LECTURE 11

Ordinary Least Squares

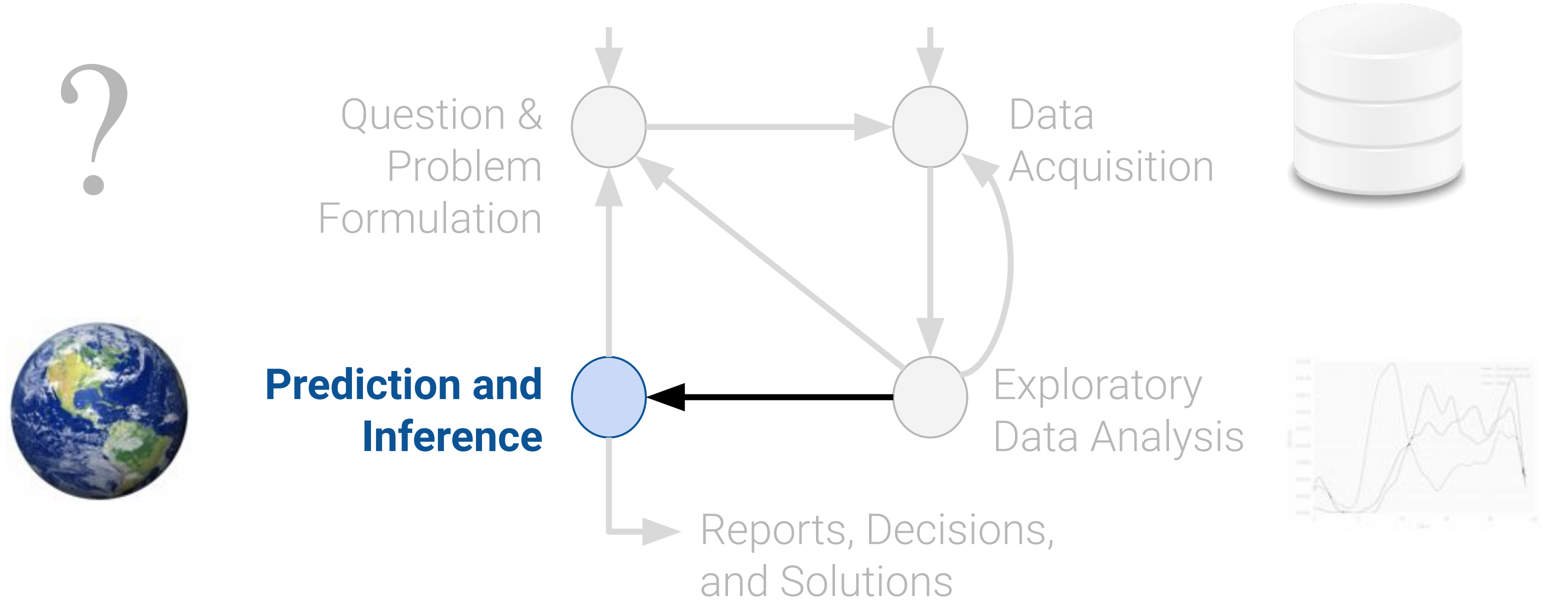
Using linear algebra to derive the multiple linear regression model.

Data 100/Data 200, Fall 2022 @ UC Berkeley

Will Fithian and Fernando Pérez

Content credit: Lisa Yan, Ani Adhikari, Deborah Nolan, Joseph Gonzalez

Plan for next few lectures: Modeling



(today)

Modeling I: Intro to Modeling, Simple Linear Regression	Modeling II: Different models, loss functions, linearization	Modeling III: Multiple Linear Regression

Linear in Theta

An expression is "**linear in theta**" if it is a **linear combination** of parameters $\theta = (\theta_0, \theta_1, \ldots, \theta_p)$.

1. $\hat{y} = \theta_0 + \theta_1(2) + \theta_2(4 \cdot 8) + \theta_3(\log 42)$

2. $\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 x_3 + \theta_3 \cdot \log x_4$

3. $\hat{y} = \theta_0 + \theta_1 \cdot x_1 + \log \theta_2 \cdot x_2 + \theta_3 \cdot \theta_4$

4. $$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 5 & 6 & 7 \\ 1 & 8 & 9 & 0 \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

5. $$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{12} & x_{13} \\ 1 & x_{12} & x_{22} & x_{23} \\ 1 & x_{13} & x_{23} & x_{33} \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

Which of the following expressions are linear in theta?

