MAE 501 *Fall 2020*

Linear Algebra in Engineering

Module 3: Orthogonality

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1 Orthogonal Vectors and Subpsaces

Definition The inner product of two n-dimensional vectors $\boldsymbol{x}$ and $\boldsymbol{y}$ is defined as

$$\boldsymbol{x}^T\boldsymbol{y} = \sum_{i=1}^{n} x_i y_i$$

Comments

- Other ways of denoting the inner product:

$$x^T y = x \cdot y$$

or

$$x^T y = (x, y)$$

- Notice that $\boldsymbol{x}^T\boldsymbol{y} = \boldsymbol{y}^T\boldsymbol{x}$

$$(x^T y)^T = y^T (x^T)^T = y^T x$$ This's is a scalar

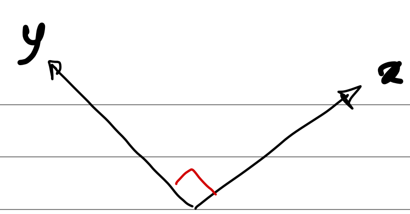
- The length, or magnitude, of an n-dimensional vector is:

$$\|x\| = \sqrt{x^T x} = \sqrt{x_1^2 + x_2^2 + \dots + x_n^2}$$

Note

Two vectors $\boldsymbol{x}$ and $\boldsymbol{y}$ are orthogonal if and only if their inner product is zero, i.e., $\boldsymbol{x}^T\boldsymbol{y} = 0$.

When are vectors orthogonal in $\mathbb{R}^2$?



x and y are orthogonal when they form a right triangle

$$\Rightarrow \|x\|^2 + \|y\|^2 = \|x-y\|^2$$

What vector is orthogonal to every other vector in $\mathbb{R}^n$?

$\boldsymbol{x}^T\boldsymbol{y} = 0$ take $\boldsymbol{y} = (1,0,0,\dots,0) \Rightarrow \boldsymbol{x}^T\boldsymbol{y} = x_1 = 0$

repeat with $\boldsymbol{y} = (0,1,0,\dots,0) \Rightarrow x_2 = 0$ and so on $\Rightarrow \boldsymbol{x} = 0$

Note

If the non-zero vectors $\boldsymbol{v}_1, \boldsymbol{v}_2, \cdots, \boldsymbol{v}_n$ are mutually orthogonal, they are linearly independent.

Proof:

$\boldsymbol{v}_i^T(c_1\boldsymbol{v}_1 + c_2\boldsymbol{v}_2 + \cdots + c_n\boldsymbol{v}_n) = 0 \Rightarrow c_i\,\boldsymbol{v}_i^T\boldsymbol{v}_i = 0$

because $\boldsymbol{v}_i^T\boldsymbol{v}_j = 0$ for $i \neq j$

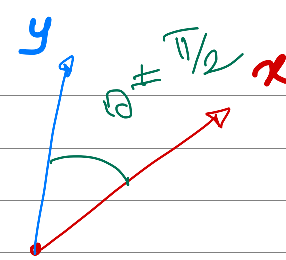
$\boldsymbol{v}_i$ is non-zero $\Rightarrow c_i = 0 \Rightarrow$ linearly independent

Comments

- Vectors in orthogonal basis $(\boldsymbol{v}_1, \boldsymbol{v}_2, \cdots, \boldsymbol{v}_n)$ of vector space $\boldsymbol{V}$ are mutually orthogonal.
- Any n mutually orthogonal vectors form a basis in $\mathbb{R}^n$.
- A vector basis $(\boldsymbol{v}_1, \boldsymbol{v}_2, \cdots, \boldsymbol{v}_n)$ is called orthonormal if the basis vectors have a magnitude equal to one, i.e, $||\boldsymbol{v}_i|| = 1$.
- What is an example of an orthonormal basis in $\mathbb{R}^2$?

  The unit vectors $\begin{bmatrix}1\\0\end{bmatrix}$ and $\begin{bmatrix}0\\1\end{bmatrix}$ mutually orthogonal and of unitary length

What if $\boldsymbol{x}$ and $\boldsymbol{y}$ are not orthogonal?



what is $\boldsymbol{x}^T\boldsymbol{y}$?

In this case $\boldsymbol{x}^T\boldsymbol{y} = ||\boldsymbol{x}||\,||\boldsymbol{y}||\cos(\theta)$

The inner product defines the angle θ between $\boldsymbol{x}$ and $\boldsymbol{y}$.

