

Lectures 8-10

# Linear algebra: Dot products and Projections

DSC 40A, Fall 2025

## Announcements

- Homework 2 was released Friday.
- Groupwork 3 is due **tonight**.
- Check out [FAQs page](#) and the [tutor-created supplemental resources](#) on the course website.

# Agenda

- Recap: Simple linear regression and correlation.
- Connections to related models.
- Dot products.
- Spans and projections.

## Question 🤔

Answer at [q.dsc40a.com](https://q.dsc40a.com)

**Remember, you can always ask questions at [q.dsc40a.com!](https://q.dsc40a.com)**

If the direct link doesn't work, click the " Lecture Questions" link in the top right corner of [dsc40a.com](https://dsc40a.com).

## Simple linear regression

- Model:  $H(x) = w_0 + w_1 x$ .
- Loss function: squared loss, i.e.  $L_{\text{sq}}(y_i, H(x_i)) = (y_i - H(x_i))^2$ .
- Average loss, i.e. empirical risk:

$$R_{\text{sq}}(w_0, w_1) = \frac{1}{n} \sum_{i=1}^n (y_i - (w_0 + w_1 x_i))^2$$

- Optimal model parameters, found by minimizing empirical risk:

$$w_1^* = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} = r \frac{\sigma_y}{\sigma_x} \quad w_0^* = \bar{y} - w_1^* \bar{x}$$

## The correlation coefficient

- The correlation coefficient,  $r$ , is defined as the average of the product of  $x$  and  $y$ , when both are in standard units.
- Let  $\sigma_x$  be the standard deviation of the  $x_i$ s, and  $\bar{x}$  be the mean of the  $x_i$ s.
- $x_i$  in standard units is  $\frac{x_i - \bar{x}}{\sigma_x}$ .
- The correlation coefficient, then, is:

$$r = \frac{1}{n} \sum_{i=1}^n \left( \frac{x_i - \bar{x}}{\sigma_x} \right) \left( \frac{y_i - \bar{y}}{\sigma_y} \right)$$

## Correlation and mean squared error

- **Claim:** Suppose that  $w_0^*$  and  $w_1^*$  are the optimal intercept and slope for the regression line. Then,

$$R_{\text{sq}}(w_0^*, w_1^*) = \sigma_y^2(1 - \mathbf{r}^2)$$

- That is, the **mean squared error** of the regression line's predictions and the correlation coefficient,  $\mathbf{r}$ , always satisfy the relationship above.
- Even if it's true, why do we care?
  - In machine learning, we often use both the **mean squared error** and  $\mathbf{r}^2$  to compare the performances of different models.
  - If we can prove the above statement, we can show that **finding models that minimize mean squared error** is equivalent to **finding models that maximize  $\mathbf{r}^2$** .

**Proof that**  $R_{\text{sq}}(w_0^*, w_1^*) = \sigma_y^2(1 - r^2)$



# Connections to related models

## Exercise

Suppose we choose the model  $H(x) = w_0$  and squared loss.

What is the optimal model parameter,  $w_0^*$ ?

## Exercise

Suppose we choose the model  $H(x) = w_1x$  and squared loss.

What is the optimal model parameter,  $w_1^*$ ?

## Comparing mean squared errors

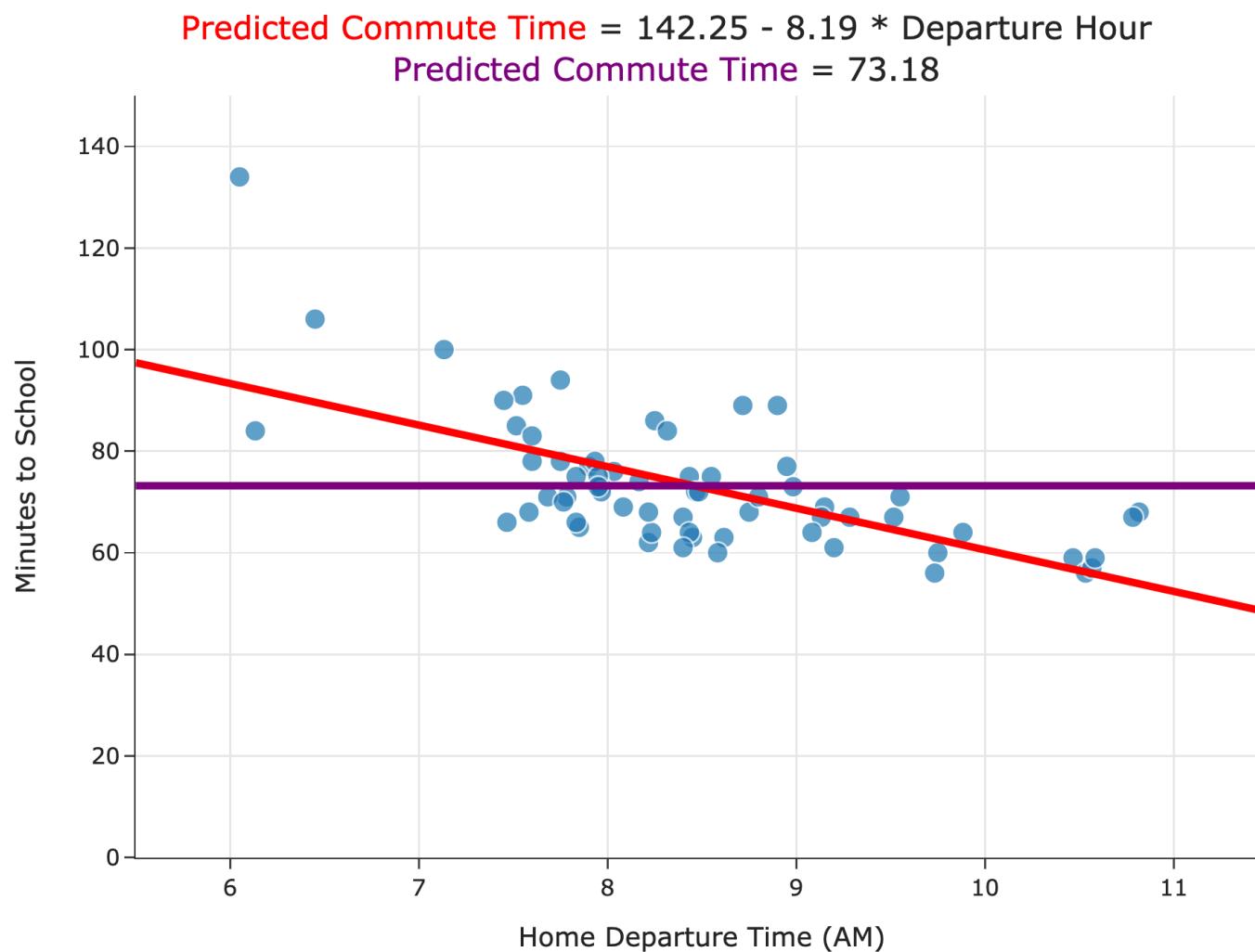
- With both:
  - the constant model,  $H(x) = h$ , and
  - the simple linear regression model,  $H(x) = w_0 + w_1x$ ,

when we chose squared loss, we minimized mean squared error to find optimal parameters:

$$R_{\text{sq}}(H) = \frac{1}{n} \sum_{i=1}^n (y_i - H(x_i))^2$$

- Which model minimizes mean squared error more?