Linear in Theta

An expression is "**linear in theta**" if it is a **linear combination** of parameters $\theta = (\theta_0, \theta_1, \ldots, \theta_p)$.

1. $\hat{y} = \theta_0 + \theta_1(2) + \theta_2(4 \cdot 8) + \theta_3(\log 42)$

$$= \begin{bmatrix} 1 & 2 & 4 \cdot 8 & \log 42 \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

2. $\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 x_3 + \theta_3 \cdot \log x_4$

$$= \begin{bmatrix} 1 & x_1 & x_2 x_3 & \log x_4 \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

3. $\hat{y} = \theta_0 + \theta_1 \cdot x_1 + \log \theta_2 \cdot x_2 + \theta_3 \cdot \theta_4$

4. $$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 5 & 6 & 7 \\ 1 & 8 & 9 & 0 \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

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"**Linear in theta**" means the expression can separate into a matrix product of two terms: **a vector of thetas**, and a matrix/vector not involving thetas.

Multiple Linear Regression

Define the **multiple linear regression** model:

$$\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_p x_p$$

Predicted value of y

This is a linear model because it is
a linear combination of parameters $\theta = (\theta_0, \theta_1, \ldots, \theta_p)$.

$$(x_1, \ldots, x_p) \longrightarrow \boxed{\theta = (\theta_0, \theta_1, \ldots, \theta_p)} \longrightarrow \hat{y}$$

single **observation**
(p features)

single
prediction

NBA 2018-2019 Dataset

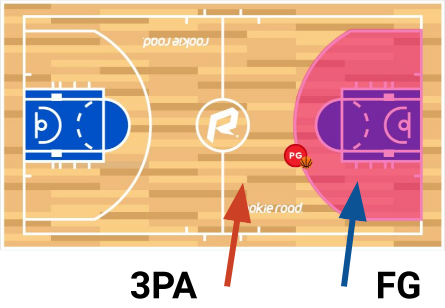
How many points does an athlete score per game?
PTS (average points/game)

To name a few factors:

- **FG**: average # 2 point field goals
- **AST**: average # of assists
- **3PA**: average # 3 point field goals attempted

	FG	AST	3PA	PTS
1	1.8	0.6	4.1	5.3
2	0.4	0.8	1.5	1.7
3	1.1	1.9	2.2	3.2
4	6.0	1.6	0.0	13.9
5	3.4	2.2	0.2	8.9
6	0.6	0.3	1.2	1.7

Rows correspond to individual players.



assist: a pass to a teammate that directly leads to a goal

Multiple Linear Regression Model

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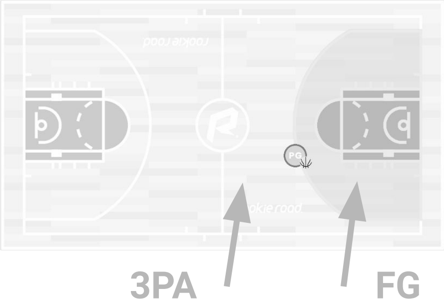

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Rows correspond to individual players.

$$\begin{bmatrix} 0.4 \\ 0.8 \\ 1.5 \end{bmatrix} \rightarrow \boxed{\theta = (\theta_0, \theta_1, \ldots, \theta_p)} \rightarrow \boxed{\hat{y}}$$

$$\begin{aligned} \hat{y} &= \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_p x_p \\ &= \theta_0 + \theta_1 \underbrace{x_1}_{\text{FG}} + \theta_2 \underbrace{x_2}_{\text{AST}} + \theta_3 \underbrace{x_3}_{\text{3PA}} \end{aligned}$$

Today's Roadmap

Lecture 11, Data 100 Fall 2022

OLS Problem Formulation

- Multiple Linear Regression Model
- Mean Squared Error

Geometric Derivation

- Lin Alg Review: Orthogonality, Span
- Least Squares Estimate Proof

Performance: Residuals, Multiple R^2

OLS Properties

- Residuals
- The Intercept Term
- Existence of a Unique Solution

Linear Algebra Resources: [Ed post]

