MT-1004
Linear Algebra

Fall 2023

Week # 10-11

National University of Computer and Emerging Sciences

November 2, 2023

Chapter 6

Orthogonality and Least Squares

Motivation

Recall: This course is about learning to:

- Solve the matrix equation $Ax = b$ (Echelon Form, Reduced Echelon Form, Column Space, Null Space)

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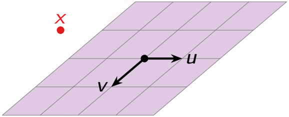

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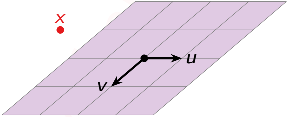

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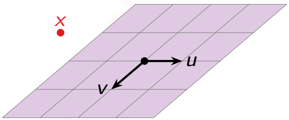

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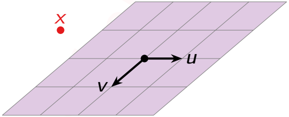

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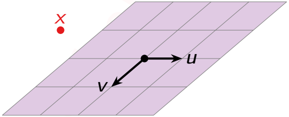

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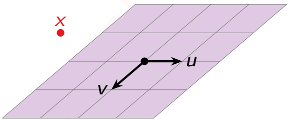

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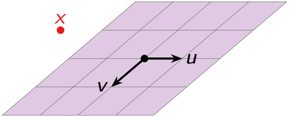

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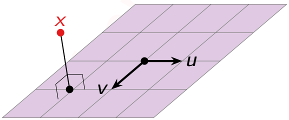

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Example

$$\begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \cdot \begin{pmatrix} 4 \\ 5 \\ 6 \end{pmatrix} = \begin{pmatrix} 4 & 5 & 6 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} = 1 \cdot 4 + 2 \cdot 5 + 3 \cdot 6 = 32.$$

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- $(cx) \cdot y = c(x \cdot y)$

The Dot Product and Length

Definition

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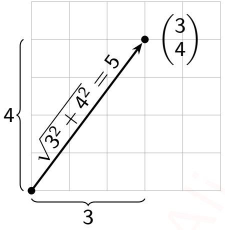

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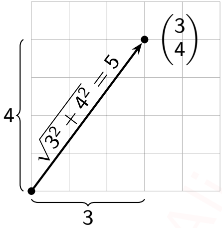

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Fact

If x is a vector and c is a scalar, then $\|cx\| = |c| \cdot \|x\|$.

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Let $x = (1, 2)$ and $y = (4, 4)$. Then

$$\mathrm{dist}(x, y) = \|y - x\| = \left\| \begin{pmatrix} 3 \\ 2 \end{pmatrix} \right\| = \sqrt{3^2 + 2^2} = \sqrt{13}.$$

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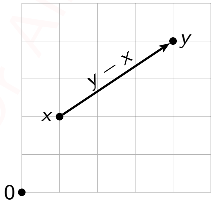

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This is in fact a unit vector:

scalar

$$\left\| \frac{x}{\|x\|} \right\| = \frac{1}{\|x\|}\|x\| = 1.$$

Unit Vectors

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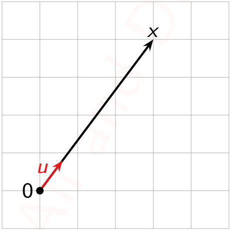
What is the unit vector in the direction of $x = \begin{pmatrix} 3 \\ 4 \end{pmatrix}$?

$$u = \frac{x}{\|x\|} = \frac{1}{\sqrt{3^2 + 4^2}} \begin{pmatrix} 3 \\ 4 \end{pmatrix} = \frac{1}{5} \begin{pmatrix} 3 \\ 4 \end{pmatrix}.$$



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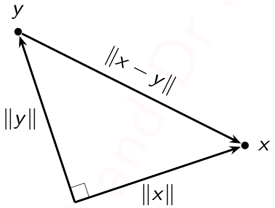

$$
\begin{aligned}
x \text{ and } y \text{ are perpendicular} &\iff \|x\|^2 + \|y\|^2 = \|x-y\|^2 \\
&\iff x\cdot x + y\cdot y = (x-y)\cdot(x-y) \\
&\iff x\cdot x + y\cdot y = x\cdot x + y\cdot y - 2x\cdot y \\
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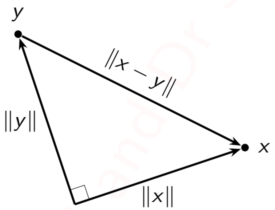

$$\begin{aligned} x \text{ and } y \text{ are perpendicular} &\iff \|x\|^2 + \|y\|^2 = \|x - y\|^2 \\ &\iff x \cdot x + y \cdot y = (x - y) \cdot (x - y) \\ &\iff x \cdot x + y \cdot y = x \cdot x + y \cdot y - 2x \cdot y \\ &\iff x \cdot y = 0 \end{aligned}$$

Fact: $x \perp y \iff \|x - y\|^2 = \|x\|^2 + \|y\|^2$

Orthogonality

Definition

A set of vectors $\{x_1, x_2, ..., x_k\}$ in R^n is called an **orthogonal set** if $x_i \cdot x_j = 0$ whenever $i \neq j$ for $i, j = 1, 2, ..., k$.

Problem: Show that $\{x_1,\ x_2,\ x_3\}$ is an orthogonal set in R^3 if

$$x_1 = \begin{bmatrix} 2 \\ 1 \\ -1 \end{bmatrix},\ x_2 = \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix},\ x_3 = \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix}.$$

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$$x_1 \cdot x_2 = 2(0) + 1(1) + (-1)(1) = 0$$
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For instance, $\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix} \perp \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}$ because $\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix} = 0.$

Problem: Find *all* vectors orthogonal to both $v = \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}$ and $w = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$.

Now we have to solve the system of two homogeneous equations

$$0 = x \cdot v = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix} = x_1 + x_2 - x_3$$
$$0 = x \cdot w = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = x_1 + x_2 + x_3.$$

In matrix form:

$$\text{The rows are } v \text{ and } w \longrightarrow \begin{pmatrix} 1 & 1 & -1 \\ 1 & 1 & 1 \end{pmatrix} \xrightarrow{\text{rref}} \begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The parametric vector form of the solution is

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = x_2 \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}.$$

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$$c_1 u_1 + c_2 u_2 + \cdots + c_m u_m = 0$$

has only the trivial solution $c_1 = c_2 = \cdots = c_m = 0$.

$$0 = u_1 \cdot (c_1 u_1 + c_2 u_2 + \cdots + c_m u_m) = c_1(u_1 \cdot u_1) + 0 + 0 + \cdots + 0.$$

Hence $c_1 = 0$. Similarly for the other c_i.

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An **orthogonal basis** for a subspace W of R^n is a basis of W that is an orthogonal set.

Orthogonal Basis

Theorem

If $\{u_1, u_2, ..., u_k\}$ is an orthogonal set of nonzero vectors in R^n, then these vectors are linearly independent.

Suppose $\{u_1, u_2, \ldots, u_m\}$ is orthogonal. We need to show that the equation

$$c_1 u_1 + c_2 u_2 + \cdots + c_m u_m = 0$$

has only the trivial solution $c_1 = c_2 = \cdots = c_m = 0$.

$$0 = u_1 \cdot (c_1 u_1 + c_2 u_2 + \cdots + c_m u_m) = c_1(u_1 \cdot u_1) + 0 + 0 + \cdots + 0.$$

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Problem Show that $\left\{ \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right\}$ forms orthogonal basis of R^2.

Orthogonal Basis
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Problem Find an orthogonal basis for the subspace W of R^3 given by

$$W = \left\{ \begin{bmatrix} x \\ y \\ z \end{bmatrix} : x - y + 2z = 0 \right\}.$$

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$$\begin{bmatrix} y - 2z \\ y \\ z \end{bmatrix} = y \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} + z \begin{bmatrix} -2 \\ 0 \\ 1 \end{bmatrix},$$

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They are not orthogonal.

Orthogonal Basis

We want to find a vector of W that is orthogonal to either $\begin{bmatrix}1\\1\\0\end{bmatrix}$ or $\begin{bmatrix}-2\\0\\1\end{bmatrix}$.

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Solving above two equations, we get

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Theorem

Let $\{x_1, x_2, ..., x_k\}$ be an orthogonal basis for a subspace W of R^n and let w be any vector in W. Then the unique scalars $c_1, c_2, ..., c_k$ such that

$$w = c_1x_1 + c_2x_2 + ... + c_kx_k$$

are given by

$$c_i = \frac{w \cdot x_i}{x_i \cdot x_i}, \quad i = 1, 2, ..., k.$$

Orthogonal Basis

Example

Problem Show that $B = \left\{ v_1 = \begin{bmatrix} 4 \\ -2 \end{bmatrix}, v_2 = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \right\}$ forms basis of R^2 and write coordinate vector of $w = \begin{bmatrix} 1 \\ -3 \end{bmatrix}$ w.r.t B.