We now know when two vectors are orthogonal. When are two subspaces orthogonal?

Definition Two subspaces $\boldsymbol{V}$ and $\boldsymbol{W}$ of the same vector space $\mathbb{R}^n$ are said orthogonal if every vector in $\boldsymbol{V}$ is orthogonal to every vector in $\boldsymbol{W}$, i.e.,

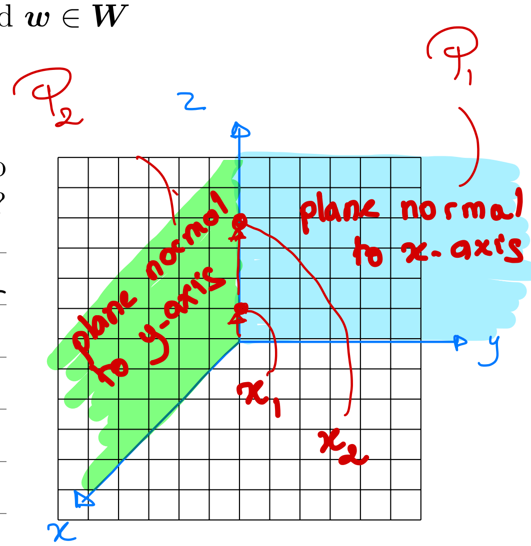
$$\boldsymbol{v}^T\boldsymbol{w} = 0 \quad \text{for every } \boldsymbol{v} \in \boldsymbol{V} \text{ and } \boldsymbol{w} \in \boldsymbol{W}$$

Example 1

Consider the two planes (subspaces) in $\mathbb{R}^3$ normal to the x and y axis. Are these two subspaces orthogonal?

No! Vectors in the intersection line are not orthogonal!

$x_1 \in P_1$, $x_2 \in P_2$ but $x_1^T x_2 \neq 0$



Are there any two planes in $\mathbb{R}^3$ that are orthogonal?

No! because any two planes (going through zero) in 3D will intersect along a line.

Note

(*) The row space is orthogonal to the nullspace: $\boldsymbol{C}(A^T) \perp \boldsymbol{N}(A)$.

(**) The column space is orthogonal to the left nullspace: $\boldsymbol{C}(A) \perp \boldsymbol{N}(A^T)$.

Proof:

(*) Take $x \in C(A^T)$ (means there is y such that $x = A^T y$)

and Take $z \in N(A)$

$$z^T x = x^T z = (A^T y)^T z = y^T A^{T^T} z = y^T \underbrace{Az}_{= 0} = y^T 0 = 0$$

(**) Take $x \in C(A)$ (means there is y such that $x = Ay$)

and Take $z \in N(A^T)$

$$x^T z = z^T x = z^T (Ay) = \underbrace{(z^T A)}_{= 0^T} y = 0^T y = 0$$

How can we show that $A\boldsymbol{x} = \boldsymbol{b}$ is solvable?

1. Show that $\boldsymbol{b}$ is in $\boldsymbol{C}(A)$.

2. Show that $\mathbf{y}^T\mathbf{b} = 0$ for all $\mathbf{y} \in \boldsymbol{N}(A^T)$

If you have a basis of $\boldsymbol{N}(A^T)$, it suffices to show that $\mathbf{b}$ is orthogonal to all basis vectors.

Example 2 Show that the the row space and nullspace are orthogonal for the rank 1 matrix:

$$A = \begin{array}{cc} \text{col}_1 & \text{col}_2 \end{array}$$
$$A = \begin{bmatrix} 1 & 2 \\ 2 & 4 \\ 3 & 6 \end{bmatrix} \quad -2\times \text{col}_1 + 1\times \text{col}_2 = \mathbf{0}$$

Here: $\boldsymbol{C}(A^T) = \left\{ \alpha\, \text{row}_1^T \right\} = \left\{ \alpha \begin{bmatrix} 1 \\ 2 \end{bmatrix} \right\}$ and $\boldsymbol{N}(A) = \left\{ \beta \begin{bmatrix} -2 \\ 1 \end{bmatrix} \right\}$