Today's Goal: Ordinary Least Squares

1. Choose a model	**Multiple Linear Regression**	
2. Choose a loss function	L2 Loss **Mean Squared Error (MSE)**	In statistics, this model + loss is called **ordinary least squares (OLS)**.
3. Fit the model	Minimize average loss with ~~calculus~~ geometry	The solution to OLS are the minimizing parameters $\hat{\theta}$, also called the **least squares estimate**.
4. Evaluate model performance	Visualize, ~~Root MSE~~ Multiple R^2	

Multiple Linear Regression Model

Lecture 11, Data 100 Fall 2022

OLS Problem Formulation

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Linear Algebra Resources: Ed post

Today's Goal: Ordinary Least Squares

1. Choose a model

Multiple Linear Regression

For each of our n datapoints:

$$\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_p x_p$$

$$\hat{\mathbb{Y}} = \mathbb{X}\theta$$

2. Choose a loss function

L2 Loss

Mean Squared Error (MSE)

Linear Algebra!!

3. Fit the model

Minimize average loss with ~~calculus~~ geometry

4. Evaluate model performance

Visualize,
~~Root MSE~~
Multiple R^2

Vector Notation

$$\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_p x_p$$

$$= \theta_0 + \sum_{j=1}^{p} \theta_j x_j$$

$$= x^T \theta \qquad x, \theta \in \mathbb{R}^{(p+1)} : x = \boxed{\begin{matrix} 1 \\ 0.4 \\ 0.8 \\ 1.5 \end{matrix}} \quad \theta = \boxed{\begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}}$$

$$= \boxed{\begin{matrix} 1 & 0.4 & 0.8 & 1.5 \end{matrix}} \boxed{\begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}} = \boxed{\hat{y}} \in \mathbb{R}$$

NBA Data

	FG	AST	3PA	PTS
1	1.8	0.6	4.1	5.3
2	0.4	0.8	1.5	1.7
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Rows correspond to individual players.

Matrix Notation

Data

	FG	AST	3PA	PTS
1	1.8	0.6	4.1	5.3
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3	1.1	1.9	2.2	3.2

To make predictions on all n datapoints in our sample:

same $\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$ for all preds

$$\hat{y}_1 = x_1^T \theta \quad \text{where } x_1^T = [1 \quad x_{11} \quad x_{12} \quad \dots \quad x_{1p}]$$ Datapoint 1

$$\hat{y}_2 = x_2^T \theta \quad \text{where } x_2^T = [1 \quad x_{21} \quad x_{22} \quad \dots \quad x_{2p}]$$ Datapoint 2

$$\vdots \qquad \vdots \qquad \qquad \vdots$$

$$\hat{y}_n = x_n^T \theta \quad \text{where } x_n^T = [1 \quad x_{n1} \quad x_{n2} \quad \dots \quad x_{np}]$$ Datapoint n

Matrix Notation

Data

	FG	AST	3PA	PTS
1	1.8	0.6	4.1	5.3
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To make predictions on all n datapoints in our sample:

$$\hat{y}_1 = \begin{bmatrix} 1 & x_{11} & x_{12} \dots & x_{1p} \end{bmatrix} \theta = x_1^T \theta$$

$$\hat{y}_2 = \begin{bmatrix} 1 & x_{21} & x_{22} & \dots & x_{2p} \end{bmatrix} \theta = x_2^T \theta$$

$$\vdots \qquad \vdots \qquad \vdots$$

$$\hat{y}_n = \begin{bmatrix} 1 & x_{n1} & x_{n2} & \dots & x_{np} \end{bmatrix} \theta = x_n^T \theta$$

same $\theta =$ for all preds $\begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$

n row vectors, each with dimension **(p+1)**

Expand out each datapoint's (transposed) input

Matrix Notation

Data

	FG	AST	3PA	PTS
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To make predictions on all n datapoints in our sample:

$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \boxed{\begin{matrix} [1 & x_{11} & x_{12} & \ldots & x_{1p}] \\ [1 & x_{21} & x_{22} & \ldots & x_{2p}] \\ & & \vdots & & \\ [1 & x_{n1} & x_{n2} & \ldots & x_{np}] \end{matrix}} \theta$$

n row vectors, each with dimension **(p+1)**

same $\theta =$ for all preds $\begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$

Vectorize predictions and parameters to encapsulate all n equations into a single matrix equation.

Matrix Notation

To make predictions on all n datapoints in our sample:

$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \mathbb{X} \, \theta$$

Design matrix with dimensions n x (p + 1)

Data

	FG	AST	3PA	PTS
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3	1.1	1.9	2.2	3.2

same $\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$ for all preds

The Design Matrix $\mathbb{X}$

We can use linear algebra to represent our predictions of all n datapoints at once.