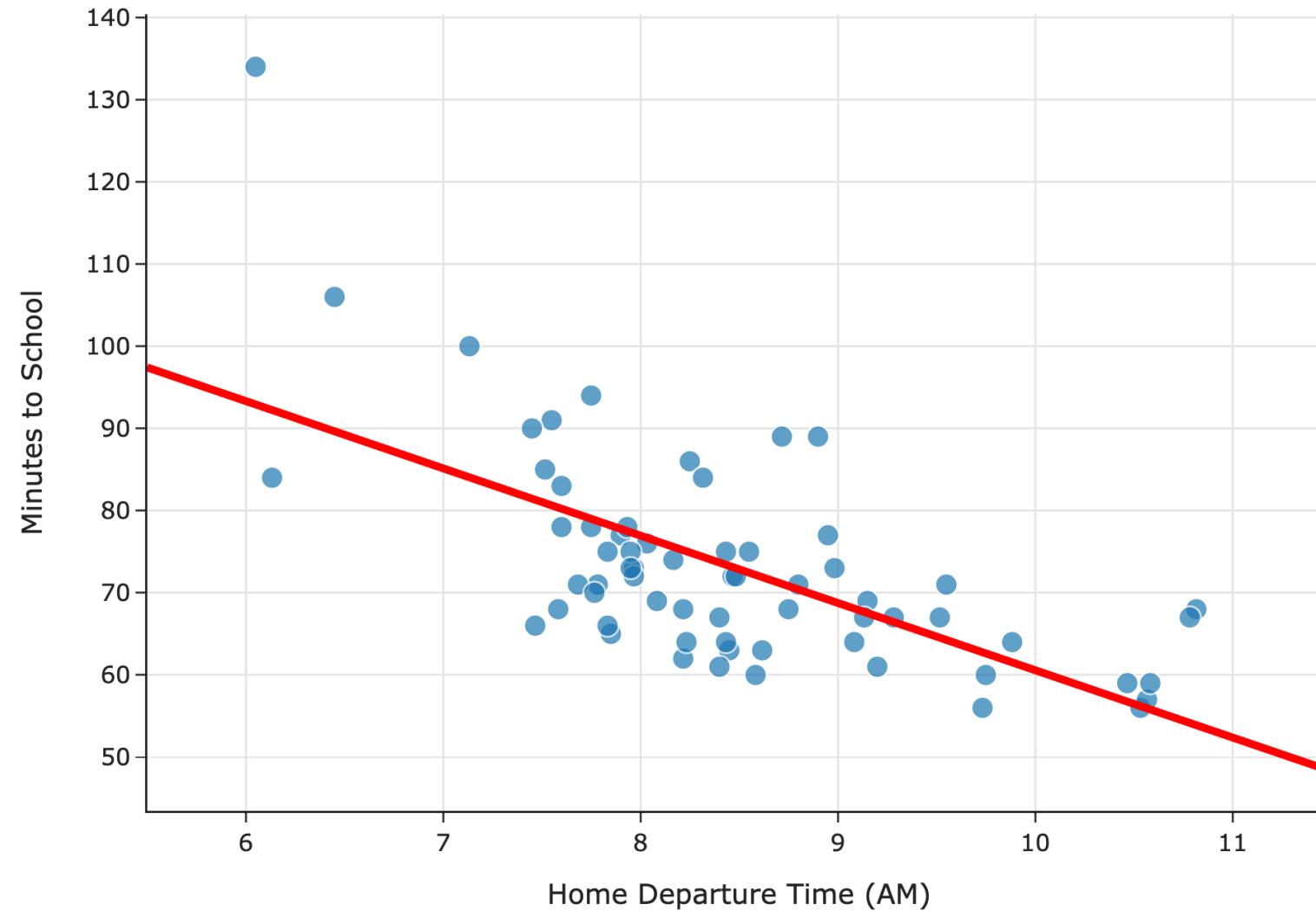
# Comparing mean squared errors



$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n (y_i - H(x_i))^2$$

- The MSE of the best simple linear regression model is  $\approx 97$
- The MSE of the best constant model is  $\approx 167$
- The simple linear regression model is a more flexible version of the constant model.

Predicted Commute Time =  $142.25 - 8.19 * \text{Departure Hour}$



# Linear algebra

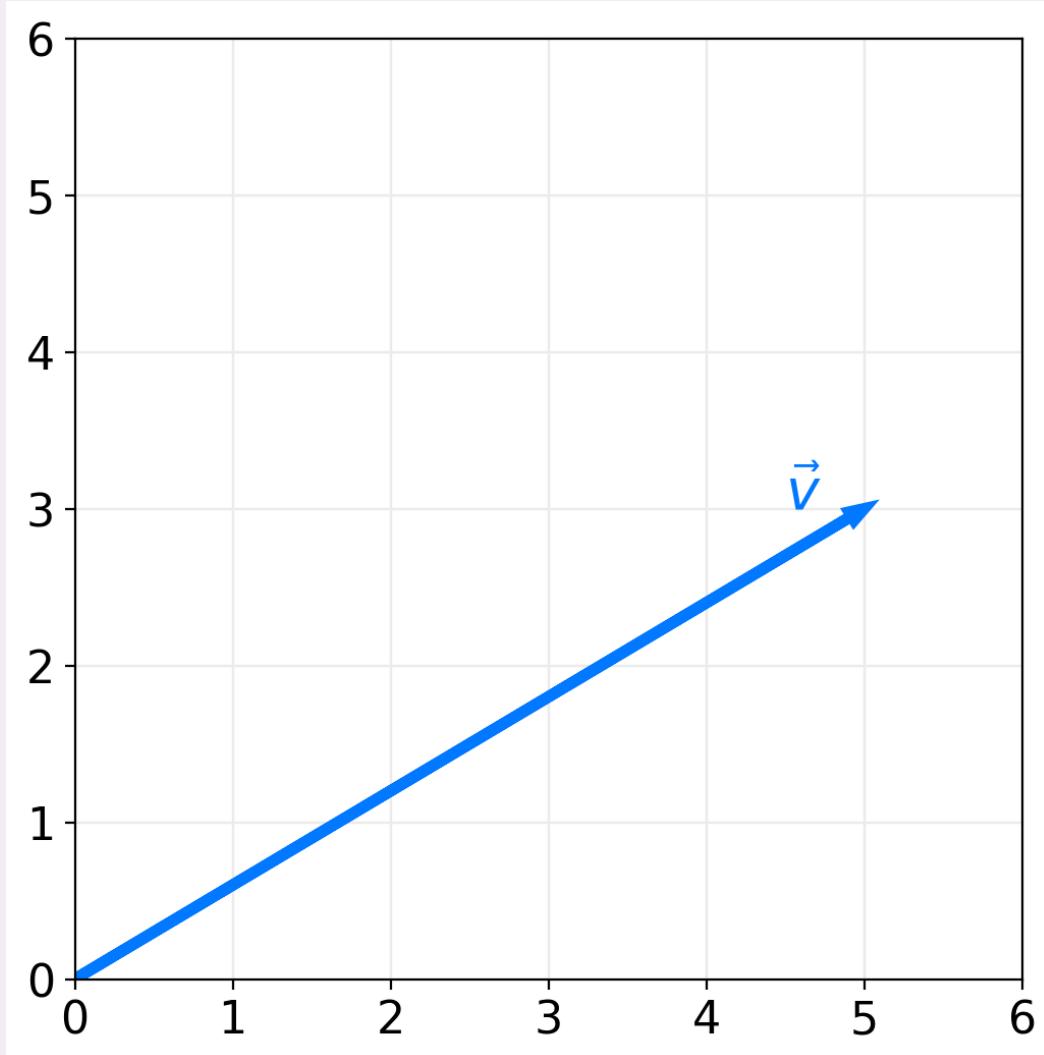
## Wait... why do we need linear algebra?

- Soon, we'll want to make predictions using more than one feature.
  - Example: Predicting commute times using departure hour and temperature.
- Thinking about linear regression in terms of **matrices and vectors** will allow us to find hypothesis functions that:
  - Use multiple features (input variables).
  - Are nonlinear in the features, e.g.  $H(x) = w_0 + w_1x + w_2x^2$ .

## Question 1: Norm

What is the length of  $\vec{v}$ ?

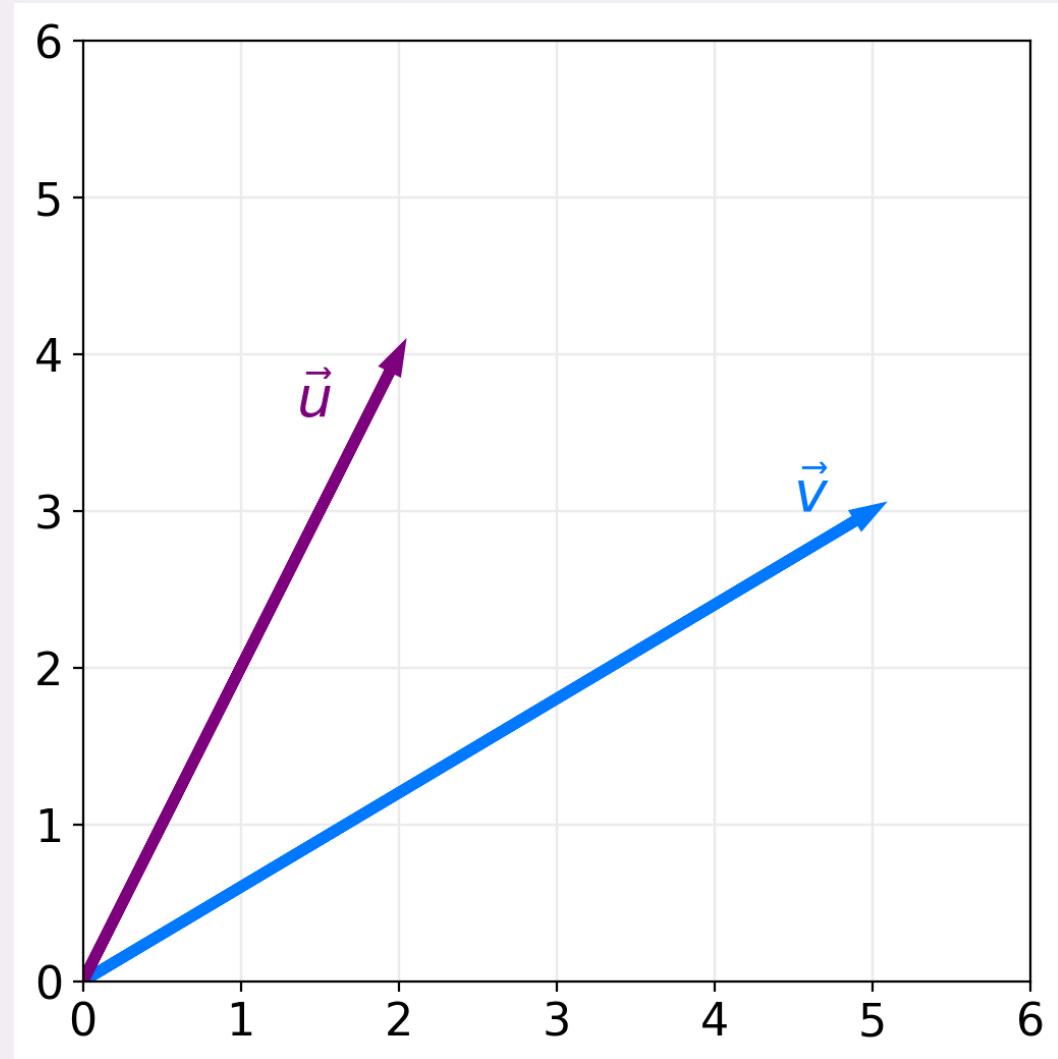
- A. 8
- B.  $\sqrt{34}$
- C.  $\sqrt{38}$
- D. 34



