quad \text{since} \quad Q^T A = Q^T QR = R$$

(So $A = QQ^T A$. But $QQ^T \neq I$. What's going on?)

Example 2x2 example

$$\vec{a} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \vec{b} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}$$



$$A = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad B = \begin{bmatrix} 1 \\ 3 \end{bmatrix} - \frac{a^T b}{a^T a} a = \begin{bmatrix} 1 \\ 3 \end{bmatrix} - \frac{4}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 3 \end{bmatrix} - \begin{bmatrix} 2 \\ 2 \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

Normalize: $q_1 = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \quad q_2 = \begin{bmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$