One step in this process is to stack all of our input features together into a **design matrix**:

$$\mathbb{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1p} \\ 1 & x_{21} & x_{22} & \dots & x_{2p} \\ 1 & x_{31} & x_{32} & \dots & x_{3p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{np} \end{bmatrix}$$

What do the **rows** and **columns** of the design matrix represent in terms of the observed data?

Field Goals
Assists
3-Point Attempts

Bias	FG	AST	3PA	PTS
1	1.8	0.6	4.1	5.3
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1	1.1	1.9	2.2	3.2
1	6.0	1.6	0.0	13.9
1	3.4	2.2	0.2	8.9
...	...	...	...	...
1	4.0	0.8	0.0	11.5
1	3.1	0.9	0.0	7.8
1	3.6	1.1	0.0	8.9
1	3.4	0.8	0.0	8.5
1	3.8	1.5	0.0	9.4

Example design matrix
708 rows x (3+1) cols

The Design Matrix $\mathbb{X}$

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A **row** corresponds to one **observation**, e.g., all (p+1) features for datapoint 3

A **column** corresponds to a **feature**, e.g. feature 1 for all n data points

Special all-ones feature often called the **intercept**

Field Goals, Assists, 3-Point Attempts

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...	...	...	...	...
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1	3.1	0.9	0.0	7.8
1	3.6	1.1	0.0	8.9
1	3.4	0.8	0.0	8.5
1	3.8	1.5	0.0	9.4

Example design matrix
708 rows x (3+1) cols

The Multiple Linear Regression Model using Matrix Notation

We can express our linear model on our entire dataset as follows:

$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1p} \\ 1 & x_{21} & x_{22} & \dots & x_{2p} \\ 1 & x_{31} & x_{32} & \dots & x_{3p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{np} \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_p \end{bmatrix}$$

$$\boxed{\hat{\mathbb{Y}} = \mathbb{X}\theta}$$

Prediction vector $\mathbb{R}^n$

Design matrix $\mathbb{R}^{n \times (p+1)}$

Parameter vector $\mathbb{R}^{(p+1)}$

Note that our **true output** is also a vector: $\mathbb{Y} \in \mathbb{R}^n$

Mean Squared Error

Lecture 11, Data 100 Fall 2022

OLS Problem Formulation

- Multiple Linear Regression Model
- **Mean Squared Error**

Geometric Derivation

- Lin Alg Review: Orthogonality, Span
- Least Squares Estimate Proof

Performance: Residuals, Multiple R^2

OLS Properties

- Residuals
- The Intercept Term
- Existence of a Unique Solution

Linear Algebra Resources: Ed post

Today's Goal: Ordinary Least Squares

1. Choose a model ✅	Multiple Linear Regression	$\hat{\mathbb{Y}} = \mathbb{X}\theta$
2. Choose a loss function	L2 Loss Mean Squared Error (MSE)	$R(\theta) = \frac{1}{n}\|\|\mathbb{Y} - \mathbb{X}\theta\|\|_2^2$
3. Fit the model	Minimize average loss with ~~calculus~~ geometry	More Linear Algebra!!
4. Evaluate model performance	Visualize, ~~Root MSE~~ Multiple R^2	

[Linear Algebra] Vector Norms and the L2 Vector Norm

The **norm** of a vector is some measure of that vector's **size**.

- The two norms we need to know for Data 100 are the L_1 and L_2 norms (sound familiar?).
- Today, we focus on L_2 norm. We'll define the L_1 norm another day.

For the n-dimensional vector $x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix}$, the **L2 vector norm** is

$$||x||_2 = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2} = \sqrt{\sum_{i=1}^{n} x_i^2}$$

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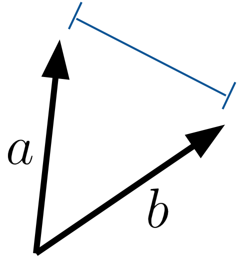
The L2 vector norm is a generalization of the Pythagorean theorem into ***n*** dimensions.

It can therefore be used as a measure of **distance** between two vectors.

- For n-dimensional vectors a, b, their distance is $||a - b||_2$.



Note: The square of the L2 norm of a vector is the sum of the squares of the vector's elements:

$$||\boldsymbol{x}||_2^2 = \sum_{i=1}^{n} \boldsymbol{x}_i^2$$

Looks like Mean Squared Error!!