## Question 2: Dot product

What is  $\vec{u} \cdot \vec{v}$ ?

- A. 22
- B. 24
- C.  $\sqrt{680}$
- D.  $\begin{bmatrix} 10 \\ 12 \end{bmatrix}$



## Question 3: Norm

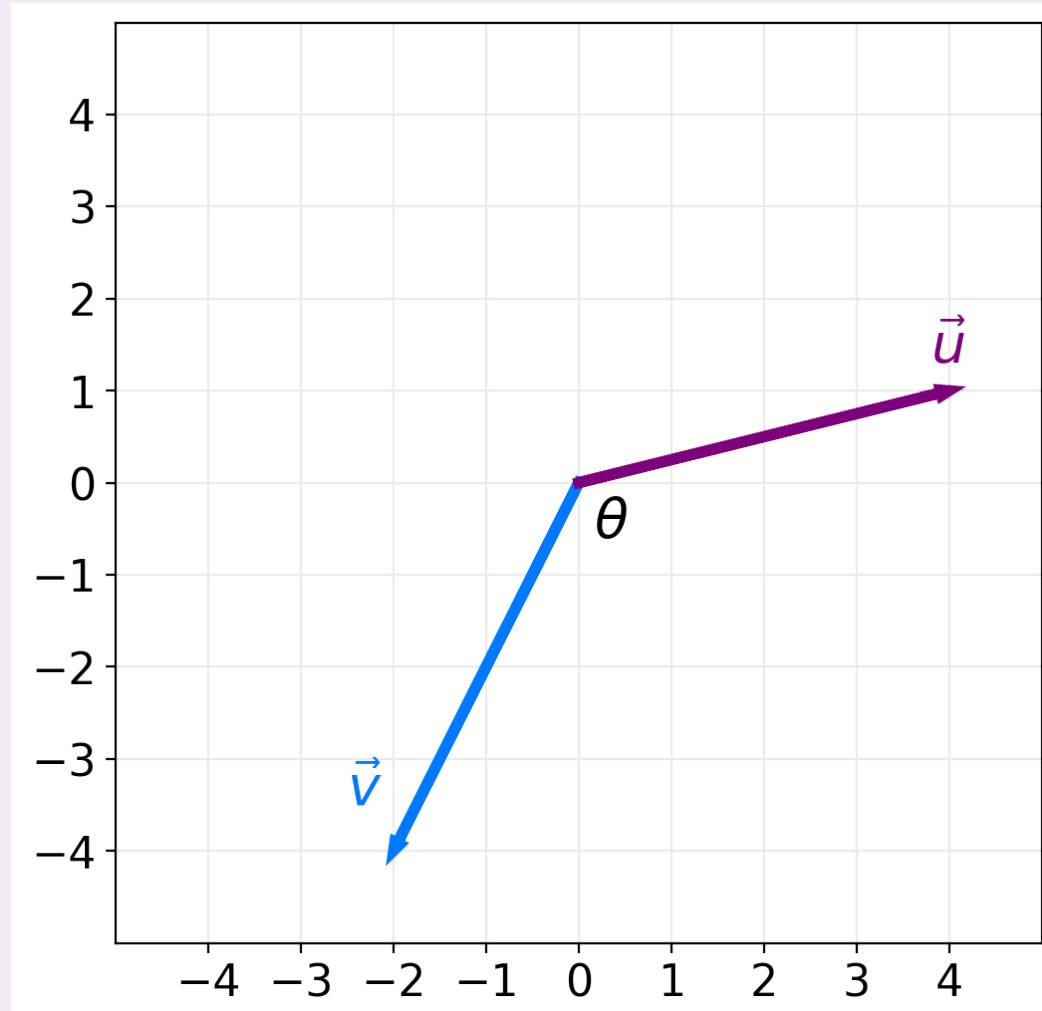
Which of these is another expression for the length of  $\vec{v}$ ?

- A.  $\vec{v} \cdot \vec{v}$
- B.  $\sqrt{\vec{v}^2}$
- C.  $\sqrt{\vec{v} \cdot \vec{v}}$
- D.  $\vec{v}^2$
- E. More than one of the above.

## Question 4: $\cos \theta$

What is  $\cos \theta$ ?

- A.  $\frac{6}{\sqrt{85}}$
- B.  $\frac{-6}{\sqrt{85}}$
- C.  $\frac{-3}{85}$
- D.  $\frac{-2}{3}$



## Question 5: Orthogonality

Which of these vectors in  $\mathbb{R}^3$  orthogonal to:

$$\vec{v} = \begin{bmatrix} 2 \\ 5 \\ -8 \end{bmatrix} ?$$

- A.  $\begin{bmatrix} -2 \\ -5 \\ 8 \end{bmatrix}$
- B.  $\begin{bmatrix} 5 \\ -8 \\ 2 \end{bmatrix}$
- C.  $\begin{bmatrix} 8 \\ 0 \\ 2 \end{bmatrix}$
- D. All of the above

## Warning

- We're **not** going to cover every single detail from your linear algebra course.
- There will be facts that you're expected to remember that we won't explicitly say.
  - For example, if  $A$  and  $B$  are two matrices, then  $AB \neq BA$ .
  - This is the kind of fact that we will only mention explicitly if it's directly relevant to what we're studying.
  - But you still need to know it, and it may come up in homework questions.
- We **will** review the topics that you really need to know well.

# Dot Products

# Vectors

- A **vector** in  $\mathbb{R}^n$  is an **ordered collection of  $n$  numbers**.
- We use lower-case letters with an arrow on top to represent vectors, and we usually write vectors as **columns**.

$$\vec{v} = \begin{bmatrix} 8 \\ 3 \\ -2 \\ 5 \end{bmatrix}$$

- Another way of writing the above vector is  $\vec{v} = [8, 3, -2, 5]^\top$ .
- Since  $\vec{v}$  has four **components**, we say  $\vec{v} \in \mathbb{R}^4$ .

# The geometric interpretation of a vector

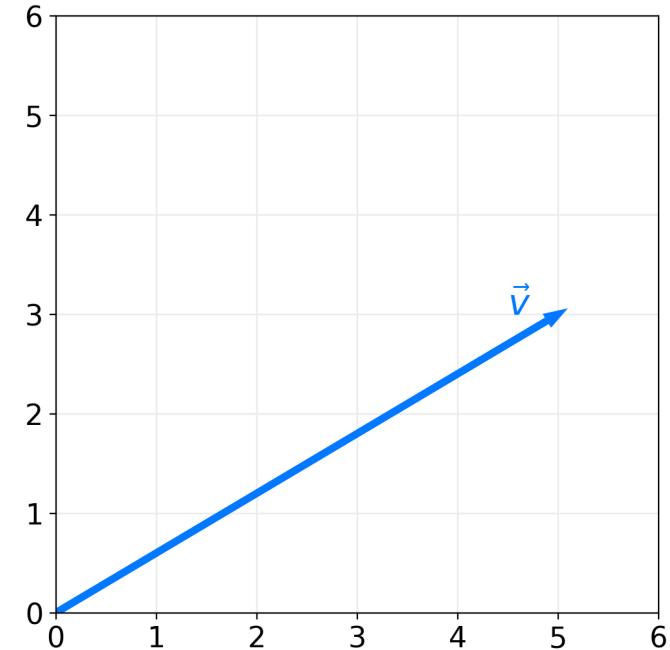
- A vector  $\vec{v} = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}$  is an arrow to the point

$(v_1, v_2, \dots, v_n)$  from the origin.