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As $v_1 \cdot v_1 = 12,\ v_2 \cdot v_2 = 5,\ w \cdot v_1 = 10,\ w \cdot v_2 = -5$. So, $c_1 = \frac{5}{6},\ c_2 = -1$.
Hence, coordinate vector of w is

$$\begin{bmatrix} \frac{5}{6} \\ -1 \end{bmatrix}.$$

Orthogonality

General procedure

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Putting the *row* vectors $v_1^T, v_2^T, \dots, v_m^T$ into a matrix, this is the same as finding all x such that

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The set of all vectors orthogonal to some vectors $v_1, v_2, \ldots, v_m$ in $\mathbf{R}^n$ is the *null space* of the $m \times n$ matrix

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In particular, this set is a subspace!

Orthogonal Complements

Definition

Let W be a subspace of R^n. Its **orthogonal complement** is

$$W^{\perp} = \{v \text{ in } \mathrm{R}^n \mid v \cdot w = 0 \text{ for all } w \text{ in } W\} \qquad \text{read "}W\text{ perp".}$$

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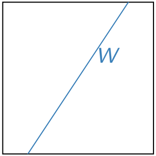
Pictures:

The orthogonal complement of a line in $\mathbb{R}^2$ is



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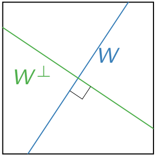

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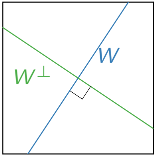

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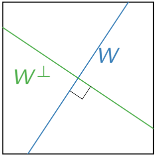

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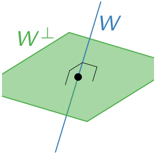

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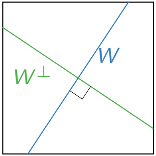

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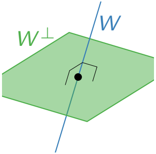

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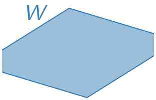

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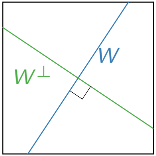

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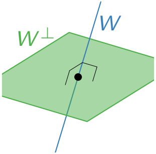

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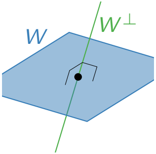

Poll

Poll

Let W be a plane in $\mathbb{R}^4$. How would you describe $W^\perp$?

A. The zero space $\{0\}$.
B. A line in $\mathbb{R}^4$.
C. A plane in $\mathbb{R}^4$.
D. A 3-dimensional space in $\mathbb{R}^4$.
E. All of $\mathbb{R}^4$.

Orthogonal Complements

Basic properties

Let W be a subspace of $\mathbb{R}^n$.

Facts:

Orthogonal Complements

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Let W be a subspace of R^n.

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3. $\dim W + \dim W^\perp = n$
4. If $W = \mathrm{Span}\{v_1, v_2, \ldots, v_m\}$, then

$$\begin{aligned} W^\perp &= \text{all vectors orthogonal to each } v_1, v_2, \ldots, v_m \\ &= \{x \text{ in } \mathrm{R}^n \mid x \cdot v_i = 0 \text{ for all } i = 1, 2, \ldots, m\} \\ &= \mathrm{Nul}\begin{pmatrix} — v_1^T — \\ — v_2^T — \\ \vdots \\ — v_m^T — \end{pmatrix}. \end{aligned}$$

Let's check 1.

- Is 0 in $W^\perp$? Yes: $0 \cdot w = 0$ for any w in W.
- Suppose x, y are in $W^\perp$. So $x \cdot w = 0$ and $y \cdot w = 0$ for all w in W. Then $(x + y) \cdot w = x \cdot w + y \cdot w = 0 + 0 = 0$ for all w in W. So $x + y$ is also in $W^\perp$.
- Suppose x is in $W^\perp$. So $x \cdot w = 0$ for all w in W. If c is a scalar, then $(cx) \cdot w = c(x \cdot 0) = c(0) = 0$ for any w in W. So cx is in $W^\perp$.

Problem: if $W = \text{Span}\left\{ \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \right\}$, compute $W^\perp$.

By property 4, we have to find the null space of the matrix whose rows are $\begin{pmatrix} 1 & 1 & -1 \end{pmatrix}$ and $\begin{pmatrix} 1 & 1 & 1 \end{pmatrix}$, which we did before:

$$\text{Nul}\begin{pmatrix} 1 & 1 & -1 \\ 1 & 1 & 1 \end{pmatrix} = \text{Span}\left\{ \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix} \right\}.$$

Orthogonal Complements
Computation

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We showed before that if A has rows $v_1^T, v_2^T, \ldots, v_m^T$, then

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$$\text{Row}\, A = \text{Col}\, A^T.$$

It is a subspace of $\mathbf{R}^n$.

We showed before that if A has rows $v_1^T, v_2^T, \ldots, v_m^T$, then

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Fact: $(\operatorname{Nul} A)^\perp = \operatorname{Row} A$ and $\operatorname{Col} A = (\operatorname{Nul} A^T)^\perp$.

Orthogonal Complements of Most of the Subspaces We've Seen

For any vectors $v_1, v_2, \ldots, v_m$:

$$\mathrm{Span}\{v_1, v_2, \ldots, v_m\}^\perp = \mathrm{Nul}\begin{pmatrix} - v_1^T - \\ - v_2^T - \\ \vdots \\ - v_m^T - \end{pmatrix}$$

For any matrix A:

$$\mathrm{Row}\,A = \mathrm{Col}\,A^T$$

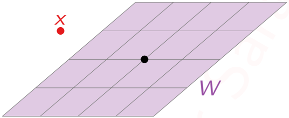
and

$$(\mathrm{Row}\,A)^\perp = \mathrm{Nul}\,A \qquad \mathrm{Row}\,A = (\mathrm{Nul}\,A)^\perp$$

$$(\mathrm{Col}\,A)^\perp = \mathrm{Nul}\,A^T \qquad \mathrm{Col}\,A = (\mathrm{Nul}\,A^T)^\perp$$

Best Approximation

Suppose you measure a data point x which you know for theoretical reasons must lie on a subspace W.



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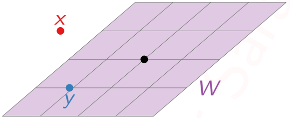

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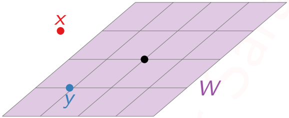

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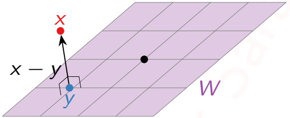

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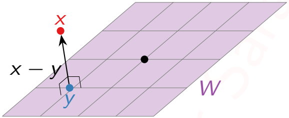

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How do you know that y is the closest point? The vector from y to x is orthogonal to W: it is in the *orthogonal complement* $W^{\perp}$.

Orthogonal Projection onto a Line

Theorem

Let $L = \mathrm{Span}\{u\}$ be a line in R^n, and let x be in R^n. The closest point to x on L is the point

$$\mathrm{proj}_L(x) = \frac{x \cdot u}{u \cdot u}\, u.$$

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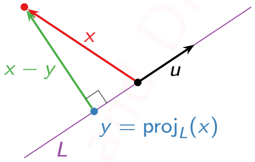

Why? Let $y = \text{proj}_L(x)$. We have to verify that $x - y$ is in $L^{\perp}$. This means proving that $u \cdot (x - y) = 0$.

$$u \cdot (x - y) = u \cdot \left(x - \frac{x \cdot u}{u \cdot u} u\right) = u \cdot x - \frac{x \cdot u}{u \cdot u}(u \cdot u) = u \cdot x - x \cdot u = 0.$$

Orthogonal Projection onto a Line

Example

Compute the orthogonal projection of $x = \begin{pmatrix} -6 \\ 4 \end{pmatrix}$ onto the line L spanned by $u = \begin{pmatrix} 3 \\ 2 \end{pmatrix}$.

$$y = \mathrm{proj}_L(x) = \frac{x \cdot u}{u \cdot u} u = \frac{-18+8}{9+4} \begin{pmatrix} 3 \\ 2 \end{pmatrix} = -\frac{10}{13} \begin{pmatrix} 3 \\ 2 \end{pmatrix}.$$

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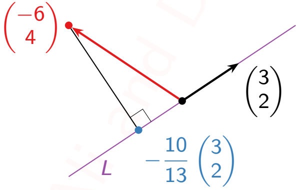

Orthogonal Sets

Definition

A set of *nonzero* vectors is **orthogonal** if each pair of vectors is orthogonal.

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Example: $\mathcal{B} = \left\{ \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \right\}$ is an orthogonal set. Check:

$$\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} = 0 \qquad \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = 0 \qquad \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = 0.$$

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Lemma

An orthogonal set of vectors is linearly independent.

Suppose $\{u_1, u_2, \ldots, u_m\}$ is orthogonal. We need to show that the equation

$$c_1 u_1 + c_2 u_2 + \cdots + c_m u_m = 0$$

has only the trivial solution $c_1 = c_2 = \cdots = c_m = 0$.

$$0 = u_1 \cdot (c_1 u_1 + c_2 u_2 + \cdots + c_m u_m) = c_1(u_1 \cdot u_1) + 0 + 0 + \cdots + 0.$$

Hence $c_1 = 0$. Similarly for the other c_i.

Orthogonal Bases

An orthogonal set $\mathcal{B} = \{u_1, u_2, \ldots, u_m\}$ forms a basis for $W = \operatorname{Span} \mathcal{B}$.