Take: $\mathbf{u} \in \boldsymbol{C}(A^T)$, $\mathbf{v} \in \boldsymbol{N}(A) \Rightarrow \mathbf{u} = \alpha \begin{bmatrix} 1 \\ 2 \end{bmatrix}$ $\mathbf{v} = \beta \begin{bmatrix} -2 \\ 1 \end{bmatrix}$

$$\mathbf{u}^T\mathbf{v} = \alpha\beta \begin{bmatrix} 1 & 2 \end{bmatrix} \begin{bmatrix} -2 \\ 1 \end{bmatrix} = \alpha\beta(-2+2) = 0$$

Definition Given a subspace $\boldsymbol{V}$ of $\mathbb{R}^n$, the space of all vectors orthogonal to $\boldsymbol{V}$ is called the orthogonal complement of $\boldsymbol{V}$ and denoted $\boldsymbol{V}^\perp$.

Example 3 What is the orthogonal complement to the yOz plane in 3D?

A line orthogonal to yOz and going through the origin $\Rightarrow$ Ox line

Comments

- If $\boldsymbol{V}$ is a subspace of $\mathbb{R}^n$ and has dimension d, what is the dimension of $\boldsymbol{V}^\perp$?

$\dim(V) + \dim(V^\perp) = \dim(\mathbb{R}^n) = n$

$\dim(V^\perp) = n-d$

- If $\boldsymbol{V}$ is a subspace of $\mathbb{R}^n$, then every vector $\boldsymbol{x} \in \mathbb{R}^n$ can be split into $\boldsymbol{x} = \boldsymbol{v} + \boldsymbol{w}$ where $\boldsymbol{v} \in \boldsymbol{V}$ and $\boldsymbol{w} \in \boldsymbol{W} = \boldsymbol{V}^\perp$.

v is the projection of x onto V

w is the projection of x onto $V^\perp = W$

Note

For a matrix A of size $m \times n$:
The row space is the orthogonal complement of the nullspace in $\mathbb{R}^n$:

$$\boldsymbol{C}(A^T)^\perp = \boldsymbol{N}(A)$$

The column space is the orthogonal complement of the left nullspace in $\mathbb{R}^m$:

$$\boldsymbol{C}(A)^\perp = \boldsymbol{N}(A^T)$$

Comments

- The dimensions of the row space and nullspace add up to n:

Row space and nullspace are subspaces of $\mathbb{R}^n$

$\underbrace{\dim(\boldsymbol{C}(A^T))}_{= \text{rank } r} + \underbrace{\dim(\boldsymbol{N}(A))}_{= n-r} = n$

- The dimensions of the column space and left nullspace add up to m:

Column space and left nullspace are subspaces of $\mathbb{R}^m$

$\underbrace{\dim(\boldsymbol{C}(A))}_{= r} + \underbrace{\dim(\boldsymbol{N}(A^T))}_{= m-r} = m$

- Any vector $\boldsymbol{x} \in \mathbb{R}^n$ can be decomposed into $\boldsymbol{x} = \boldsymbol{x}_r + \boldsymbol{x}_n$ with $\boldsymbol{x}_r$ in the row space of A and $\boldsymbol{x}_n$ in the nullspace of A.

x_r belongs to row space $\Rightarrow$ there is y such that $x_r = A^T y$

x_n belongs to nullspace $\Rightarrow$ $A x_n = 0$

- The matrix A maps the row space to the column space

$$Ax = A(x_r + x_n) = A x_r$$

belongs to columnspace

belongs to row space

Row space $\xrightarrow{A}$ column space

Nullspace $\xrightarrow{A}$ $\{0\}$

2 Projection

We start with the following observation: $A\boldsymbol{x} = \boldsymbol{b}$ has a solution only if $\boldsymbol{b}$ is in the column space. However, an arbitrary $\boldsymbol{b} \in \mathbb{R}^n$ may not belong to the column space. So how can we "change" it, to make it fit in $\boldsymbol{C}(A)$?