- The **length**, or  $L_2$  **norm**, of  $\vec{v}$  is:

$$\|\vec{v}\| = \sqrt{v_1^2 + v_2^2 + \dots + v_n^2}$$

- A vector is sometimes described as an object with a **magnitude/length** and **direction**.



## Dot product: coordinate definition

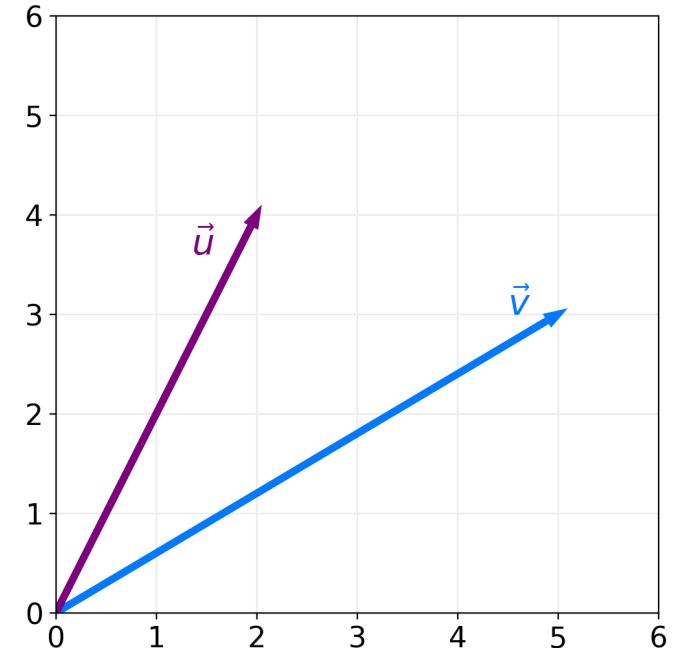
- The **dot product** of two vectors  $\vec{u}$  and  $\vec{v}$  in  $\mathbb{R}^n$  is written as:

$$\vec{u} \cdot \vec{v} = \vec{u}^\top \vec{v}$$

- The computational definition of the dot product:

$$\vec{u} \cdot \vec{v} = \sum_{i=1}^n u_i v_i = u_1 v_1 + u_2 v_2 + \dots + u_n v_n$$

- The result is a **scalar**, i.e. a single number.



## Dot product: geometric definition

- The computational definition of the dot product:

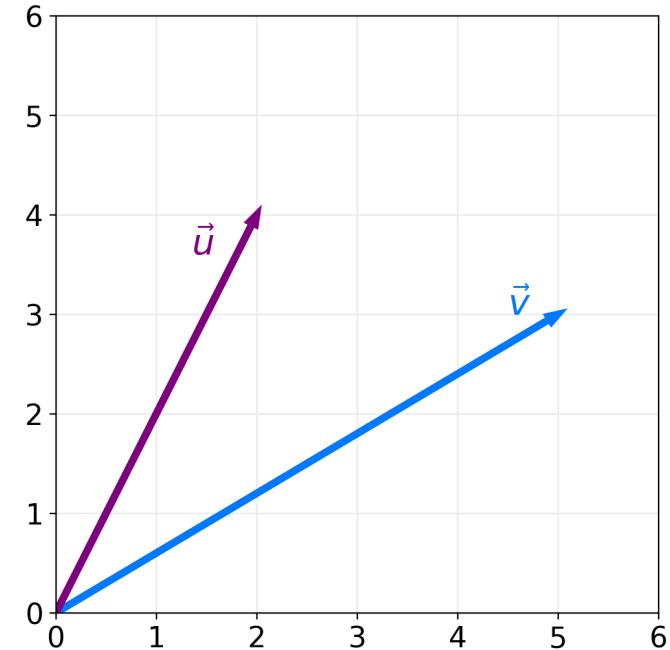
$$\vec{u} \cdot \vec{v} = \sum_{i=1}^n u_i v_i = u_1 v_1 + u_2 v_2 + \dots + u_n v_n$$

- The geometric definition of the dot product:

$$\vec{u} \cdot \vec{v} = \|\vec{u}\| \|\vec{v}\| \cos \theta$$

where  $\theta$  is the angle between  $\vec{u}$  and  $\vec{v}$ .

- The two definitions are equivalent! This equivalence allows us to find the angle  $\theta$  between two vectors.



## Orthogonal vectors

- Recall:  $\cos 90^\circ = 0$ .
- Since  $\vec{u} \cdot \vec{v} = \|\vec{u}\| \|\vec{v}\| \cos \theta$ , if the angle between two vectors is  $90^\circ$ , their dot product is  $\|\vec{u}\| \|\vec{v}\| \cos 90^\circ = 0$ .
- If the angle between two vectors is  $90^\circ$ , we say they are perpendicular, or more generally, **orthogonal**.
- Key idea:

two vectors are **orthogonal**  $\iff \vec{u} \cdot \vec{v} = 0$

## Exercise

Find a non-zero vector in  $\mathbb{R}^3$  orthogonal to:

$$\vec{v} = \begin{bmatrix} 2 \\ 5 \\ -8 \end{bmatrix}$$

# Spans and projections

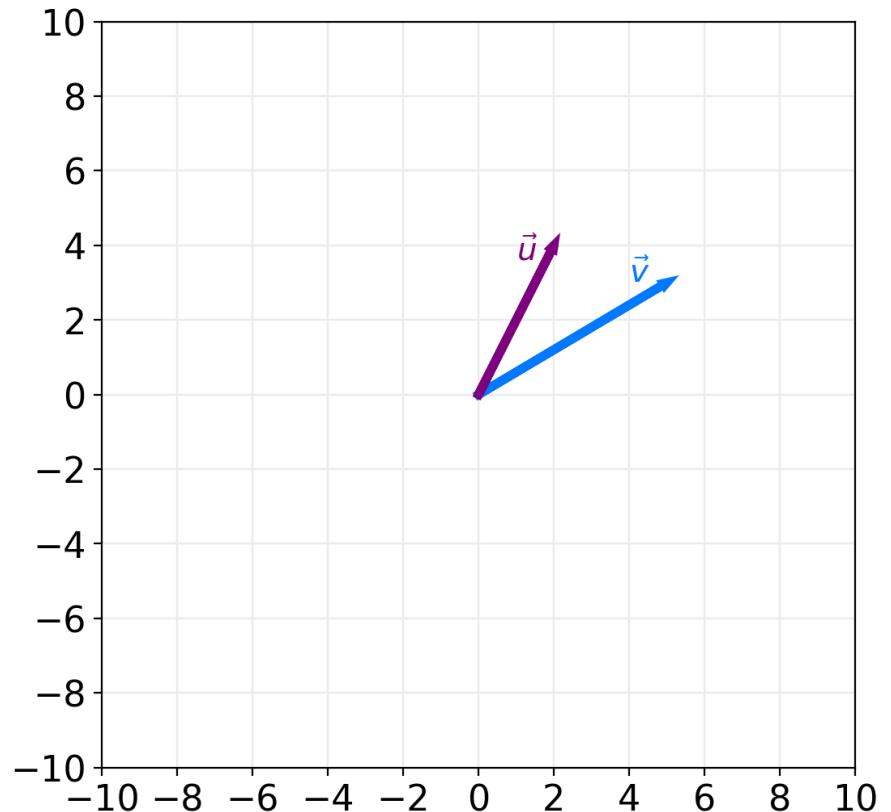
## Adding and scaling vectors

- The sum of two vectors  $\vec{u}$  and  $\vec{v}$  in  $\mathbb{R}^n$  is the **element-wise sum** of their components:

$$\vec{u} + \vec{v} = \begin{bmatrix} u_1 + v_1 \\ u_2 + v_2 \\ \vdots \\ u_n + v_n \end{bmatrix}$$

- If  $c$  is a scalar, then:

$$c\vec{v} = \begin{bmatrix} cv_1 \\ cv_2 \\ \vdots \\ cv_n \end{bmatrix}$$



## Linear combinations

Let  $\vec{v}_1, \vec{v}_2, \dots, \vec{v}_d$  all be vectors in  $\mathbb{R}^n$ .

A **linear combination** of  $\vec{v}_1, \vec{v}_2, \dots, \vec{v}_d$  is any vector of the form:

$$a_1\vec{v}_1 + a_2\vec{v}_2 + \dots + a_d\vec{v}_d$$

where  $a_1, a_2, \dots, a_d$  are all scalars.

## Span

- Let  $\vec{v}_1, \vec{v}_2, \dots, \vec{v}_d$  all be vectors in  $\mathbb{R}^n$ .
- The **span** of  $\vec{v}_1, \vec{v}_2, \dots, \vec{v}_d$  is the set of all vectors that can be created using linear combinations of those vectors.
- Formal definition:

$$\text{span}(\vec{v}_1, \vec{v}_2, \dots, \vec{v}_d) = \{a_1\vec{v}_1 + a_2\vec{v}_2 + \dots + a_d\vec{v}_d : a_1, a_2, \dots, a_n \in \mathbb{R}\}$$

## Exercise

Let  $\vec{v}_1 = \begin{bmatrix} 2 \\ -3 \end{bmatrix}$  and let  $\vec{v}_2 = \begin{bmatrix} -1 \\ 4 \end{bmatrix}$ . Is  $\vec{y} = \begin{bmatrix} 9 \\ 1 \end{bmatrix}$  in  $\text{span}(\vec{v}_1, \vec{v}_2)$ ?