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Theorem

Let $\mathcal{B} = \{u_1, u_2, \ldots, u_m\}$ be an orthogonal set, and let x be a vector in $W = \operatorname{Span}\mathcal{B}$. Then

$$x = \sum_{i=1}^{m} \frac{x \cdot u_i}{u_i \cdot u_i}\, u_i = \frac{x \cdot u_1}{u_1 \cdot u_1}\, u_1 + \frac{x \cdot u_2}{u_2 \cdot u_2}\, u_2 + \cdots + \frac{x \cdot u_m}{u_m \cdot u_m}\, u_m.$$

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In other words, the $\mathcal{B}$-coordinates of x are $\left(\frac{x \cdot u_1}{u_1 \cdot u_1}, \frac{x \cdot u_2}{u_2 \cdot u_2}, \ldots, \frac{x \cdot u_m}{u_m \cdot u_m} \right)$.

Why? If $x = c_1 u_1 + c_2 u_2 + \cdots + c_m u_m$, then

$$x \cdot u_1 = c_1(u_1 \cdot u_1) + 0 + \cdots + 0 \implies c_1 = \frac{x \cdot u_1}{u_1 \cdot u_1}.$$

Similarly for the other c_i.

Orthogonal Bases

Geometric reason

Theorem

Let $\mathcal{B} = \{u_1, u_2, \ldots, u_m\}$ be an orthogonal set, and let x be a vector in $W = \operatorname{Span} \mathcal{B}$. Then

proj$_{L_2}(u_2)$

$$x = \sum_{i=1}^{m} \frac{x \cdot u_i}{u_i \cdot u_i} u_i = \frac{x \cdot u_1}{u_1 \cdot u_1} u_1 + \boxed{\frac{x \cdot u_2}{u_2 \cdot u_2} u_2} + \cdots + \frac{x \cdot u_m}{u_m \cdot u_m} u_m.$$

If L_i is the line spanned by u_i, then this says

$$x = \operatorname{proj}_{L_1}(x) + \operatorname{proj}_{L_2}(x) + \cdots + \operatorname{proj}_{L_m}(x).$$

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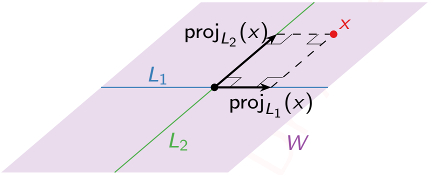

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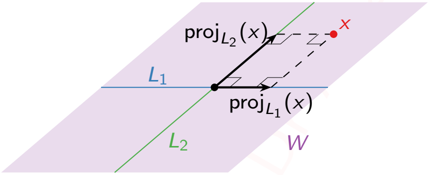

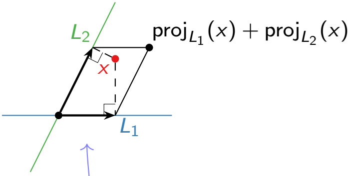

Warning: This only works for an *orthogonal* basis.

Orthogonal Bases

Example

Problem: Find the $\mathcal{B}$-coordinates of $x = \binom{0}{3}$, where

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$$x = \frac{x \cdot u_1}{u_1 \cdot u_1} u_1 + \frac{x \cdot u_2}{u_2 \cdot u_2} u_2 = \frac{3 \cdot 2}{1^2 + 2^2} u_1 + \frac{3 \cdot 2}{(-4)^2 + 2^2} u_2 = \frac{6}{5} u_1 + \frac{6}{20} u_2.$$

So the $\mathcal{B}$-coordinates are $\frac{6}{5}, \frac{6}{20}$.

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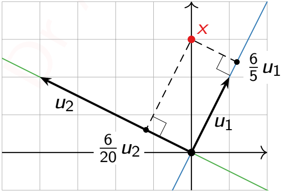

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Answer:

$$\begin{aligned}
[x]_{\mathcal{B}} &= \left(\frac{x \cdot u_1}{u_1 \cdot u_1}, \frac{x \cdot u_2}{u_2 \cdot u_2}, \frac{x \cdot u_3}{u_3 \cdot u_3} \right) \\
&= \left(\frac{6 \cdot 1 + 1 \cdot 1 - 8 \cdot 1}{1^2 + 1^2 + 1^2}, \frac{6 \cdot 1 + 1 \cdot (-2) - 8 \cdot 1}{1^2 + (-2)^2 + 1^2}, \frac{6 \cdot 1 + 1 \cdot 0 + (-8) \cdot (-1)}{1^2 + 0^2 + (-1)^2} \right) \\
&= \left(-\frac{1}{3}, -\frac{2}{3}, 7 \right).
\end{aligned}$$

Check:

$$\begin{pmatrix} 6 \\ 1 \\ -8 \end{pmatrix} = -\frac{1}{3} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} - \frac{2}{3} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} + 7 \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}.$$

✔

Orthonormal Basis

Definition

A set of vectors in R^n is called an **orthonormal set** if it is an orthogonal set of unit vectors.

Theorem

Let $\{x_1, x_2, ..., x_k\}$ be an orthonormal basis for a subspace W of R^n and let w be any vector in W. Then the unique scalars $c_1, c_2, ..., c_k$ such that

$$w = c_1 x_1 + c_2 x_2 + ... + c_k x_k$$

are given by

$$c_i = w \cdot x_i, \quad i = 1, 2, ..., k.$$

Theorem

The matrix Q (square or rectangular) has orthonormal columns if and only if $Q^TQ = I$

Proof.

If Q has orthonormal columns then,

$$(Q^TQ)_{ij} = q_i \cdot q_j = I.$$

Conversely,
If $Q^TQ = I$, then

$$q_i \cdot q_j = \begin{cases} 1, & \text{if } i \neq j \\ 0, & \text{if} i = j. \end{cases}$$

Orthogonal Matrices

Theorem

Any square matrix Q whose columns form an orthonormal set is called **Orthogonal Matrix**.

Theorem

Let Q be an $n \times n$ matrix. Then the following statements are equivalent:

1. Q is orthogonal.
2. $Q^T = Q^{-1}$.
3. $\|Q\mathbf{x}\| = \|\mathbf{x}\|$.
4. $Q\mathbf{x} \cdot Q\mathbf{y} = \mathbf{x} \cdot \mathbf{y}$.

   where $\mathbf{x}$ and $\mathbf{y}$ are from R^n.

Orthogonal Matrices

Theorem

Let Q be an orthogonal matrix.

1. Q^{-1} is orthogonal.
2. $det(Q) = \pm 1$
3. If λ is an eigenvalue of Q, then $|\lambda| = 1$.
4. Product of orthogonal matrices of same size is another orthogonal matrix.
5. Rows of Q forms an orthonormal set.

Orthogonal Matrices

Examples

- $\begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & cos\theta \end{bmatrix}$.
- $\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$.

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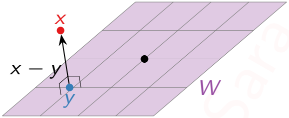

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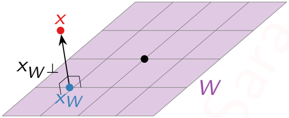

Reformulation: Every vector x can be decompsed uniquely as

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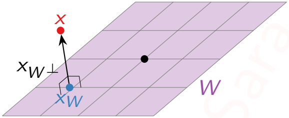

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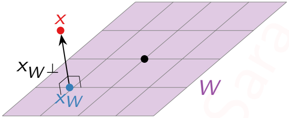

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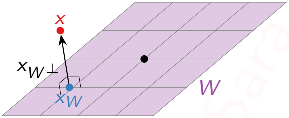

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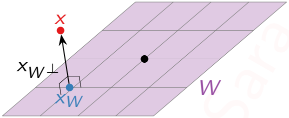

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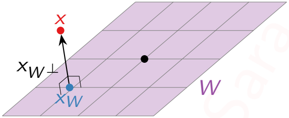

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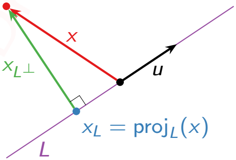

Orthogonal Projections

Definition

Let W be a subspace of R^n, and let $\{u_1, u_2, \ldots, u_m\}$ be an *orthogonal* basis for W. The **orthogonal projection** of a vector x onto W is

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Theorem

Let W be a subspace of R^n, and let x be a vector in R^n. Then $\mathrm{proj}_W(x)$ is the closest point to x in W. Therefore

$$\boxed{x_W = \mathrm{proj}_W(x) \qquad x_{W^\perp} = x - \mathrm{proj}_W(x).}$$

Why? Let $y = \mathrm{proj}_W(x)$. We need to show that $x - y$ is in $W^\perp$. In other words, $u_i \cdot (x - y) = 0$ for each i. Let's do u_1:

$$u_1 \cdot (x - y) = u_1 \cdot \left(x - \sum_{i=1}^{m} \frac{x \cdot u_i}{u_i \cdot u_i}\, u_i \right) = u_1 \cdot x - \frac{x \cdot u_1}{u_1 \cdot u_1}(u_1 \cdot u_1) - 0 - \cdots = 0.$$

Orthogonal Projections

Easy example

What is the projection of $x = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$ onto the xy-plane?