Recall that thee orthogonal complement of $\boldsymbol{C}(A)$ is the left nullspace. Therefore, for an arbitrary $\boldsymbol{b} \in \mathbb{R}^n$ we can write

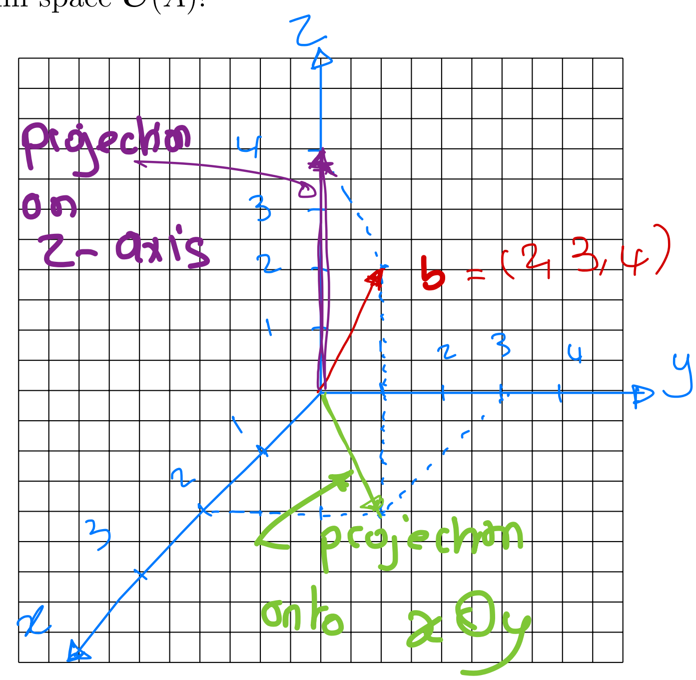
$$b = b_c + b_\ell \quad \text{where } b_c \in C(A) \text{ and } b_\ell \in N(A^T)$$

$\boldsymbol{b}_c$ is called the *projection* of $\boldsymbol{b}$ onto the column space $\boldsymbol{C}(A)$!

What is the projection of $\boldsymbol{b} = (2, 3, 4)$ onto the z axis? onto the xy plane?

The projection of b on xOy is $(2,3,0)$

The projection of b on the z axis is $(0,0,4)$



Which matrix P produces the projection of $\boldsymbol{b}$ onto the z axis?

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 3 \\ 4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 4 \end{bmatrix}$$

Which matrix P produces the projection of $\boldsymbol{b}$ onto the xy ~~axis~~ plane?

$$P b = \begin{bmatrix} 2 \\ 3 \\ 0 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 2 \\ 3 \\ 4 \end{bmatrix} = \begin{bmatrix} 2 \\ 3 \\ 0 \end{bmatrix}$$

How to systematically find P for an arbitrary subspace?

Note

The projection matrix onto a line oriented along a vector $\boldsymbol{a}$ is

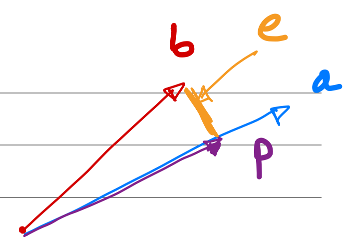
$$P = \frac{\overbrace{\boldsymbol{a}\boldsymbol{a}^T}^{\text{matrix of size } n\times n}}{\underbrace{\boldsymbol{a}^T\boldsymbol{a}}_{\text{inner product } = \|\boldsymbol{a}\|^2}}.$$

The projection of a vector $\boldsymbol{b}$ on this line is

$$P\boldsymbol{b} = \boldsymbol{a}\frac{\boldsymbol{a}^T\boldsymbol{b}}{\boldsymbol{a}^T\boldsymbol{a}}.$$

Proof:

Consider $\mathbf{p}$ projection of $\mathbf{b}$ on the line



$\Rightarrow \mathbf{p} = \underbrace{\hat{x}}_{\text{scaling factor}}\,\mathbf{a}$

The residual (or error) $\mathbf{e} = \mathbf{b} - \mathbf{p} \perp \mathbf{a} \Rightarrow \mathbf{a}^T\mathbf{e} = 0$

$\Rightarrow \mathbf{a}^T(\mathbf{b} - \mathbf{p}) = 0 \Rightarrow \mathbf{a}^T\mathbf{b} - \mathbf{a}^T(\hat{x}\mathbf{a}) \Rightarrow \hat{x} = \mathbf{a}^T\mathbf{b}/\mathbf{a}^T\mathbf{a}$

$\Rightarrow \quad \mathbf{p} = \underbrace{\boxed{\dfrac{\mathbf{a}\,\mathbf{a}^T}{\mathbf{a}^T\mathbf{a}}}}_{\text{projection matrix}}\mathbf{b}$: projection vector

Comments

- Check with previous example!