If so, write  $\vec{y}$  as a linear combination of  $\vec{v}_1$  and  $\vec{v}_2$ .

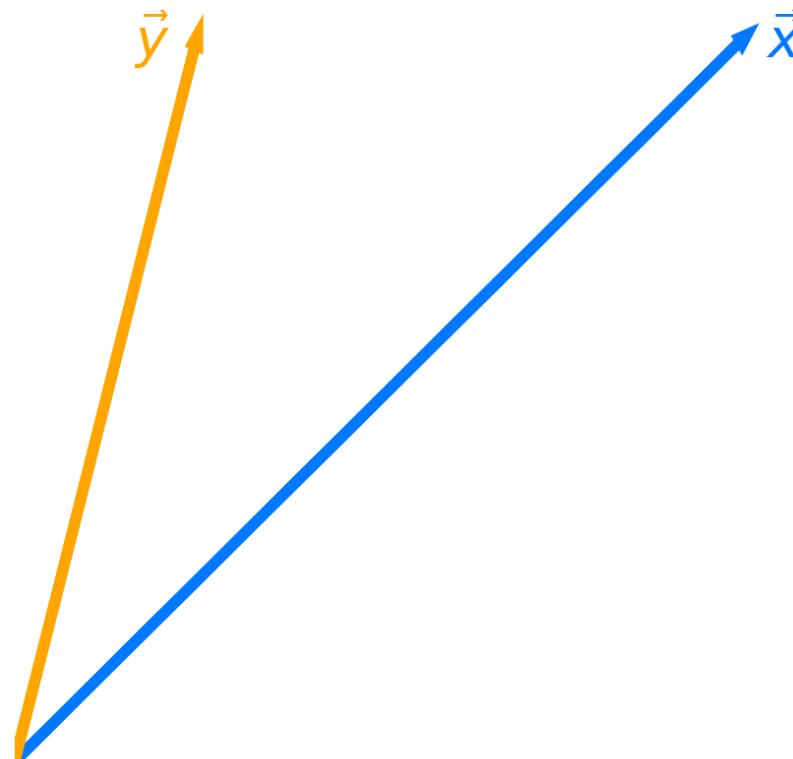
## Projecting onto a single vector

- Let  $\vec{x}$  and  $\vec{y}$  be two vectors in  $\mathbb{R}^n$ .
- The span of  $\vec{x}$  is the set of all vectors of the form:

$$w\vec{x}$$

where  $w \in \mathbb{R}$  is a scalar.

- **Question:** What vector in  $\text{span}(\vec{x})$  is closest to  $\vec{y}$ ?
- The vector in  $\text{span}(\vec{x})$  that is closest to  $\vec{y}$  is the \_\_\_\_\_ projection of  $\vec{y}$  onto  $\text{span}(\vec{x})$ .



## Projection error

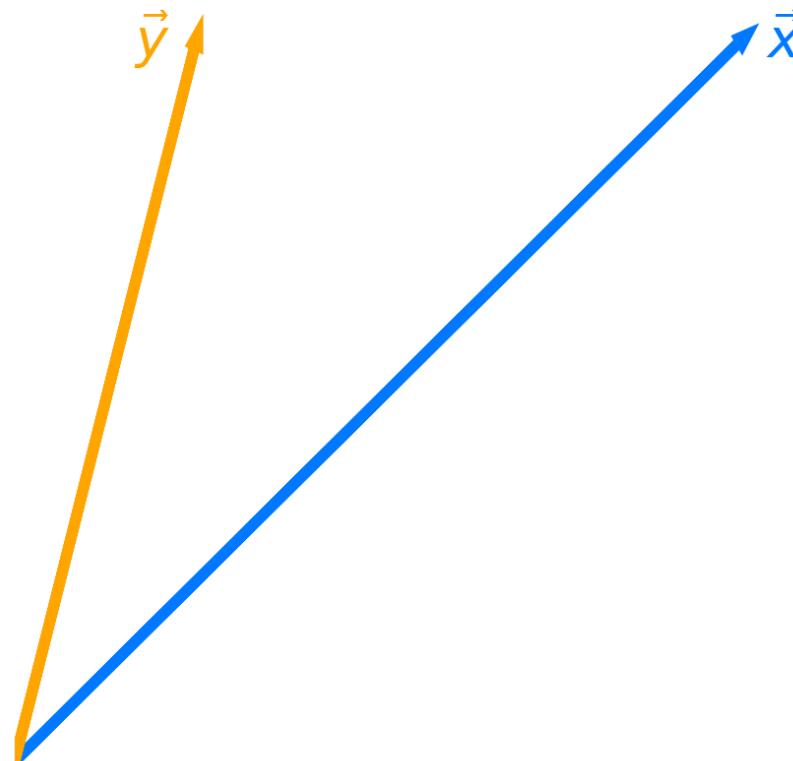
- Let  $\vec{e} = \vec{y} - w\vec{x}$  be the **projection error**: that is, the vector that connects  $\vec{y}$  to  $\text{span}(\vec{x})$ .
- **Goal:** Find the  $w$  that makes  $\vec{e}$  as short as possible.
  - That is, minimize:

$$\|\vec{e}\|$$

- Equivalently, minimize:

$$\|\vec{y} - w\vec{x}\|$$

- **Idea:** To make  $\vec{e}$  as short as possible, it should be **orthogonal** to  $w\vec{x}$ .



## Minimizing projection error

- Goal: Find the  $w$  that makes  $\vec{e} = \vec{y} - w\vec{x}$  as short as possible.
- Idea: To make  $\vec{e}$  as short as possible, it should be **orthogonal** to  $w\vec{x}$ .
- Can we prove that making  $\vec{e}$  orthogonal to  $w\vec{x}$  minimizes  $\|\vec{e}\|$ ?

## Minimizing projection error

- Goal: Find the  $w$  that makes  $\vec{e} = \vec{y} - w\vec{x}$  as short as possible.
- Now we know that to minimize  $\|\vec{e}\|$ ,  $\vec{e}$  must be orthogonal to  $w\vec{x}$ .
- Given this fact, how can we solve for  $w$ ?

# Orthogonal projection

- **Question:** What vector in  $\text{span}(\vec{x})$  is closest to  $\vec{y}$ ?
- **Answer:** It is the vector  $w^* \vec{x}$ , where:

$$w^* = \frac{\vec{x} \cdot \vec{y}}{\vec{x} \cdot \vec{x}}$$

- Note that  $w^*$  is the solution to a minimization problem, specifically, this one:

$$\text{error}(w) = \|\vec{e}\| = \|\vec{y} - w\vec{x}\|$$

- We call  $w^* \vec{x}$  the **orthogonal projection of  $\vec{y}$  onto  $\text{span}(\vec{x})$** .
  - Think of  $w^* \vec{x}$  as the "shadow" of  $\vec{y}$ .

## Exercise

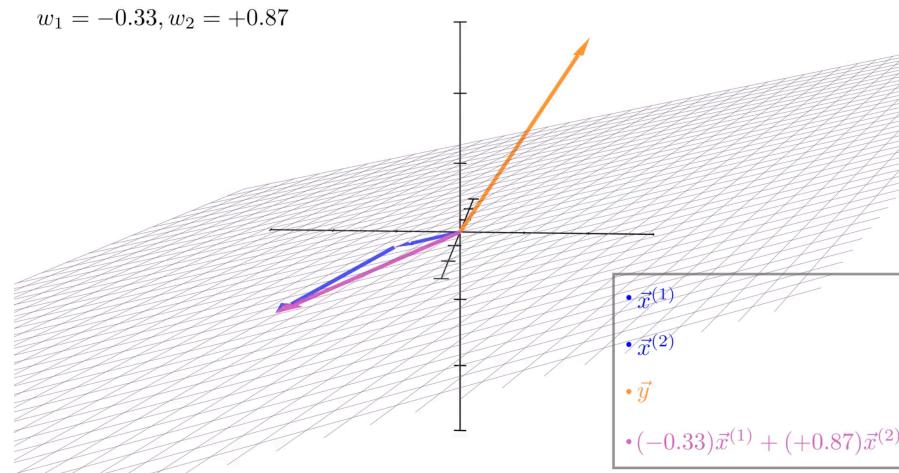
Let  $\vec{a} = \begin{bmatrix} 5 \\ 2 \end{bmatrix}$  and  $\vec{b} = \begin{bmatrix} -1 \\ 9 \end{bmatrix}$ .

What is the orthogonal projection of  $\vec{a}$  onto  $\text{span}(\vec{b})$ ?