Mean Squared Error with L2 Norms

We can rewrite mean squared error as a squared L2 norm:

$$R(\theta) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$
$$= \frac{1}{n}||\mathbb{Y} - \hat{\mathbb{Y}}||_2^2$$

With our linear model $\hat{\mathbb{Y}} = \mathbb{X}\theta$:

$$R(\theta) = \frac{1}{n}||\mathbb{Y} - \mathbb{X}\theta||_2^2$$

Ordinary Least Squares

The **least squares estimate** $\hat{\theta}$ is the parameter that **minimizes** the objective function $R(\theta)$:

$$R(\theta) = \frac{1}{n}||\mathbb{Y} - \mathbb{X}\theta||_2^2$$

How should we interpret the OLS problem?

A. Minimize the mean squared error for the linear model $\hat{\mathbb{Y}} = \mathbb{X}\theta$

B. Minimize the **distance** between true and predicted values $\mathbb{Y}$ and $\hat{\mathbb{Y}}$

C. Minimize the **length** of the residual vector, $e = \mathbb{Y} - \hat{\mathbb{Y}} = \begin{bmatrix} y_1 - \hat{y_1} \\ y_2 - \hat{y_2} \\ \vdots \\ y_n - \hat{y_n} \end{bmatrix}$

D. All of the above

E. Something else

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Important for today

Geometric Derivation

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Linear Algebra Resources: [Ed post]

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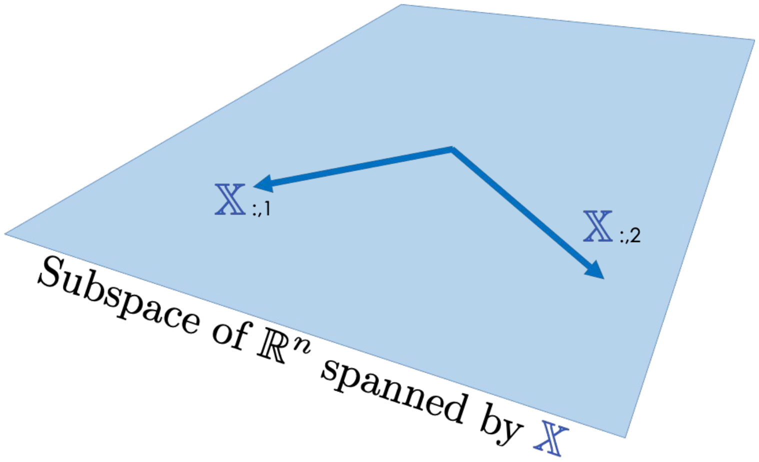
1. Choose a model	Multiple Linear Regression	$\hat{\mathbb{Y}} = \mathbb{X}\theta$
2. Choose a loss function	L2 Loss Mean Squared Error (MSE)	$R(\theta) = \frac{1}{n}\lvert\lvert\mathbb{Y} - \mathbb{X}\theta\rvert\rvert_2^2$
3. Fit the model	Minimize average loss with ~~calculus~~ geometry	The calculus derivation requires matrix calculus (out of scope, but here's a link if you're interested). Instead, we will derive $\hat{\theta}$ using a **geometric argument**.
4. Evaluate model performance	Visualize, ~~Root MSE~~ Multiple R^2	

The set of all possible linear combinations of the columns of X is called the **span** of the columns of X (denoted $\mathbf{span}(\mathbb{X})$), also called the **column space**.

- Intuitively, this is all of the vectors you can "reach" using the columns of X.
- If each column of X has length n, $\mathbf{span}(\mathbb{X})$ is a subspace of $\mathbb{R}^n$.