  Projection on z axis:

  $$P\mathbf{b} = \frac{\begin{bmatrix}0\\0\\1\end{bmatrix}\begin{bmatrix}0 & 0 & 1\end{bmatrix}}{1^2}\begin{bmatrix}2\\3\\4\end{bmatrix} = \begin{bmatrix}0 & 0 & 0\\0 & 0 & 0\\0 & 0 & 1\end{bmatrix}\begin{bmatrix}2\\3\\4\end{bmatrix} = \begin{bmatrix}0\\0\\4\end{bmatrix}$$

- What is the column space of the projection matrix onto a line?

  $$C(P) = \text{Span}\{\mathbf{a}\} = \{\alpha\,\mathbf{a}\}$$

- What is its rank?

  $\text{rank} = \dim\left(C(P)\right) = 1$

  remember that all matrices of rank 1 can be written as $A = \mathbf{u}\mathbf{v}^T$

- What happens if we project a second time?

$p = \hat{x} a$ with $\hat{x} = a^T b / a^T a$

$p' = \frac{a a^T}{a^T a}(\hat{x} a) = \hat{x} \frac{a \cancel{a^T a}}{\cancel{a^T a}} = \hat{x} a = p \Rightarrow$ $P^2 b = P b$ $\boxed{P^2 = P}$

- $I - P$ is also a projection matrix! It projects on the perpendicular subspace.

Check $(I-P)^2 = I - P - \cancel{P} + \cancel{P^2} = I - P \Rightarrow$ projection matrix

In previous example $P_{xOy} = I - P_{z\,axis}$

Note

The projection matrix onto a subspace spanned by n linearly independent vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\cdots$, $\boldsymbol{a}_n$ is

$$P = A(A^T A)^{-1} A^T$$

where $A = [\boldsymbol{a}_1\ \boldsymbol{a}_2\ \cdots\ \boldsymbol{a}_n]$.

Proof:

Let p projection of b onto subspace $\Rightarrow$ there is $\hat{x}$ such that $p = A\hat{x}$

The error $e = b - p = b - A\hat{x} \perp$ subspace $\Rightarrow a_i^T (b - A\hat{x}) = 0$

In matrix form: $A^T b - A^T A \hat{x} = 0 \Rightarrow \boxed{A^T A \hat{x} = A^T b}$

$\Rightarrow \hat{x} = (A^T A)^{-1} A^T b \Rightarrow p = A\hat{x} = \underbrace{A (A^T A)^{-1} A^T}_{\text{Projection matrix onto subspace}} b$

Note: $(A^T A)^{-1}$ exists if and only if the a_i are linearly independent.

Example 4 For the previous example, find the projection matrix onto the xy plane.

Plane xOy is spanned by $(1,0,0)$ and $(0,1,0) \Rightarrow A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}$

$A^T A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \Rightarrow (A^T A)^{-1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

The projection matrix $P = A(A^TA)^{-1}A^T$

$$P = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$ exactly what we found before!

Comments

- Check that here too $\boxed{P^2 = P}$.

$$P^2 = A(A^TA)^{-1}\underbrace{A^TA(A^TA)^{-1}}_{I}A^T = A(A^TA)^{-1} I A^T = A(A^TA)^{-1}A^T = P$$

- When solving $A\boldsymbol{x} = \boldsymbol{b}$, the right hand side $\boldsymbol{b}$ can be split into its projection on the column space of A and an error vector.

$$\boldsymbol{b} = \boldsymbol{b_c} + \boldsymbol{e} \qquad \boldsymbol{b_c} = \text{projection of } \boldsymbol{b} \text{ onto } \boldsymbol{C}(A)$$

$$\boldsymbol{b_c} = P\boldsymbol{b} = A\boxed{(A^TA)^{-1}A^T\boldsymbol{b}} = A\boxed{\hat{\boldsymbol{x}}}$$

- The error $\boldsymbol{e} = \boldsymbol{b} - A\hat{\boldsymbol{x}} = \boldsymbol{b} - P\boldsymbol{b}$ belongs to the left nullspace of A.
- The distance from $\boldsymbol{b}$ to the column space $\boldsymbol{C}(A)$ is $||\boldsymbol{e}||$.
- Careful! A^{-1} does not exist in general! So the following would be a mistake:

$$P = A(A^TA)^{-1}A^T = A\cancel{A^{-1}}\cancel{(A^T)^{-1}}A^T = I\,I = I$$

classic mistake!

(A^TA) may be invertible, but A is generally not.