Your answer should be of the form  $w^* \vec{b}$ , where  $w^*$  is a scalar.

# Moving to multiple dimensions

- Let's now consider three vectors,  $\vec{y}$ ,  $\vec{x}^{(1)}$ , and  $\vec{x}^{(2)}$ , all in  $\mathbb{R}^n$ .
- **Question:** What vector in  $\text{span}(\vec{x}^{(1)}, \vec{x}^{(2)})$  is closest to  $\vec{y}$ ?
  - Vectors in  $\text{span}(\vec{x}^{(1)}, \vec{x}^{(2)})$  are of the form  $w_1 \vec{x}^{(1)} + w_2 \vec{x}^{(2)}$ , where  $w_1, w_2 \in \mathbb{R}$  are scalars.
- Before trying to answer, let's watch  [this animation that Jack, one of our tutors, made.](#)



## Minimizing projection error in multiple dimensions

- **Question:** What vector in  $\text{span}(\vec{x}^{(1)}, \vec{x}^{(2)})$  is closest to  $\vec{y}$ ?

- That is, what vector minimizes  $\|\vec{e}\|$ , where:

$$\vec{e} = \vec{y} - w_1 \vec{x}^{(1)} - w_2 \vec{x}^{(2)}$$

- **Answer:** It's the vector such that  $w_1 \vec{x}^{(1)} + w_2 \vec{x}^{(2)}$  is **orthogonal** to  $\vec{e}$ .
- **Issue:** Solving for  $w_1$  and  $w_2$  in the following equation is difficult:

$$\left( w_1 \vec{x}^{(1)} + w_2 \vec{x}^{(2)} \right) \cdot \underbrace{\left( \vec{y} - w_1 \vec{x}^{(1)} - w_2 \vec{x}^{(2)} \right)}_{\vec{e}} = 0$$

## Minimizing projection error in multiple dimensions

- It's hard for us to solve for  $w_1$  and  $w_2$  in:

$$\left( w_1 \vec{x}^{(1)} + w_2 \vec{x}^{(2)} \right) \cdot \underbrace{\left( \vec{y} - w_1 \vec{x}^{(1)} - w_2 \vec{x}^{(2)} \right)}_{\vec{e}} = 0$$

- **Observation:** All we really need is for  $\vec{x}^{(1)}$  and  $\vec{x}^{(2)}$  to individually be orthogonal to  $\vec{e}$ .
  - That is, it's sufficient for  $\vec{e}$  to be orthogonal to the spanning vectors themselves.
- If  $\vec{x}^{(1)} \cdot \vec{e} = 0$  and  $\vec{x}^{(2)} \cdot \vec{e} = 0$ , then:

## Minimizing projection error in multiple dimensions

- **Question:** What vector in  $\text{span}(\vec{x}^{(1)}, \vec{x}^{(2)})$  is closest to  $\vec{y}$ ?
- **Answer:** It's the vector such that  $w_1\vec{x}^{(1)} + w_2\vec{x}^{(2)}$  is **orthogonal** to  $\vec{e} = \vec{y} - w_1\vec{x}^{(1)} - w_2\vec{x}^{(2)}$ .
- **Equivalently,** it's the vector such that  $\vec{x}^{(1)}$  and  $\vec{x}^{(2)}$  are both orthogonal to  $\vec{e}$ :

$$\begin{aligned}\vec{x}^{(1)} \cdot \left( \vec{y} - w_1\vec{x}^{(1)} - w_2\vec{x}^{(2)} \right) &= 0 \\ \vec{x}^{(2)} \cdot \underbrace{\left( \vec{y} - w_1\vec{x}^{(1)} - w_2\vec{x}^{(2)} \right)}_{\vec{e}} &= 0\end{aligned}$$

- This is a system of two equations, two unknowns ( $w_1$  and  $w_2$ ), but it still looks difficult to solve.

## Now what?

- We're looking for the scalars  $w_1$  and  $w_2$  that satisfy the following equations:

$$\vec{x}^{(1)} \cdot \left( \vec{y} - w_1 \vec{x}^{(1)} - w_2 \vec{x}^{(2)} \right) = 0$$
$$\vec{x}^{(2)} \cdot \underbrace{\left( \vec{y} - w_1 \vec{x}^{(1)} - w_2 \vec{x}^{(2)} \right)}_{\vec{e}} = 0$$

- In this example, we just have two spanning vectors,  $\vec{x}^{(1)}$  and  $\vec{x}^{(2)}$ .
- If we had any more, this system of equations would get extremely messy, extremely quickly.
- Idea: Rewrite the above system of equations as a **single equation, involving matrix-vector products**.

# Matrices

# Matrices

- An  $n \times d$  **matrix** is a table of numbers with  $n$  rows and  $d$  columns.
- We use upper-case letters to denote matrices.

$$A = \begin{bmatrix} 2 & 5 & 8 \\ -1 & 5 & -3 \end{bmatrix}$$

- Since  $A$  has two rows and three columns, we say  $A \in \mathbb{R}^{2 \times 3}$ .
- **Key idea:** Think of a matrix as **several column vectors, stacked next to each other**.

## Matrix addition and scalar multiplication

- We can add two matrices only if they have the same dimensions.
- Addition occurs elementwise:

$$\begin{bmatrix} 2 & 5 & 8 \\ -1 & 5 & -3 \end{bmatrix} + \begin{bmatrix} 1 & 2 & 3 \\ 0 & 1 & 2 \end{bmatrix} = \begin{bmatrix} 3 & 7 & 11 \\ -1 & 6 & -1 \end{bmatrix}$$

- Scalar multiplication occurs elementwise, too:

$$2 \begin{bmatrix} 2 & 5 & 8 \\ -1 & 5 & -3 \end{bmatrix} = \begin{bmatrix} 4 & 10 & 16 \\ -2 & 10 & -6 \end{bmatrix}$$

## Matrix-matrix multiplication

- Key idea: We can multiply matrices  $A$  and  $B$  if and only if:

$$\# \text{ columns in } A = \# \text{ rows in } B$$

- If  $A$  is  $n \times d$  and  $B$  is  $d \times p$ , then  $AB$  is  $n \times p$ .
- Example: If  $A$  is as defined below, what is  $A^T A$ ?

$$A = \begin{bmatrix} 2 & 5 & 8 \\ -1 & 5 & -3 \end{bmatrix}$$

## Question 🤔

Answer at [q.dsc40a.com](https://q.dsc40a.com)

Assume  $A$ ,  $B$ , and  $C$  are all matrices. Select the **incorrect** statement below.

- A.  $A(B + C) = AB + AC$ .
- B.  $A(BC) = (AB)C$ .
- C.  $AB = BA$ .
- D.  $(A + B)^T = A^T + B^T$ .
- E.  $(AB)^T = B^T A^T$ .

## Matrix-vector multiplication

- A vector  $\vec{v} \in \mathbb{R}^n$  is a matrix with  $n$  rows and 1 column.

$$\vec{v} = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}$$

- Suppose  $A \in \mathbb{R}^{n \times d}$ .
  - What must the dimensions of  $\vec{v}$  be in order for the product  $A\vec{v}$  to be valid?
  - What must the dimensions of  $\vec{v}$  be in order for the product  $\vec{v}^T A$  to be valid?

## One view of matrix-vector multiplication

- One way of thinking about the product  $A\vec{v}$  is that it is the **dot product of  $\vec{v}$  with every row of  $A$** .
- Example: What is  $A\vec{v}$ ?

$$A = \begin{bmatrix} 2 & 5 & 8 \\ -1 & 5 & -3 \end{bmatrix} \quad \vec{v} = \begin{bmatrix} 2 \\ -1 \\ -5 \end{bmatrix}$$

## Another view of matrix-vector multiplication

- Another way of thinking about the product  $A\vec{v}$  is that it is a **linear combination of the columns of  $A$ , using the weights in  $\vec{v}$** .
- Example: What is  $A\vec{v}$ ?

$$A = \begin{bmatrix} 2 & 5 & 8 \\ -1 & 5 & -3 \end{bmatrix} \quad \vec{v} = \begin{bmatrix} 2 \\ -1 \\ -5 \end{bmatrix}$$

## Matrix-vector products create linear combinations of columns!

- Key idea: It'll be very useful to think of the matrix-vector product  $A\vec{v}$  as a linear combination of the columns of  $A$ , using the weights in  $\vec{v}$ .