A linear combination of columns

$$\hat{\mathbb{Y}} = \mathbb{X}\,\theta$$

So far, we've thought of our model as horizontally stacked predictions per datapoint:

$$\begin{array}{c} n \\ \begin{bmatrix} \hat{\mathbb{Y}} \end{bmatrix} \\ 1 \end{array} = \begin{bmatrix} — x_1^T — \\ — x_2^T — \\ \vdots \\ — x_n^T — \end{bmatrix} \begin{array}{c} \begin{bmatrix} \theta \end{bmatrix} \\ 1 \end{array} \begin{array}{c} p+1 \end{array} =$$

We can also think of $\hat{\mathbb{Y}}$ as a **linear combination of feature vectors**, scaled by **parameters**.

$$\begin{array}{c} n \\ \begin{bmatrix} \hat{\mathbb{Y}} \end{bmatrix} \\ 1 \end{array} = \begin{array}{c} n \\ \begin{bmatrix} \mathbb{X}_{:,1} & \mathbb{X}_{:,2} \end{bmatrix} \\ p+1 \end{array} \begin{array}{c} p+1 \\ \begin{bmatrix} \theta \end{bmatrix} \\ 1 \end{array} = \theta_1 \mathbb{X}_{:,1} + \theta_2 \mathbb{X}_{:,2}$$

A linear combination of columns

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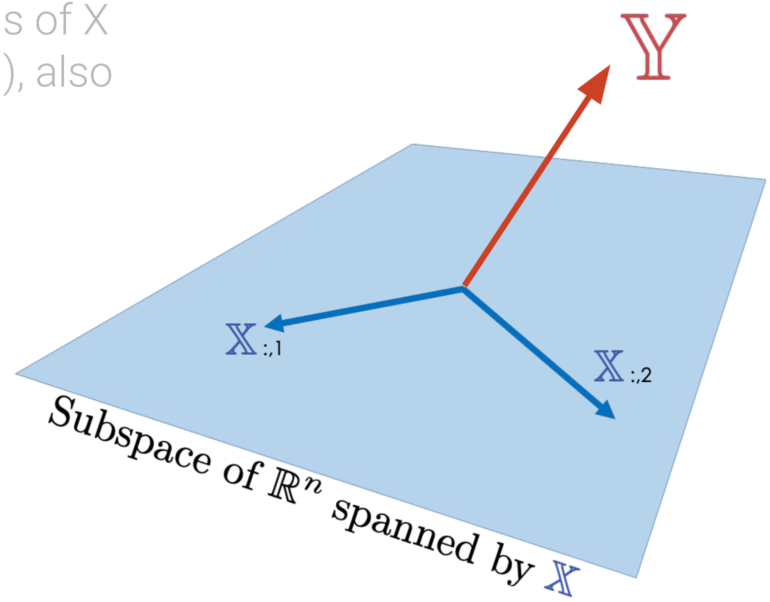
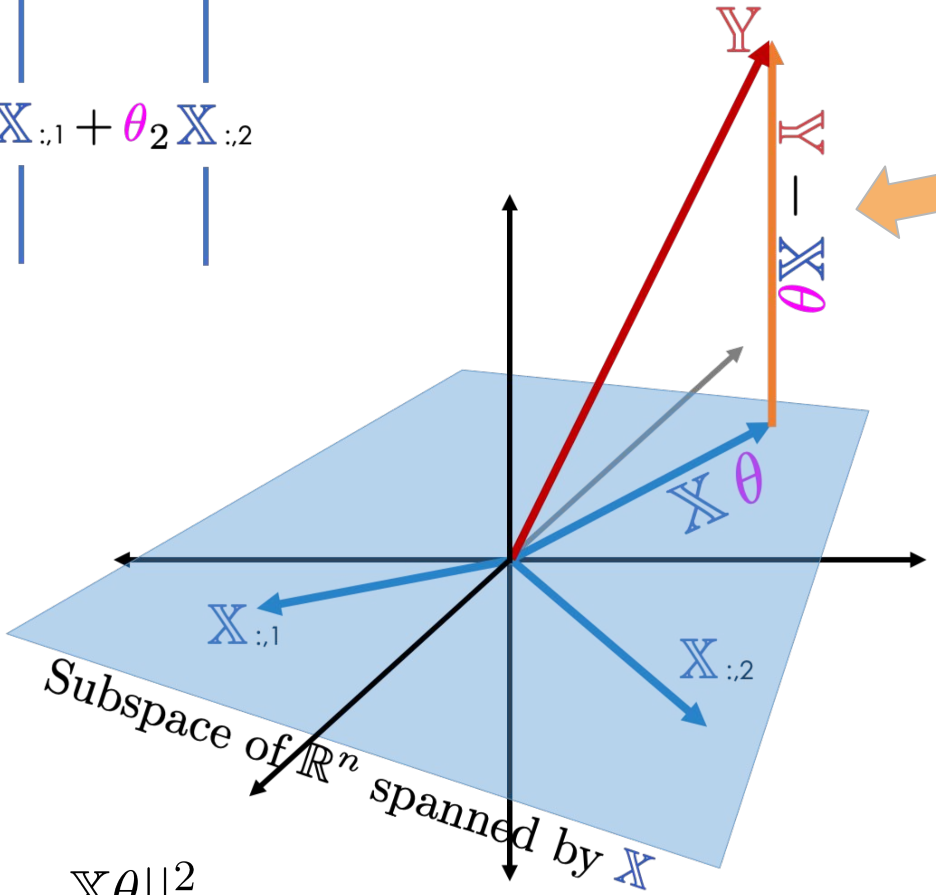