Answer: The xy-plane is $W = \mathrm{Span}\{e_1, e_2\}$, and $\{e_1, e_2\}$ is an orthogonal basis.

$$x_W = \mathrm{proj}_W \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} = \frac{x \cdot e_1}{e_1 \cdot e_1} e_1 + \frac{x \cdot e_2}{e_2 \cdot e_2} e_2 = \frac{1 \cdot 1}{1^2} e_1 + \frac{1 \cdot 2}{1^2} e_2 = \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix}.$$

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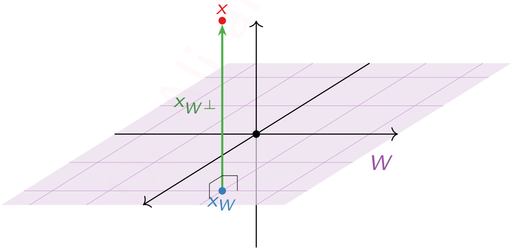
So this is the same projection as before.



Orthogonal Projections

More complicated example

What is the projection of $x = \begin{pmatrix} -1.1 \\ 1.4 \\ 1.45 \end{pmatrix}$ onto $W = \text{Span}\left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1.1 \\ -.2 \end{pmatrix} \right\}$?

Answer: The basis is orthogonal, so

$$x_W = \text{proj}_W \begin{pmatrix} -1.1 \\ 1.4 \\ 1.45 \end{pmatrix} = \frac{x \cdot u_1}{u_1 \cdot u_1} u_1 + \frac{x \cdot u_2}{u_2 \cdot u_2} u_2$$

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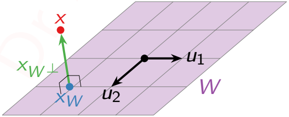

Orthogonal Projections

Picture

Let W be a subspace of R^n, and let $\{u_1, u_2, \ldots, u_m\}$ be an orthogonal basis for W. Let $L_i = \mathrm{Span}\{u_i\}$. Then

$$\mathrm{proj}_W(x) = \sum_{i=1}^{m} \frac{x \cdot u_i}{u_i \cdot u_i}\, u_i = \sum_{i=1}^{m} \mathrm{proj}_{L_i}(x).$$

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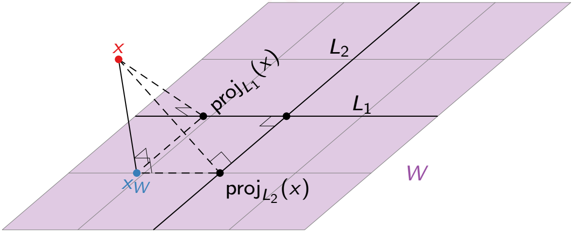
So the orthogonal projection is formed by adding orthogonal projections onto perpendicular lines.



First we restate the property we've been using all along.

Best Approximation Theorem

Let W be a subspace of R^n, and let x be a vector in R^n. Then $y = \mathrm{proj}_W(x)$ is the closest point in W to x, in the sense that

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Orthogonal Projections
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4. The range of proj_W is W.

Poll

Let W be a subspace of $\mathbb{R}^n$.

Poll

Let A be the matrix for proj_W. What is/are the eigenvalue(s) of A?

A. 0 B. 1 C. -1 D. $0, 1$ E. $1, -1$ F. $0, -1$ G. $-1, 0, 1$

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We have $\dim W + \dim W^\perp = n$, so that gives n linearly independent eigenvectors already.

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So the answer is D.

What is the matrix for $\mathrm{proj}_W \colon \mathrm{R}^3 \to \mathrm{R}^3$, where

$$W = \mathrm{Span}\left\{ \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \right\}?$$

Answer: Recall how to compute the matrix for a linear transformation:

$$A = \begin{pmatrix} | & | & | \\ \mathrm{proj}_W(e_1) & \mathrm{proj}_W(e_2) & \mathrm{proj}_W(e_3) \\ | & | & | \end{pmatrix}.$$

We compute:

$$\mathrm{proj}_W(e_1) = \frac{e_1 \cdot u_1}{u_1 \cdot u_1} u_1 + \frac{e_1 \cdot u_2}{u_2 \cdot u_2} u_2 = \frac{1}{2} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} + \frac{1}{3} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 5/6 \\ 1/3 \\ -1/6 \end{pmatrix}$$

$$\mathrm{proj}_W(e_2) = \frac{e_2 \cdot u_1}{u_1 \cdot u_1} u_1 + \frac{e_2 \cdot u_2}{u_2 \cdot u_2} u_2 = 0 + \frac{1}{3} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1/3 \\ 1/3 \\ 1/3 \end{pmatrix}$$

$$\mathrm{proj}_W(e_3) = \frac{e_3 \cdot u_1}{u_1 \cdot u_1} u_1 + \frac{e_3 \cdot u_2}{u_2 \cdot u_2} u_2 = -\frac{1}{2} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} + \frac{1}{3} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} -1/6 \\ 1/3 \\ 5/6 \end{pmatrix}$$

Therefore $A = \begin{pmatrix} 5/6 & 1/3 & -1/6 \\ 1/3 & 1/3 & 1/3 \\ -1/6 & 1/3 & 5/6 \end{pmatrix}$.

Orthogonal Projections

Matrix facts

Let W be an m-dimensional subspace of $\mathbb{R}^n$, let $\text{proj}_W \colon \mathbb{R}^n \to W$ be the projection, and let A be the matrix for proj_L.

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Let W be an m-dimensional subspace of $\mathbf{R}^n$, let $\text{proj}_W \colon \mathbf{R}^n \to W$ be the projection, and let A be the matrix for proj_L.

Fact 1: A is diagonalizable with eigenvalues 0 and 1; it is similar to the diagonal matrix with m ones and $n - m$ zeros on the diagonal.

Why? Let $v_1, v_2, \ldots, v_m$ be a basis for W, and let $v_{m+1}, v_{m+2}, \ldots, v_n$ be a basis for $W^\perp$. These are (linearly independent) eigenvectors with eigenvalues 1 and 0, respectively, and they form a basis for $\mathbf{R}^n$ because there are n of them.

Example: If W is a plane in $\mathbf{R}^3$, then A is similar to projection onto the xy-plane:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Orthogonal Projections

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Let W be an m-dimensional subspace of $\mathbf{R}^n$, let $\text{proj}_W \colon \mathbf{R}^n \to W$ be the projection, and let A be the matrix for proj_L.

Fact 1: A is diagonalizable with eigenvalues 0 and 1; it is similar to the diagonal matrix with m ones and $n-m$ zeros on the diagonal.

Why? Let $v_1, v_2, \ldots, v_m$ be a basis for W, and let $v_{m+1}, v_{m+2}, \ldots, v_n$ be a basis for $W^\perp$. These are (linearly independent) eigenvectors with eigenvalues 1 and 0, respectively, and they form a basis for $\mathbf{R}^n$ because there are n of them.

Example: If W is a plane in $\mathbf{R}^3$, then A is similar to projection onto the xy-plane:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Fact 2: $A^2 = A$.

Why? Projecting twice is the same as projecting once:

$$\text{proj}_W \circ \text{proj}_W = \text{proj}_W \implies A \cdot A = A.$$

What is the distance from e_1 to $W = \text{Span}\left\{ \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \right\}$?

Answer: The closest point on W to e_1 is $\text{proj}_W(e_1) = \begin{pmatrix} 5/6 \\ 1/3 \\ -1/6 \end{pmatrix}$.

The distance from e_1 to this point is

$$\begin{aligned}
\text{dist}\big(e_1, \text{proj}_W(e_1)\big) &= \|(e_1)_{W^\perp}\| \\
&= \left\| \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} - \begin{pmatrix} 5/6 \\ 1/3 \\ -1/6 \end{pmatrix} \right\| \\
&= \left\| \begin{pmatrix} 1/6 \\ -1/3 \\ -1/6 \end{pmatrix} \right\| \\
&= \sqrt{(1/6)^2 + (-1/3)^2 + (-1/6)^2} \\
&= \frac{1}{\sqrt{6}}.
\end{aligned}$$

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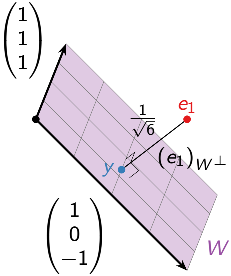

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All of the procedures we learned require an *orthogonal* basis $\{u_1, u_2, \ldots, u_m\}$.

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Problem: What if your basis isn't orthogonal?

Solution: The Gram–Schmidt process: take any basis and make it orthogonal.

The Gram–Schmidt Process

Let $\{v_1, v_2, \ldots, v_m\}$ be a basis for a subspace W of R^n. Define:

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Remark

In fact, for every i between 1 and n, the set $\{u_1, u_2, \dots, u_i\}$ is an orthogonal basis for $\mathrm{Span}\{v_1, v_2, \dots, v_i\}$.

The Gram–Schmidt Process

Two vectors

Find an orthogonal basis $\{u_1, u_2\}$ for $W = \mathrm{Span}\{v_1, v_2\}$, where

$$v_1 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \quad \text{and} \quad v_2 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}.$$

Run Gram–Schmidt:

$$\text{1. } u_1 = v_1 \qquad \text{2. } u_2 = v_2 - \frac{v_2 \cdot u_1}{u_1 \cdot u_1} u_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} - \frac{2}{2} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

Why does this work?