- The matrix A^TA is invertible if and only if A has linearly independent columns.
- When A has independent columns, A^TA is square, symmetric and invertible. Moreover, A^TA has the same nullspace as A.

3 Least Squares

As we have seen in module 2, when $\boldsymbol{b}$ is outside the column space, the system $A\boldsymbol{x} = \boldsymbol{b}$ is not solvable. Even though it sounds like defeat, we will not abandon yet. Our goal in this section is to find a "best" solution $\hat{\boldsymbol{x}}$ that approximates $A\hat{\boldsymbol{x}} \simeq \boldsymbol{b}$ reasonably well.

Let's start with the following example:

$$x = b_1$$
$$2x = b_2$$
$$3x = b_3$$

There are more equations than unknowns. What would be a few strategies to make this system solvable?

We could drop eq 2 and 3 and solve
or drop eq 1 and 3
or drop eq 1 and 2

We don't have a way of telling which eq to drop or which eq is more important!

Our approach will consist in choosing a solution $\hat{x}$ that minimizes an average error:

$e_1 = x - b_1$
$e_2 = 2x - b_2$ $\quad E^2 = e_1^2 + e_2^2 + e_3^2 = (x-b_1)^2 + (2x-b_2)^2 + (3x-b_3)^2$
$e_3 = 3x - b_3$

(sum of squares)

Minimizing the error leads to

E^2 is minumum when $\frac{\partial E^2}{\partial x}(\hat{x}) = 0$!

$\frac{\partial E^2}{\partial x}(\hat{x}) = 2(\hat{x}-b_1) + 2(2\hat{x}-b_2)\cdot 2 + 2(3\hat{x}-b_3)\cdot 3 = 0$

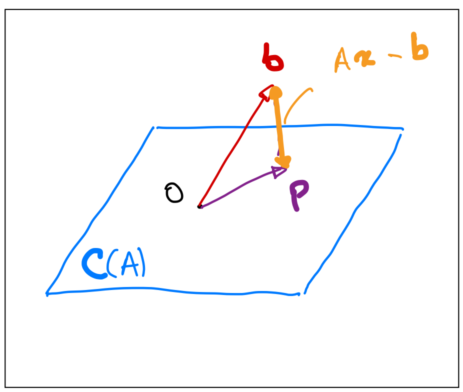
$\Rightarrow \hat{x}(1+4+9) = b_1 + 2b_2 + 3b_3$

$\Rightarrow \hat{x} = \frac{b_1 + 2b_2 + 3b_3}{1+4+9} = \frac{\mathbf{a}^T\mathbf{b}}{\mathbf{a}^T\mathbf{a}}$ with $\mathbf{a} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$

In general if A is a $m \times n$ matrix and $\boldsymbol{b} \notin \boldsymbol{C}(A)$, we can define

$$E(\boldsymbol{x}) = ||A\boldsymbol{x} - \boldsymbol{b}||$$

which represents the error for a given $\boldsymbol{x}$. Geometrically, E represents the distance between $\boldsymbol{b}$ to $A\boldsymbol{x}$.



What is $\hat{\boldsymbol{x}}$ that minimizes the error?

1. By geometry:

Error is minimum when $A\hat{\mathbf{x}} = \mathbf{p}$ projection of $\mathbf{b}$ onto $C(A)$

In the previous section, we saw that $\hat{\mathbf{x}}$ is solution to

$$\boxed{A^TA\hat{\mathbf{x}} = A^T\mathbf{b}}$$

2. By calculus

$$\frac{\partial E^2}{\partial x_i} = 0 = \frac{\partial}{\partial x_i}\left(\sum_j\left(\sum_k a_{jk}\hat{x}_k - b_j\right)^2\right) = \sum_j 2a_{ji}\left(\sum_k a_{jk}\hat{x}_k - b_j\right)$$

$$\underbrace{\sum_j a_{ji}\sum_k a_{jk}\hat{x}_k}_{A^TA\hat{\mathbf{x}}} = \underbrace{\sum_j a_{ji}b_j}_{A^T\mathbf{b}} \Rightarrow \boxed{A^TA\hat{\mathbf{x}} = A^T\mathbf{b}}$$

3. By algebra

$\mathbf{b} = \mathbf{b}_c + \mathbf{b}_e$ $\quad \mathbf{b}_c \in C(A)$ and $\mathbf{b}_e \in N(A^T)$

while $A\mathbf{x} = \mathbf{b} = \mathbf{b}_c + \mathbf{b}_e$ is not solvable, $A\hat{\mathbf{x}} = \mathbf{b}_c$ is solvable! To select the solvable part:

$$A^TA\mathbf{x} = A^T\mathbf{b}_c + \cancel{A^T\mathbf{b}_e}^{\to 0} \Rightarrow A^TA\hat{\mathbf{x}} = A^T\mathbf{b}$$
$$= A^T\mathbf{b}$$

Comments

- What is the minimum error when $A\boldsymbol{x} = \boldsymbol{b}$ is solvable?