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1d} \\ a_{21} & a_{22} & \dots & a_{2d} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nd} \end{bmatrix} \quad \vec{v} = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_d \end{bmatrix}$$

↓

$$A\vec{v} = v_1 \begin{bmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{n1} \end{bmatrix} + v_2 \begin{bmatrix} a_{12} \\ a_{22} \\ \vdots \\ a_{n2} \end{bmatrix} + \dots + v_d \begin{bmatrix} a_{1d} \\ a_{2d} \\ \vdots \\ a_{nd} \end{bmatrix}$$

# Spans and projections, revisited

## Moving to multiple dimensions

- Let's now consider three vectors,  $\vec{y}$ ,  $\vec{x}^{(1)}$ , and  $\vec{x}^{(2)}$ , all in  $\mathbb{R}^n$ .
- **Question:** What vector in  $\text{span}(\vec{x}^{(1)}, \vec{x}^{(2)})$  is closest to  $\vec{y}$ ?
  - That is, what values of  $w_1$  and  $w_2$  minimize  $\|\vec{e}\| = \|\vec{y} - w_1\vec{x}^{(1)} - w_2\vec{x}^{(2)}\|$ ?

## Matrix-vector products create linear combinations of columns!

$$\vec{x}^{(1)} = \begin{bmatrix} 2 \\ 5 \\ 3 \end{bmatrix} \quad \vec{x}^{(2)} = \begin{bmatrix} -1 \\ 0 \\ 4 \end{bmatrix} \quad \vec{y} = \begin{bmatrix} 1 \\ 3 \\ 9 \end{bmatrix}$$

- Combining  $\vec{x}^{(1)}$  and  $\vec{x}^{(2)}$  into a single matrix gives:

$$X = \begin{bmatrix} | & | \\ \vec{x}^{(1)} & \vec{x}^{(2)} \\ | & | \end{bmatrix} = \begin{bmatrix} \text{---} & \text{---} \\ \text{---} & \text{---} \\ \text{---} & \text{---} \end{bmatrix}$$

- Then, if  $\vec{w} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$ , linear combinations of  $\vec{x}^{(1)}$  and  $\vec{x}^{(2)}$  can be written as  $X\vec{w}$ .
- The **span of the columns of  $X$** , or  $\text{span}(X)$ , consists of all vectors that can be written in the form  $X\vec{w}$ .

## Minimizing projection error in multiple dimensions

$$X = \begin{bmatrix} | & | \\ \vec{x}^{(1)} & \vec{x}^{(2)} \\ | & | \end{bmatrix} = \begin{bmatrix} 2 & -1 \\ 5 & 0 \\ 3 & 4 \end{bmatrix} \quad \vec{y} = \begin{bmatrix} 1 \\ 3 \\ 9 \end{bmatrix}$$

- **Goal:** Find the vector  $\vec{w} = [w_1 \quad w_2]^T$  such that  $\|\vec{e}\| = \|\vec{y} - X\vec{w}\|$  is minimized.
- As we've seen,  $\vec{w}$  must be such that:

$$\vec{x}^{(1)} \cdot \left( \vec{y} - w_1 \vec{x}^{(1)} - w_2 \vec{x}^{(2)} \right) = 0$$
$$\vec{x}^{(2)} \cdot \underbrace{\left( \vec{y} - w_1 \vec{x}^{(1)} - w_2 \vec{x}^{(2)} \right)}_{\vec{e}} = 0$$

- How can we use our knowledge of matrices to rewrite this system of equations as a single equation?

## Simplifying the system of equations, using matrices

$$X = \begin{bmatrix} | & | \\ \vec{x}^{(1)} & \vec{x}^{(2)} \\ | & | \end{bmatrix} = \begin{bmatrix} 2 & -1 \\ 5 & 0 \\ 3 & 4 \end{bmatrix} \quad \vec{y} = \begin{bmatrix} 1 \\ 3 \\ 9 \end{bmatrix}$$

$$\vec{x}^{(1)} \cdot \left( \vec{y} - w_1 \vec{x}^{(1)} - w_2 \vec{x}^{(2)} \right) = 0$$

$$\vec{x}^{(2)} \cdot \underbrace{\left( \vec{y} - w_1 \vec{x}^{(1)} - w_2 \vec{x}^{(2)} \right)}_{\vec{e}} = 0$$

## Simplifying the system of equations, using matrices

$$X = \begin{bmatrix} | & | \\ \vec{x}^{(1)} & \vec{x}^{(2)} \\ | & | \end{bmatrix} = \begin{bmatrix} 2 & -1 \\ 5 & 0 \\ 3 & 4 \end{bmatrix} \quad \vec{y} = \begin{bmatrix} 1 \\ 3 \\ 9 \end{bmatrix}$$

1.  $w_1 \vec{x}^{(1)} + w_2 \vec{x}^{(2)}$  can be written as  $X \vec{w}$ , so  $\vec{e} = \vec{y} - X \vec{w}$ .
2. The condition that  $\vec{e}$  must be orthogonal to each column of  $X$  is equivalent to condition that  $X^T \vec{e} = 0$ .



## The normal equations

$$\mathbf{X} = \begin{bmatrix} | & | \\ \vec{x}^{(1)} & \vec{x}^{(2)} \\ | & | \end{bmatrix} = \begin{bmatrix} 2 & -1 \\ 5 & 0 \\ 3 & 4 \end{bmatrix} \quad \vec{y} = \begin{bmatrix} 1 \\ 3 \\ 9 \end{bmatrix}$$

- **Goal:** Find the vector  $\vec{w} = [w_1 \quad w_2]^T$  such that  $\|\vec{e}\| = \|\vec{y} - \mathbf{X}\vec{w}\|$  is minimized.
- We now know that it is the vector  $\vec{w}^*$  such that:

$$\begin{aligned} \mathbf{X}^T \vec{e} &= 0 \\ \mathbf{X}^T (\vec{y} - \mathbf{X}\vec{w}^*) &= 0 \\ \mathbf{X}^T \vec{y} - \mathbf{X}^T \mathbf{X} \vec{w}^* &= 0 \\ \implies \mathbf{X}^T \mathbf{X} \vec{w}^* &= \mathbf{X}^T \vec{y} \end{aligned}$$

- The last statement is referred to as the **normal equations**.

## The general solution to the normal equations

$$X \in \mathbb{R}^{n \times d} \quad \vec{y} \in \mathbb{R}^n$$

- **Goal, in general:** Find the vector  $\vec{w} \in \mathbb{R}^d$  such that  $\|\vec{e}\| = \|\vec{y} - X\vec{w}\|$  is minimized.
- We now know that it is the vector  $\vec{w}^*$  such that:

$$\begin{aligned} X^T \vec{e} &= 0 \\ \implies X^T X \vec{w}^* &= X^T \vec{y} \end{aligned}$$

- Assuming  $X^T X$  is invertible, this is the vector:

$$\boxed{\vec{w}^* = (X^T X)^{-1} X^T \vec{y}}$$

- This is a big assumption, because it requires  $X^T X$  to be **full rank**.
- If  $X^T X$  is not full rank, then there are infinitely many solutions to the normal equations,  $X^T X \vec{w}^* = X^T \vec{y}$ .

## What does it mean?

- **Original question:** What vector in  $\text{span}(\vec{x}^{(1)}, \vec{x}^{(2)})$  is closest to  $\vec{y}$ ?
- **Final answer:** It is the vector  $\mathbf{X}\vec{w}^*$ , where:

$$\vec{w}^* = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \vec{y}$$

- Revisiting our example:

$$\mathbf{X} = \begin{bmatrix} | & | \\ \vec{x}^{(1)} & \vec{x}^{(2)} \\ | & | \end{bmatrix} = \begin{bmatrix} 2 & -1 \\ 5 & 0 \\ 3 & 4 \end{bmatrix} \quad \vec{y} = \begin{bmatrix} 1 \\ 3 \\ 9 \end{bmatrix}$$

- Using a computer gives us  $\vec{w}^* = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \vec{y} \approx \begin{bmatrix} 0.7289 \\ 1.6300 \end{bmatrix}$ .
- So, the vector in  $\text{span}(\vec{x}^{(1)}, \vec{x}^{(2)})$  closest to  $\vec{y}$  is  $0.7289\vec{x}^{(1)} + 1.6300\vec{x}^{(2)}$ .