- First we take $u_1 = v_1$.
- Now we're sad because $u_1 \cdot v_2 \neq 0$, so we can't take $u_2 = v_2$.
- Fix: let $L_1 = \mathrm{Span}\{u_1\}$, and let $u_2 = (v_2)_{L_1^\perp} = v_2 - \mathrm{proj}_{L_1}(v_2)$.
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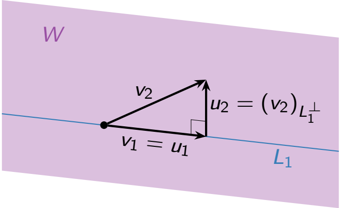

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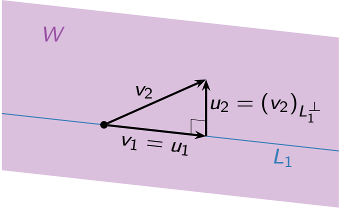

Important: $\mathrm{Span}\{u_1, u_2\} = \mathrm{Span}\{v_1, v_2\} = W$: this is an *orthogonal* basis for the *same* subspace.

The Gram–Schmidt Process

Three vectors

Find an orthogonal basis $\{u_1, u_2, u_3\}$ for $W = \mathrm{Span}\{v_1, v_2, v_3\} = \mathrm{R}^3$, where

$$v_1 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \qquad v_2 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \qquad v_3 = \begin{pmatrix} 3 \\ 1 \\ 1 \end{pmatrix}.$$

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The Gram–Schmidt Process

Three vectors

Find an orthogonal basis $\{u_1, u_2, u_3\}$ for $W = \text{Span}\{v_1, v_2, v_3\} = \mathbb{R}^3$, where

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The Gram–Schmidt Process

Three vectors, continued

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Why does this work?

- Once we have u_1 and u_2, then we're sad because v_3 is not orthogonal to u_1 and u_2.
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- By construction, $u_1 \cdot u_3 = 0 = u_2 \cdot u_3$ because $W_2 \perp u_3$.

Check:

$$u_1 \cdot u_2 = 0 \ ✓$$
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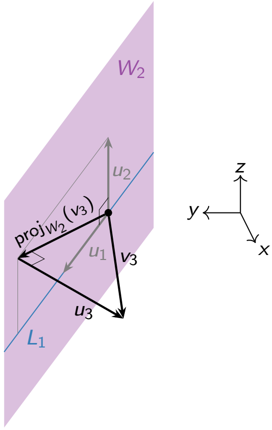

The Gram–Schmidt Process

Three vectors in $\mathbb{R}^4$

Find an orthogonal basis $\{u_1, u_2, u_3\}$ for $W = \text{Span}\{v_1, v_2, v_3\}$, where

$$v_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \qquad v_2 = \begin{pmatrix} -1 \\ 4 \\ 4 \\ -1 \end{pmatrix} \qquad v_3 = \begin{pmatrix} 4 \\ -2 \\ -2 \\ 0 \end{pmatrix}.$$

Run Gram–Schmidt:

1. $u_1 = v_1$
2. $u_2 = v_2 - \frac{v_2 \cdot u_1}{u_1 \cdot u_1} u_1 = \begin{pmatrix} -1 \\ 4 \\ 4 \\ -1 \end{pmatrix} - \frac{6}{4} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} -5/2 \\ 5/2 \\ 5/2 \\ -5/2 \end{pmatrix}$
3. $u_3 = v_3 - \frac{v_3 \cdot u_1}{u_1 \cdot u_1} u_1 - \frac{v_3 \cdot u_2}{u_2 \cdot u_2} u_2$

$$= \begin{pmatrix} 4 \\ -2 \\ -2 \\ 0 \end{pmatrix} - \frac{0}{24} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} - \frac{-20}{25} \begin{pmatrix} -5/2 \\ 5/2 \\ 5/2 \\ -5/2 \end{pmatrix} = \begin{pmatrix} 2 \\ 0 \\ 0 \\ -2 \end{pmatrix}$$

Poll

Poll

What happens if you try to run Gram–Schmidt on a linearly *de*pendent set of vectors $\{v_1, v_2, \ldots, v_m\}$?

A. You get an inconsistent equation.

B. For some i you get $u_i = u_{i-1}$.

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If $\{v_1, v_2, \dots, v_m\}$ is linearly dependent, then some v_i is in $\mathrm{Span}\{v_1, v_2, \dots, v_{i-1}\} = \mathrm{Span}\{u_1, u_2, \dots, u_{i-1}\}$.

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This means

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$$\implies u_i = v_i - \mathrm{proj}_{\mathrm{Span}\{u_1,u_2,\ldots,u_{i-1}\}}(v_i) = 0.$$

In this case, you can simply discard u_i and v_i and continue: so Gram–Schmidt produces an orthogonal basis from any spanning set!

QR Factorization

QR Factorization Theorem

Let A be a matrix with linearly independent columns. Then

$$A = QR$$

where Q has orthonormal columns and R is upper-triangular with positive diagonal entries.

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Recall: A set of vectors $\{v_1, v_2, \ldots, v_m\}$ is **orthonormal** if they are orthogonal unit vectors: $v_i \cdot v_j = 0$ when $i \neq j$, and $v_i \cdot v_i = 1$.

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The columns of A are a basis for $W = \operatorname{Col} A$. The columns of Q come from Gram–Schmidt as applied to the columns of A, after normalizing to unit vectors. The columns of R come from the steps in Gram–Schmidt.

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Let A be a matrix with linearly independent columns. Then

$$A = QR$$

where Q has orthonormal columns and R is upper-triangular with positive diagonal entries.

Recall: A set of vectors $\{v_1, v_2, \ldots, v_m\}$ is **orthonormal** if they are orthogonal unit vectors: $v_i \cdot v_j = 0$ when $i \neq j$, and $v_i \cdot v_i = 1$.

Check: A matrix Q has orthonormal columns if and only if $Q^T Q = I$.

The columns of A are a basis for $W = \operatorname{Col} A$. The columns of Q come from Gram–Schmidt as applied to the columns of A, after normalizing to unit vectors. The columns of R come from the steps in Gram–Schmidt.

Here is the procedure for producing a QR factorization.

QR Factorization

Example

Find the QR factorization of $A = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}$.

QR Factorization
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(The columns of A are the vectors v_1, v_2, v_3 from a previous example.)

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Step 1: Run Gram–Schmidt

$$u_1 = v_1 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

$$u_2 = v_2 - \frac{v_2 \cdot u_1}{u_1 \cdot u_1} u_1 = v_2 - 1\, u_1 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\begin{aligned} u_3 &= v_3 - \frac{v_3 \cdot u_1}{u_1 \cdot u_1} u_1 - \frac{v_3 \cdot u_2}{u_2 \cdot u_2} u_2 \\ &= v_3 - 2\, u_1 - 1\, u_2 = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \end{aligned}$$

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Find the QR factorization of $A = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}$.

(The columns of A are the vectors v_1, v_2, v_3 from a previous example.)

Step 1: Run Gram–Schmidt and solve for v_1, v_2, v_3 in terms of u_1, u_2, u_3.

$$u_1 = v_1 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \qquad v_1 = u_1$$

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QR Factorization

Example, continued

$$v_1 = 1\,u_1 \qquad v_2 = 1\,u_1 + 1\,u_2 \qquad v_3 = 2\,u_1 + 1\,u_2 + 1\,u_3$$

Step 2: Write $A = \widehat{Q}\widehat{R}$, where $\widehat{Q}$ has *orthogonal* columns u_1, u_2, u_3 and $\widehat{R}$ is upper-triangular with 1s on the diagonal.

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Do this by putting the above equations in matrix form:

$$A \longrightarrow \begin{pmatrix} | & | & | \\ v_1 & v_2 & v_3 \\ | & | & | \end{pmatrix} = \underbrace{\begin{pmatrix} | & | & | \\ u_1 & u_2 & u_3 \\ | & | & | \end{pmatrix}}_{\widehat{Q}} \underbrace{\begin{pmatrix} 1 & 1 & 2 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}}_{\widehat{R}}$$

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$$\text{first column of } A = \begin{pmatrix} | & | & | \\ u_1 & u_2 & u_3 \\ | & | & | \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = 1 u_1 = v_1$$

QR Factorization

Example, continued

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QR Factorization
Example, continued

$$v_1 = 1u_1 \qquad v_2 = 1u_1 + 1u_2 \qquad v_3 = 2u_1 + 1u_2 + 1u_3$$

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$$\text{third column of } A = \begin{pmatrix} | & | & | \\ u_1 & u_2 & u_3 \\ | & | & | \end{pmatrix}\begin{pmatrix} 2 \\ 1 \\ 1 \end{pmatrix} = 2u_1 + 1u_2 + 1u_3 = v_3$$

QR Factorization

Example, continued

$$A = \widehat{Q}\widehat{R} \qquad \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 1 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 & 2 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}$$

Step 3: Scale the columns of $\widehat{Q}$ to get unit vectors, and scale the rows of $\widehat{R}$ by the opposite factor, to get Q and R.

QR Factorization

Example, continued

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QR Factorization

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$$\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix} = \begin{pmatrix} 1/\sqrt{2} & 0 & 1 \\ 1/\sqrt{2} & 0 & -1 \\ 0/\sqrt{2} & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \cdot \sqrt{2} & 1 \cdot \sqrt{2} & 2 \cdot \sqrt{2} \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}.$$

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Example, continued

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Note that the entries in the ith column of Q multiply by the entries in the ith row of R, so this doesn't change the product.