  $E = \|A\mathbf{x} - \mathbf{b}\| = 0$ if $\mathbf{x}$ is solution

- The approximate solution $\hat{\boldsymbol{x}}$ is called the *least-square* because it makes $||A\boldsymbol{x} - \boldsymbol{b}||$ as small as possible.
- The vector $\boldsymbol{e} = \boldsymbol{b} - A\hat{\boldsymbol{x}}$ is called the error vector or residual vector.

Note

The solutions to the *normal equations*

$$\boxed{A^TA\hat{\boldsymbol{x}} = A^T\boldsymbol{b}}$$

correspond to the least square solutions $\hat{\boldsymbol{x}}$. When A has linearly independent columns, A^TA is invertible and the least square solution is unique and given by:

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

Example 5 Three measurements $b_1 = 1$, $b_2 = 2$ and $b_3 = 2$ are recorded at times $t_1 = 1$, $t_2 = 2$ and $t_3 = 3$ respectively. We would like to fit a line to the measurements of form $C + Dt = b$. What is the best C and D in the least square sense?

$$\begin{aligned} C + D1 &= 1 \\ C + D2 &= 2 \\ C + D3 &= 2 \end{aligned} \Rightarrow \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} \Rightarrow A^TA\hat{x} = A^T b$$

$$A^TA = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} = \begin{bmatrix} 3 & 6 \\ 6 & 14 \end{bmatrix}$$

$$A^T b = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} = \begin{bmatrix} 5 \\ 11 \end{bmatrix}$$

$$\left[\begin{array}{cc|c} \boxed{3} & 6 & 5 \\ 6 & 14 & 11 \end{array}\right] \rightarrow \left[\begin{array}{cc|c} \boxed{3} & 6 & 5 \\ 0 & \boxed{2} & 1 \end{array}\right] \rightarrow \left[\begin{array}{cc|c} 3 & 0 & 2 \\ 0 & 1 & 1/2 \end{array}\right] \rightarrow \left[\begin{array}{cc|c} 1 & 0 & 2/3 \\ 0 & 1 & 1/2 \end{array}\right]$$

$$\Rightarrow \hat{C} = 2/3 \text{ and } \hat{D} = 1/2$$

4 Orthonormal bases and Gram-Schmidt

Definition The vectors $\boldsymbol{q}_1, \boldsymbol{q}_2, \cdots, \boldsymbol{q}_n$ are orthonormal if

$$\boldsymbol{q}_i^T \boldsymbol{q}_j = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases}$$

Comments

- A matrix with orthonormal columns is denoted Q.
- A *square* matrix with orthonormal columns is called orthogonal matrix.

What is Q^TQ?

$$\begin{bmatrix} \text{---} \boldsymbol{q}_1^T \text{---} \\ \text{---} \boldsymbol{q}_2^T \text{---} \\ \vdots \\ \text{---} \boldsymbol{q}_n^T \text{---} \end{bmatrix} \begin{bmatrix} | & | & & | \\ \boldsymbol{q}_1 & \boldsymbol{q}_2 & \cdots & \boldsymbol{q}_n \\ | & | & & | \end{bmatrix} = \begin{bmatrix} & & & \\ & & & \end{bmatrix}$$

Note

Orthogonal (square) matrices have the fundamental property: $Q^{-1} = Q^T$

Comments

- If a square matrix has orthonormal columns, it has orthonormal rows and vice versa!
- Even if Q is rectangular, we still have $Q^TQ = I$. In this case, Q^T is called the *left-inverse* of Q.
- What's an orthogonal matrix that we have already seen?