## An optimization problem, solved

- We just used linear algebra to solve an **optimization problem**.
- Specifically, the function we minimized is:

$$\text{error}(\vec{w}) = \|\vec{y} - \mathbf{X}\vec{w}\|$$

- This is a function whose input is a vector,  $\vec{w}$ , and whose output is a scalar!
- The input,  $\vec{w}^*$ , to **error**( $\vec{w}$ ) that minimizes it is:

$$\vec{w}^* = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \vec{y}$$

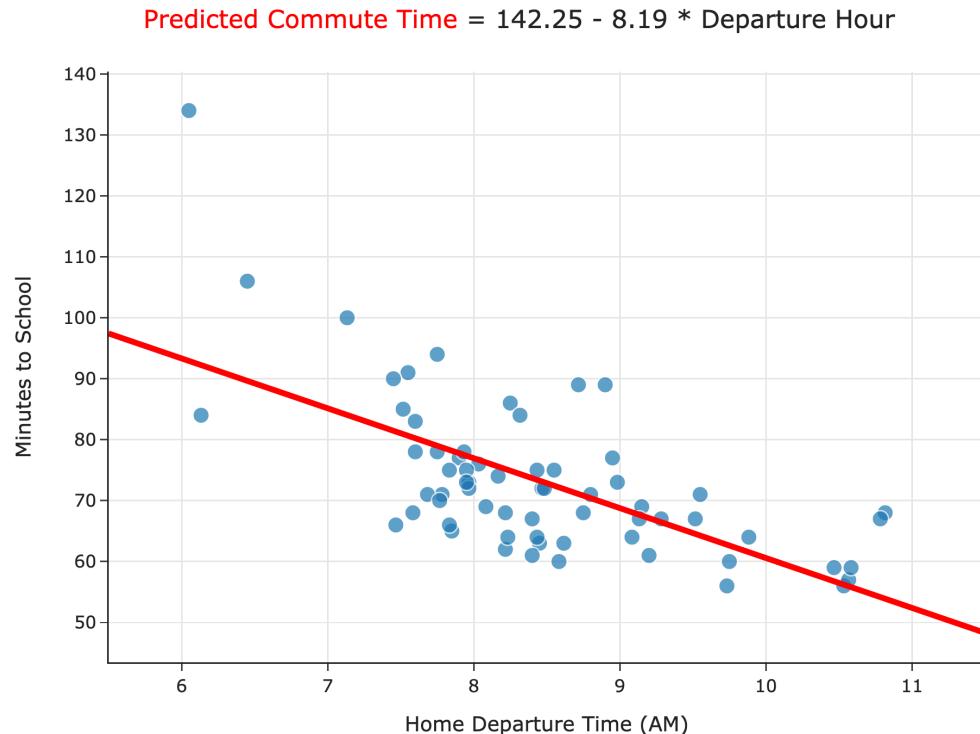
- We're going to use this frequently!

# Regression and linear algebra

## Wait... why do we need linear algebra?

- Soon, we'll want to make predictions using more than one feature.
  - Example: Predicting commute times using departure hour and temperature.
- Thinking about linear regression in terms of **matrices and vectors** will allow us to find hypothesis functions that:
  - Use multiple features (input variables).
  - Are non-linear in the features, e.g.  $H(x) = w_0 + w_1x + w_2x^2$ .
- Let's see if we can put what we've just learned to use.

# Simple linear regression, revisited



- **Model:**  $H(x) = w_0 + w_1x$ .
- **Loss function:**  $(y_i - H(x_i))^2$ .
- To find  $w_0^*$  and  $w_1^*$ , we minimized empirical risk, i.e. average loss:
$$R_{\text{sq}}(H) = \frac{1}{n} \sum_{i=1}^n (y_i - H(x_i))^2$$
- **Observation:**  $R_{\text{sq}}(w_0, w_1)$  kind of looks like the formula for the norm of a vector,  
$$\|\vec{v}\| = \sqrt{v_1^2 + v_2^2 + \dots + v_n^2}.$$

# Regression and linear algebra

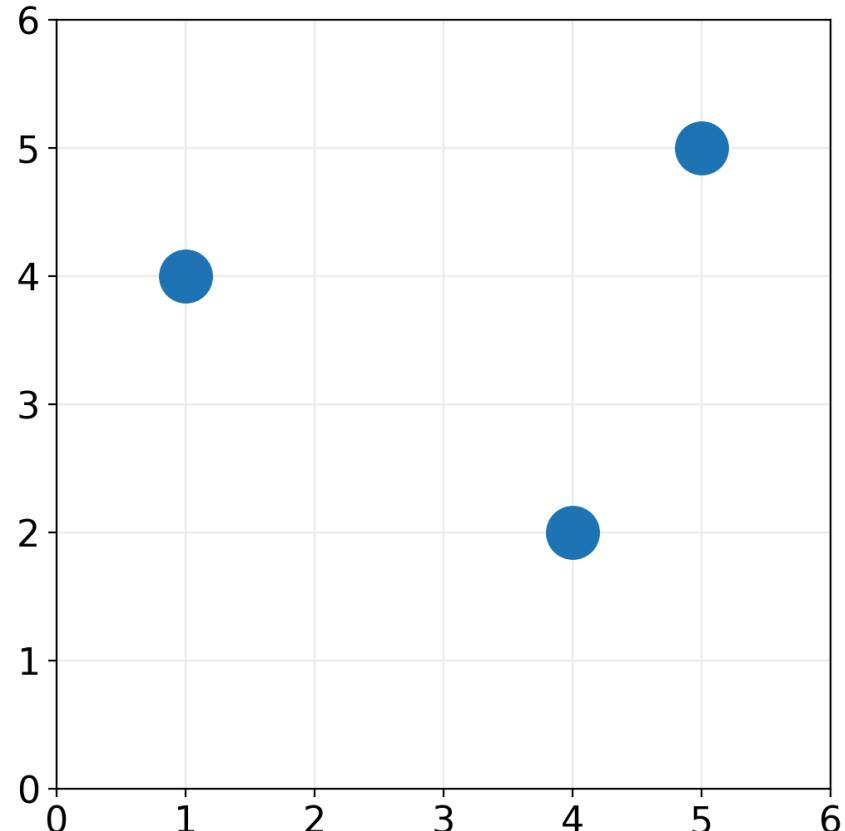
Let's define a few new terms:

- The **observation vector** is the vector  $\vec{y} \in \mathbb{R}^n$ . This is the vector of observed "actual values".
- The **hypothesis vector** is the vector  $\vec{h} \in \mathbb{R}^n$  with components  $H(x_i)$ . This is the vector of predicted values.
- The **error vector** is the vector  $\vec{e} \in \mathbb{R}^n$  with components:

$$e_i = y_i - H(x_i)$$

## Example

Consider  $H(x) = 2 + \frac{1}{2}x$ .



$$\vec{y} =$$

$$\vec{h} =$$

$$\vec{e} = \vec{y} - \vec{h} =$$

$$R_{\text{sq}}(\mathbf{H}) = \frac{1}{n} \sum_{i=1}^n (\mathbf{y}_i - \mathbf{H}(x_i))^2$$

$$=$$

# Regression and linear algebra

Let's define a few new terms:

- The **observation vector** is the vector  $\vec{y} \in \mathbb{R}^n$ . This is the vector of observed "actual values".
- The **hypothesis vector** is the vector  $\vec{h} \in \mathbb{R}^n$  with components  $H(x_i)$ . This is the vector of predicted values.
- The **error vector** is the vector  $\vec{e} \in \mathbb{R}^n$  with components:

$$e_i = y_i - H(x_i)$$

- **Key idea:** We can rewrite the mean squared error of  $H$  as:

$$R_{\text{sq}}(H) = \frac{1}{n} \sum_{i=1}^n (y_i - H(x_i))^2 = \frac{1}{n} \|\vec{e}\|^2 = \frac{1}{n} \|\vec{y} - \vec{h}\|^2$$

## The hypothesis vector

- The **hypothesis vector** is the vector  $\vec{h} \in \mathbb{R}^n$  with components  $H(x_i)$ . This is the vector of predicted values.
- For the linear hypothesis function  $H(x) = w_0 + w_1 x$ , the hypothesis vector can be written:

$$\vec{h} = \begin{bmatrix} w_0 + w_1 x_1 \\ w_0 + w_1 x_2 \\ \vdots \\ w_0 + w_1 x_n \end{bmatrix} =$$

## Rewriting the mean squared error

- Define the **design matrix**  $\mathbf{X} \in \mathbb{R}^{n \times 2}$  as:

$$\mathbf{X} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}$$

- Define the **parameter vector**  $\vec{w} \in \mathbb{R}^2$  to be  $\vec{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}$ .
- Then,  $\vec{h} = \mathbf{X}\vec{w}$ , so the mean squared error becomes:

$$R_{\text{sq}}(\mathbf{H}) = \frac{1}{n} \|\vec{y} - \vec{h}\|^2 \implies \boxed{R_{\text{sq}}(\vec{w}) = \frac{1}{n} \|\vec{y} - \mathbf{X}\vec{w}\|^2}$$

## What's next?

- To find the optimal model parameters for simple linear regression,  $w_0^*$  and  $w_1^*$ , we previously minimized:

$$R_{\text{sq}}(w_0, w_1) = \frac{1}{n} \sum_{i=1}^n (\textcolor{orange}{y}_i - (w_0 + w_1 \textcolor{blue}{x}_i))^2$$

- Now that we've reframed the simple linear regression problem in terms of linear algebra, we can find  $w_0^*$  and  $w_1^*$  by minimizing:

$$R_{\text{sq}}(\vec{w}) = \frac{1}{n} \|\vec{\textcolor{orange}{y}} - \textcolor{blue}{X} \vec{w}\|^2$$

- We've already solved this problem! Assuming  $\textcolor{blue}{X}^T \textcolor{blue}{X}$  is invertible, the best  $\vec{w}$  is:

$$\vec{w}^* = (\textcolor{blue}{X}^T \textcolor{blue}{X})^{-1} \textcolor{blue}{X}^T \vec{\textcolor{orange}{y}}$$