QR Factorization

Example, continued

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The final QR decomposition is:

$$A = QR \qquad Q = \begin{pmatrix} 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 0 & 1 & 0 \end{pmatrix} \qquad R = \begin{pmatrix} \sqrt{2} & \sqrt{2} & 2\sqrt{2} \\ 0 & 1 & 1 \\ 0 & 0 & \sqrt{2} \end{pmatrix}$$

QR Factorization
Another example

Find the QR factorization of $A = \begin{pmatrix} 1 & -1 & 4 \\ 1 & 4 & -2 \\ 1 & 4 & -2 \\ 1 & -1 & 0 \end{pmatrix}$.

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(The columns are vectors from a previous example.)

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$$u_1 = v_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \qquad v_1 = u_1$$

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QR Factorization

Another example, continued

$$v_1 = 1\, u_1 \qquad v_2 = \frac{3}{2}\, u_1 + 1\, u_2 \qquad v_3 = 0\, u_1 - \frac{4}{5}\, u_2 + 1\, u_3$$

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Step 3: Normalize the columns of $\widehat{Q}$ and the rows of $\widehat{R}$ to get Q and R:

$$Q = \begin{pmatrix} | & | & | \\ u_1/\|u_1\| & u_2/\|u_2\| & u_3/\|u_3\| \\ | & | & | \end{pmatrix} = \begin{pmatrix} 1/2 & -1/2 & 1/\sqrt{2} \\ 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \\ 1/2 & -1/2 & -1/\sqrt{2} \end{pmatrix}$$

$$R = \begin{pmatrix} 1 \cdot \|u_1\| & 3/2 \cdot \|u_1\| & 0 \cdot \|u_1\| \\ 0 & 1 \cdot \|u_2\| & -4/5 \cdot \|u_2\| \\ 0 & 0 & 1 \cdot \|u_3\| \end{pmatrix} = \begin{pmatrix} 2 & 3 & 0 \\ 0 & 5 & -4 \\ 0 & 0 & 2\sqrt{2} \end{pmatrix}$$

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Another example, continued

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QR Factorization

Application: computing determinants

Let A be an *invertible* $n \times n$ matrix. Consider its QR factorization

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But R is upper-triangular, so it's easy to compute its determinant!

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Then $A\widehat{x} = \widehat{b}$ is a consistent equation.

A solution $\widehat{x}$ to $A\widehat{x} = \widehat{b}$ is a **least squares solution.**

Least Squares Solutions

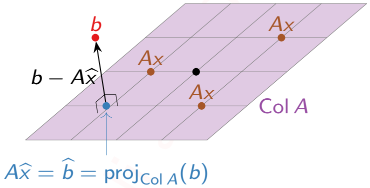
Let A be an $m \times n$ matrix.

Definition

A **least squares solution** to $Ax = b$ is a vector $\widehat{x}$ in $\mathbb{R}^n$ such that

$$\|b - A\widehat{x}\| \leq \|b - Ax\|$$

for all x in $\mathbb{R}^n$.



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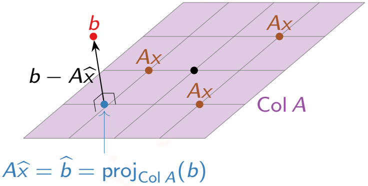
Note that $b - A\widehat{x}$ is in $(\mathrm{Col}\, A)^{\perp}$.



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Let A be an $m \times n$ matrix.

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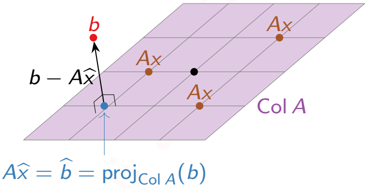

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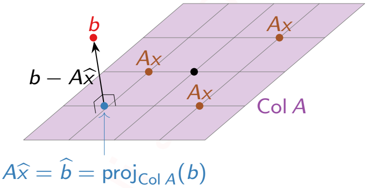

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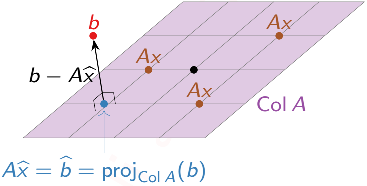

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This is because $\widehat{b}$ is the closest vector to b such that $A\widehat{x} = \widehat{b}$ is consistent.

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The least squares solutions to $Ax = b$ are the solutions to

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Why is this true?

- We want to find $\widehat{x}$ such that $A\widehat{x} = \text{proj}_{\text{Col}\,A}(b)$.
- This means $b - A\widehat{x}$ is in $(\text{Col}\,A)^{\perp}$.
- Recall that $(\text{Col}\,A)^{\perp} = \text{Nul}(A^T)$.
- So $b - A\widehat{x}$ is in $(\text{Col}\,A)^{\perp}$ if and only if $A^T(b - A\widehat{x}) = 0$.
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Alternative when A has orthogonal columns $v_1, v_2, \ldots, v_n$:

$$\widehat{b} = \mathrm{proj}_{\mathrm{Col}\,A}(b) = \sum_{i=1}^{n} \frac{b \cdot v_i}{v_i \cdot v_i}\, v_i$$

The right hand side equals $A\widehat{x}$, where $\widehat{x} = \left(\frac{b \cdot v_1}{v_1 \cdot v_1}, \frac{b \cdot v_2}{v_2 \cdot v_2}, \cdots, \frac{b \cdot v_n}{v_n \cdot v_n}\right)$.

Least Squares Solutions

Example

Find the least squares solutions to $Ax = b$ where:

$$A = \begin{pmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{pmatrix} \qquad b = \begin{pmatrix} 6 \\ 0 \\ 0 \end{pmatrix}.$$

We have

$$A^T A = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 2 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{pmatrix} = \begin{pmatrix} 3 & 3 \\ 3 & 5 \end{pmatrix}$$

and

$$A^T b = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 2 \end{pmatrix} \begin{pmatrix} 6 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 6 \\ 0 \end{pmatrix}.$$

Row reduce:

$$\left(\begin{array}{cc|c} 3 & 3 & 6 \\ 3 & 5 & 0 \end{array}\right) \rightsquigarrow \left(\begin{array}{cc|c} 1 & 0 & 5 \\ 0 & 1 & -3 \end{array}\right).$$

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So the only least squares solution is $\widehat{x} = \begin{pmatrix} 5 \\ -3 \end{pmatrix}$.

Least Squares Solutions

Example, continued

How close did we get?

$$\widehat{b} = A\widehat{x} = \begin{pmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} 5 \\ -3 \end{pmatrix} = \begin{pmatrix} 5 \\ 2 \\ -1 \end{pmatrix}$$

The distance from b is

$$\|b - A\widehat{x}\| = \left\| \begin{pmatrix} 6 \\ 0 \\ 0 \end{pmatrix} - \begin{pmatrix} 5 \\ 2 \\ -1 \end{pmatrix} \right\| = \left\| \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} \right\| = \sqrt{1^2 + (-2)^2 + 1^2} = \sqrt{6}.$$

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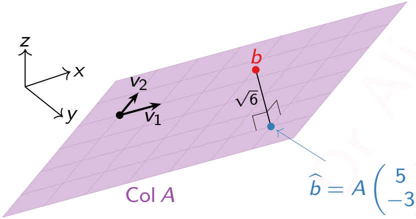

$\widehat{b} = A\begin{pmatrix} 5 \\ -3 \end{pmatrix}$

Let

$$v_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \quad \text{and} \quad v_2 = \begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix}$$

be the columns of A, and let $\mathcal{B} = \{v_1, v_2\}$.

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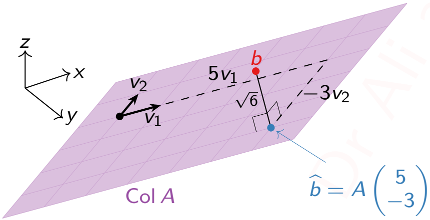

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Note $\widehat{x} = \binom{5}{-3}$ is just the $\mathcal{B}$-coordinates of $\widehat{b}$, in Col $A = \text{Span}\{v_1, v_2\}$.

Least Squares Solutions

Second example

Find the least squares solutions to $Ax = b$ where:

$$A = \begin{pmatrix} 2 & 0 \\ -1 & 1 \\ 0 & 2 \end{pmatrix} \qquad b = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}.$$

We have

$$A^T A = \begin{pmatrix} 2 & -1 & 0 \\ 0 & 1 & 2 \end{pmatrix} \begin{pmatrix} 2 & 0 \\ -1 & 1 \\ 0 & 2 \end{pmatrix} = \begin{pmatrix} 5 & -1 \\ -1 & 5 \end{pmatrix}$$

and

$$A^T b = \begin{pmatrix} 2 & -1 & 0 \\ 0 & 1 & 2 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = \begin{pmatrix} 2 \\ -2 \end{pmatrix}.$$

Row reduce:

$$\left(\begin{array}{cc|c} 5 & -1 & 2 \\ -1 & 5 & -2 \end{array}\right) \rightsquigarrow \left(\begin{array}{cc|c} 1 & 0 & 1/3 \\ 0 & 1 & -1/3 \end{array}\right).$$

Find the least squares solutions to $Ax = b$ where:

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Least Squares Solutions

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When does $Ax = b$ have a *unique* least squares solution $\widehat{x}$?