Orthogonal matrices have the two following important geometrical properties

1. They preserve lengths

2. They preserve angles

In addition, if $\boldsymbol{q}_1, \boldsymbol{q}_2, \cdots, \boldsymbol{q}_n$ is an orthonormal basis of $\boldsymbol{V}$ and $\boldsymbol{b} \in \boldsymbol{V}$, then finding the decomposition of $\boldsymbol{b}$ on the basis becomes simple:

Example 6 Show that the rotation matrix is orthogonal.

$$R = \begin{bmatrix} \cos(\theta) & -\sin(\theta) & 0 \\ \sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Let's revisit the least-squares. The least square solution satisfies $A^T A\hat{\boldsymbol{x}} = A^T b$ What if A was an orthogonal matrix?

Example 7 Let's revisit example 4 and shift the measurement times such that $\sum t_i = 0$

$$\begin{array}{llcll} t_1 = 1 & \to b_1 = 1 & & t_1 = -1 & \to b_1 = 1 \\ t_2 = 2 & \to b_2 = 2 & \to & t_2 = 0 & \to b_2 = 2 \\ t_3 = 3 & \to b_3 = 2 & & t_3 = 1 & \to b_3 = 2 \end{array}$$

Find the best C and D for the line fit $C + Dt_i = b_i$.

Unfortunately, A is generally not an orthogonal matrix. Again, we will not accept defeat, and we will seek to produce an orthogonal matrix out of any arbitrary matrix. This is the so-called QR factorization where A is expressed as $A = QR$ the product of an orthogonal matrix Q (rectangular) and an *upper-triangular & invertible* matrix R.

Why does it matter?

So how do we get this form? This is known as the Gram-Schmidt process. Suppose we are given 3 independent vectors $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$:

Step 1: To get $\boldsymbol{q}_1$, start by normalizing $\boldsymbol{a}$.

Step 2: To get $\boldsymbol{q}_2$, remove from $\boldsymbol{b}$ its projection on $\boldsymbol{q}_1$, and normalize.

Step 3: To get $\boldsymbol{q}_3$, remove from $\boldsymbol{c}$ its projections on $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$, and normalize.

Note

Gram-Schmidt: Given a family of independent vectors $\boldsymbol{a}_j$, subtract from every new vector its components in the directions that are already set:

$$\begin{aligned}\boldsymbol{A}_j &= \boldsymbol{a}_j - (\boldsymbol{q}_1^T\boldsymbol{a}_j)\boldsymbol{q}_1 - (\boldsymbol{q}_2^T\boldsymbol{a}_j)\boldsymbol{q}_2 - (\boldsymbol{q}_{j-1}^T\boldsymbol{a}_j)\boldsymbol{q}_{j-1}\\ \boldsymbol{q}_j &= \frac{\boldsymbol{A}_j}{\sqrt{\boldsymbol{A}_j^T\boldsymbol{A}_j}}\end{aligned}$$

Now let's take $\boldsymbol{a}_j$ as the columns of a matrix A and build $\boldsymbol{q}_j$ with the Gram-Schmidt process. Projecting the columns $\boldsymbol{a}_j$ on the orthonormal vectors $\boldsymbol{q}_j$:

which allows us write

$$A = \begin{bmatrix} | & | & & | \\ \boldsymbol{a}_1 & \boldsymbol{a}_2 & \cdots & \boldsymbol{a}_n \\ | & | & & | \end{bmatrix} = \begin{bmatrix} | & | & & | \\ \boldsymbol{q}_1 & \boldsymbol{q}_2 & \cdots & \boldsymbol{q}_n \\ | & | & & | \end{bmatrix} \begin{bmatrix} \boldsymbol{q}_1^T\boldsymbol{a}_1 & \boldsymbol{q}_1^T\boldsymbol{a}_2 & \cdots & \boldsymbol{q}_1^T\boldsymbol{a}_n \\ 0 & \boldsymbol{q}_2^T\boldsymbol{a}_2 & \cdots & \boldsymbol{q}_2^T\boldsymbol{a}_n \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \boldsymbol{q}_n^T\boldsymbol{a}_n \end{bmatrix}$$

Note

Every $m \times n$ matrix with independent columns can be factored in $A = QR$. The columns of Q are orthonormal and R is an upper-triangular and invertible matrix.

Comments

- Why is R invertible?

- When $m = n$ all matrices are square, Q is an orthogonal matrix.
- The system $R\hat{\boldsymbol{x}} = Q^T\boldsymbol{b}$ is fast to solve since R is upper triangular. Only back-substitutions are needed.