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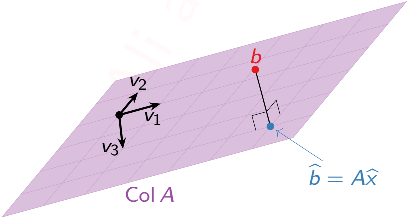
Why? If the columns of A are linearly *de*pendent, then $A\widehat{x} = \widehat{b}$ has many solutions:



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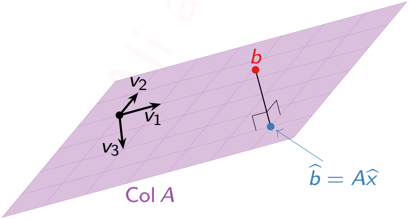


Note: $A^T A$ is always a square matrix, but it need not be invertible.

Application

Data modeling: best fit line

Find the best fit line through $(0, 6)$, $(1, 0)$, and $(2, 0)$.

The general equation of a line is

$$y = C + Dx.$$

So we want to solve:

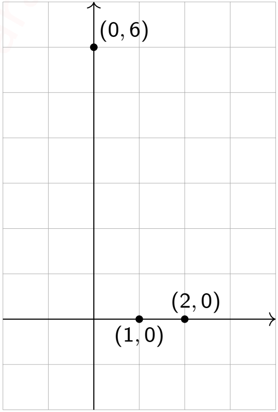
$$\begin{aligned} 6 &= C + D \cdot 0 \\ 0 &= C + D \cdot 1 \\ 0 &= C + D \cdot 2. \end{aligned}$$

In matrix form:

$$\begin{pmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} 6 \\ 0 \\ 0 \end{pmatrix}.$$

We already saw: the least squares solution is $\binom{5}{-3}$. So the best fit line is

$$y = -3x + 5.$$



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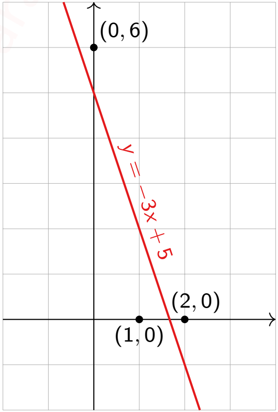

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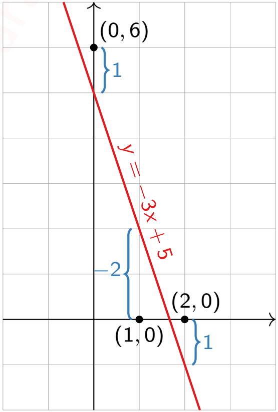

$$A\begin{pmatrix} 5 \\ -3 \end{pmatrix} - \begin{pmatrix} 6 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}$$

Poll

Poll

What does the best fit line minimize?

A. The sum of the squares of the distances from the data points to the line.

B. The sum of the squares of the vertical distances from the data points to the line.

C. The sum of the squares of the horizontal distances from the data points to the line.

D. The maximal distance from the data points to the line.

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Answer: B. See the picture on the previous slide.

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So we want to solve:

$$\begin{aligned}
(0)^2 + \quad A(2)^2 + \quad B(0)(2) + \quad C(0) + \quad D(2) + E &= 0 \\
(2)^2 + \quad A(1)^2 + \quad B(2)(1) + \quad C(2) + \quad D(1) + E &= 0 \\
(1)^2 + A(-1)^2 + \quad B(1)(-1) + \quad C(1) + D(-1) + E &= 0 \\
(-1)^2 + A(-2)^2 + B(-1)(-2) + C(-1) + D(-2) + E &= 0 \\
(-3)^2 + \quad A(1)^2 + \quad B(-3)(1) + C(-3) + \quad D(1) + E &= 0
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(1)^2 + A(-1)^2 + B(1)(-1) + C(1) + D(-1) + E &= 0 \\
(-1)^2 + A(-2)^2 + B(-1)(-2) + C(-1) + D(-2) + E &= 0 \\
(-3)^2 + A(1)^2 + B(-3)(1) + C(-3) + D(1) + E &= 0
\end{aligned}$$

In matrix form:

$$\begin{pmatrix} 4 & 0 & 0 & 2 & 1 \\ 1 & 2 & 2 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 4 & 2 & -1 & -2 & 1 \\ 1 & -3 & -3 & 1 & 1 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \\ E \end{pmatrix} = \begin{pmatrix} 0 \\ -4 \\ -1 \\ -1 \\ -9 \end{pmatrix}.$$

Application

Best fit ellipse, continued

$$A = \begin{pmatrix} 4 & 0 & 0 & 2 & 1 \\ 1 & 2 & 2 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 4 & 2 & -1 & -2 & 1 \\ 1 & -3 & -3 & 1 & 1 \end{pmatrix} \qquad b = \begin{pmatrix} 0 \\ -4 \\ -1 \\ -1 \\ -9 \end{pmatrix}.$$

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$$A^T A = \begin{pmatrix} 35 & 6 & -4 & 1 & 11 \\ 6 & 18 & 10 & -4 & 0 \\ -4 & 10 & 15 & 0 & -1 \\ 1 & -4 & 0 & 11 & 1 \\ 11 & 0 & -1 & 1 & 5 \end{pmatrix} \qquad A^T b = \begin{pmatrix} -18 \\ 18 \\ 19 \\ -10 \\ -15 \end{pmatrix}$$

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Row reduce:

$$\left(\begin{array}{ccccc|c} 35 & 6 & -4 & 1 & 11 & -18 \\ 6 & 18 & 10 & -4 & 0 & 18 \\ -4 & 10 & 15 & 0 & -1 & 19 \\ 1 & -4 & 0 & 11 & 1 & -10 \\ 11 & 0 & -1 & 1 & 5 & -15 \end{array}\right) \rightsquigarrow \left(\begin{array}{ccccc|c} 1 & 0 & 0 & 0 & 0 & 16/7 \\ 0 & 1 & 0 & 0 & 0 & -8/7 \\ 0 & 0 & 1 & 0 & 0 & 15/7 \\ 0 & 0 & 0 & 1 & 0 & -6/7 \\ 0 & 0 & 0 & 0 & 1 & -52/7 \end{array}\right)$$

Application

Best fit ellipse, continued

$$A = \begin{pmatrix} 4 & 0 & 0 & 2 & 1 \\ 1 & 2 & 2 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 4 & 2 & -1 & -2 & 1 \\ 1 & -3 & -3 & 1 & 1 \end{pmatrix} \qquad b = \begin{pmatrix} 0 \\ -4 \\ -1 \\ -1 \\ -9 \end{pmatrix}.$$

$$A^T A = \begin{pmatrix} 35 & 6 & -4 & 1 & 11 \\ 6 & 18 & 10 & -4 & 0 \\ -4 & 10 & 15 & 0 & -1 \\ 1 & -4 & 0 & 11 & 1 \\ 11 & 0 & -1 & 1 & 5 \end{pmatrix} \qquad A^T b = \begin{pmatrix} -18 \\ 18 \\ 19 \\ -10 \\ -15 \end{pmatrix}$$

Row reduce:

$$\left(\begin{array}{ccccc|c} 35 & 6 & -4 & 1 & 11 & -18 \\ 6 & 18 & 10 & -4 & 0 & 18 \\ -4 & 10 & 15 & 0 & -1 & 19 \\ 1 & -4 & 0 & 11 & 1 & -10 \\ 11 & 0 & -1 & 1 & 5 & -15 \end{array}\right) \rightsquigarrow \left(\begin{array}{ccccc|c} 1 & 0 & 0 & 0 & 0 & 16/7 \\ 0 & 1 & 0 & 0 & 0 & -8/7 \\ 0 & 0 & 1 & 0 & 0 & 15/7 \\ 0 & 0 & 0 & 1 & 0 & -6/7 \\ 0 & 0 & 0 & 0 & 1 & -52/7 \end{array}\right)$$

Best fit ellipse:

$$x^2 + \frac{16}{7}y^2 - \frac{8}{7}xy + \frac{15}{7}x - \frac{6}{7}y - \frac{52}{7} = 0$$

Application

Best fit ellipse, continued

$$A = \begin{pmatrix} 4 & 0 & 0 & 2 & 1 \\ 1 & 2 & 2 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 4 & 2 & -1 & -2 & 1 \\ 1 & -3 & -3 & 1 & 1 \end{pmatrix} \qquad b = \begin{pmatrix} 0 \\ -4 \\ -1 \\ -1 \\ -9 \end{pmatrix}.$$

$$A^T A = \begin{pmatrix} 35 & 6 & -4 & 1 & 11 \\ 6 & 18 & 10 & -4 & 0 \\ -4 & 10 & 15 & 0 & -1 \\ 1 & -4 & 0 & 11 & 1 \\ 11 & 0 & -1 & 1 & 5 \end{pmatrix} \qquad A^T b = \begin{pmatrix} -18 \\ 18 \\ 19 \\ -10 \\ -15 \end{pmatrix}$$

Row reduce:

$$\left(\begin{array}{ccccc|c} 35 & 6 & -4 & 1 & 11 & -18 \\ 6 & 18 & 10 & -4 & 0 & 18 \\ -4 & 10 & 15 & 0 & -1 & 19 \\ 1 & -4 & 0 & 11 & 1 & -10 \\ 11 & 0 & -1 & 1 & 5 & -15 \end{array}\right) \rightsquigarrow \left(\begin{array}{ccccc|c} 1 & 0 & 0 & 0 & 0 & 16/7 \\ 0 & 1 & 0 & 0 & 0 & -8/7 \\ 0 & 0 & 1 & 0 & 0 & 15/7 \\ 0 & 0 & 0 & 1 & 0 & -6/7 \\ 0 & 0 & 0 & 0 & 1 & -52/7 \end{array}\right)$$

Best fit ellipse:

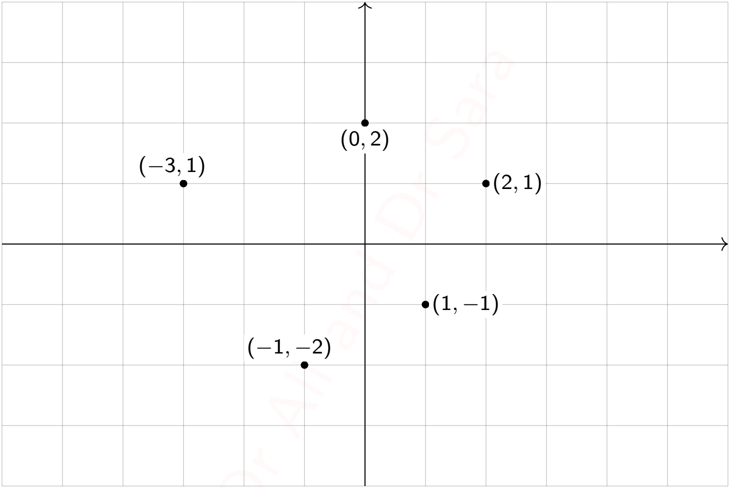
$$x^2 + \frac{16}{7}y^2 - \frac{8}{7}xy + \frac{15}{7}x - \frac{6}{7}y - \frac{52}{7} = 0$$

or

$$7x^2 + 16y^2 - 8xy + 15x - 6y - 52 = 0.$$

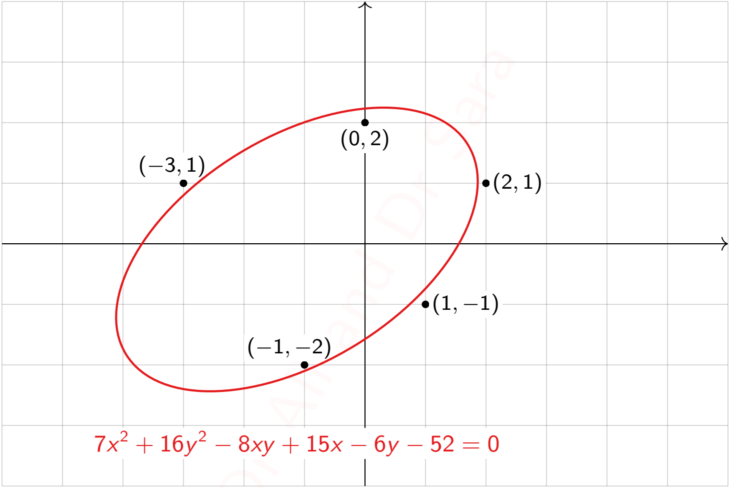
Application

Best fit ellipse, picture



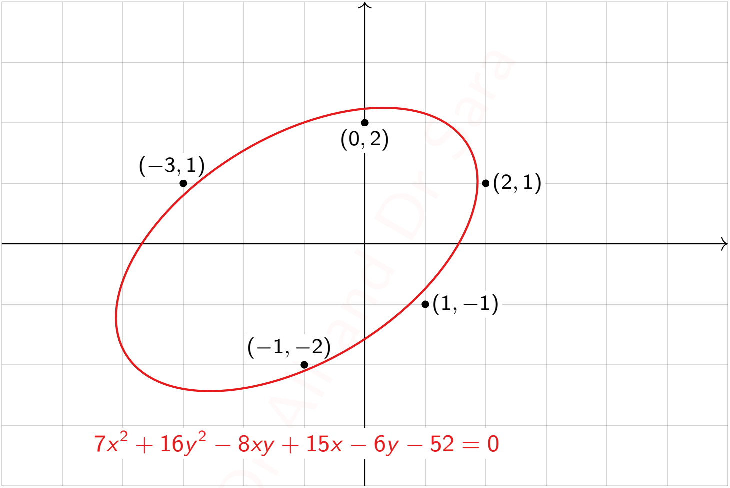
Application

Best fit ellipse, picture



Application

Best fit ellipse, picture



Remark: Gauss invented the method of least squares to do exactly this: he predicted the (elliptical) orbit of the asteroid Ceres as it passed behind the sun in 1801.

What least squares problem $Ax = b$ finds the best parabola through the points $(-1, 0.5)$, $(1, -1)$, $(2, -0.5)$, $(3, 2)$?

The general equation for a parabola is

$$y = Ax^2 + Bx + C.$$

So we want to solve:

$$\begin{aligned} 0.5 &= A(-1)^2 + B(-1) + C \\ -1 &= A(1)^2 + B(1) + C \\ -0.5 &= A(2)^2 + B(2) + C \\ 2 &= A(3)^2 + B(3) + C \end{aligned}$$

In matrix form:

$$\begin{pmatrix} 1 & -1 & 1 \\ 1 & 1 & 1 \\ 4 & 2 & 1 \\ 9 & 3 & 1 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \end{pmatrix} = \begin{pmatrix} 0.5 \\ -1 \\ -0.5 \\ 2 \end{pmatrix}.$$

Application

Best fit parabola

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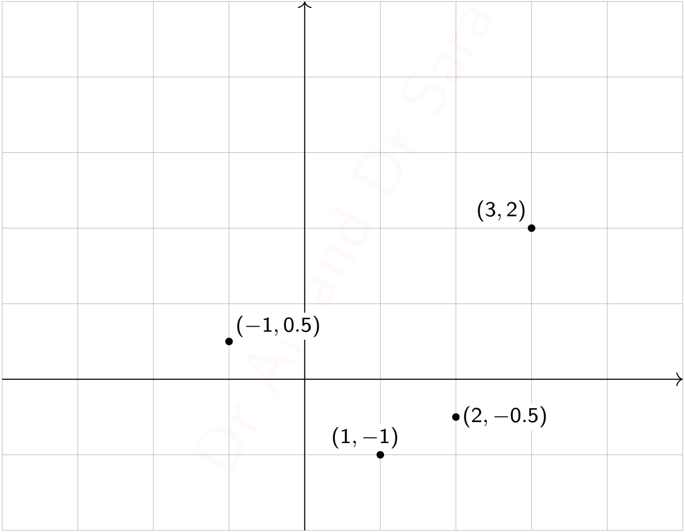
Answer:

$$88y = 53x^2 - \frac{379}{5}x - 82$$

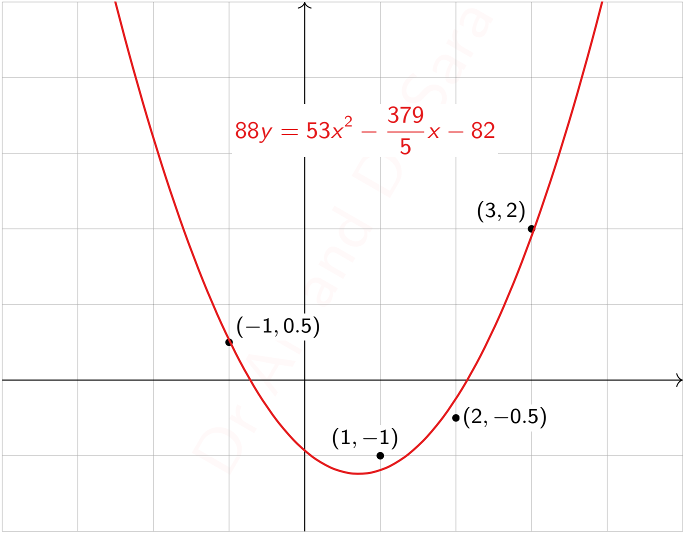
Application

Best fit parabola, picture



Application

Best fit parabola, picture



What least squares problem $Ax = b$ finds the best linear function $f(x, y)$ fitting the following data?

x	y	$f(x,y)$
1	0	0
0	1	1
-1	0	3
0	-1	4

The general equation for a linear function in two variables is

$$f(x, y) = Ax + By + C.$$

So we want to solve

$$\begin{aligned} A(1) + \quad B(0) + C &= 0 \\ A(0) + \quad B(1) + C &= 1 \\ A(-1) + \quad B(0) + C &= 3 \\ A(0) + B(-1) + C &= 4 \end{aligned}$$

In matrix form:

$$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ -1 & 0 & 1 \\ 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 3 \\ 4 \end{pmatrix}.$$

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In matrix form:

$$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ -1 & 0 & 1 \\ 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 3 \\ 4 \end{pmatrix}.$$

Answer:

$$f(x, y) = -\frac{3}{2}x - \frac{3}{2}y + 2$$