Our prediction $\hat{\mathbb{Y}} = \mathbb{X}\theta$ is a **linear combination** of the columns of $\mathbb{X}$. Therefore $\hat{\mathbb{Y}} \in \text{span}(\mathbb{X})$.

Interpret: Our linear prediction $\hat{\mathbb{Y}}$ will be in $\text{span}(\mathbb{X})$, even if the true values $\mathbb{Y}$ might not be.

Goal: Find the vector in $\text{span}(\mathbb{X})$ that is **closest** to $\mathbb{Y}$.

$$\hat{\mathbb{Y}} = \theta_1 \mathbb{X}_{:,1} + \theta_2 \mathbb{X}_{:,2}$$



This is the residual vector, $e = \mathbb{Y} - \hat{\mathbb{Y}}$.

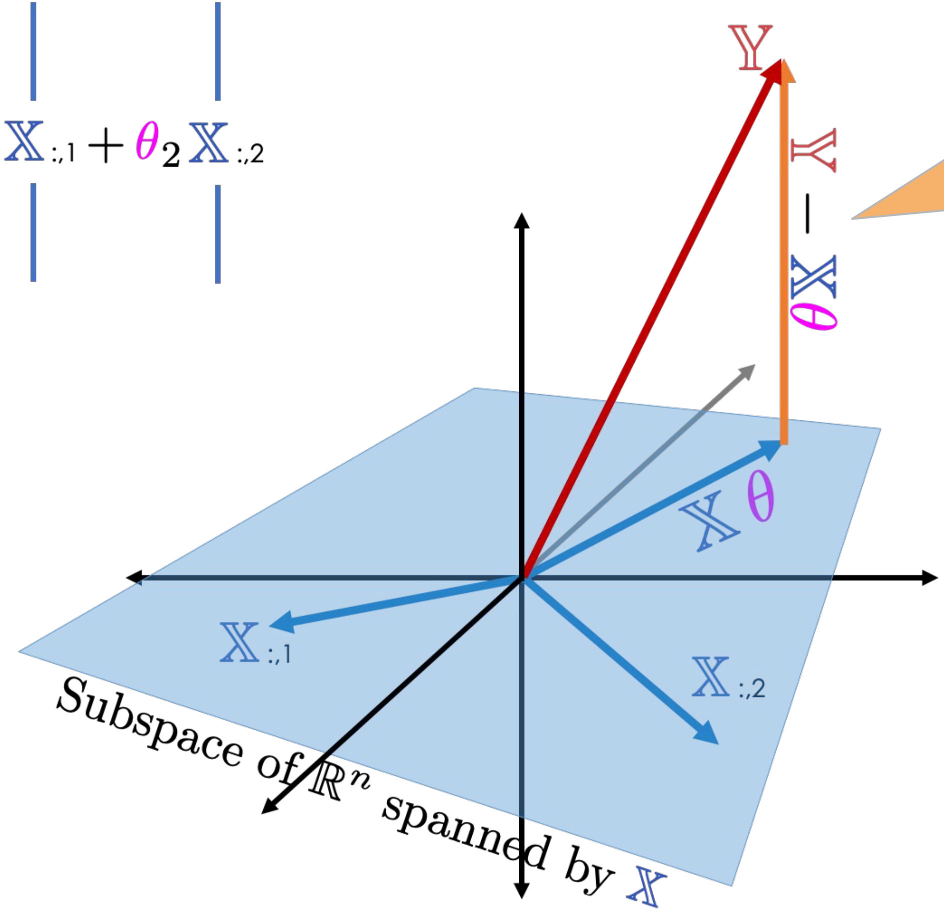
Goal:

Minimize the L_2 norm of the residual vector.

i.e., get the predictions $\hat{\mathbb{Y}}$ to be “as close” to our true y values as possible.

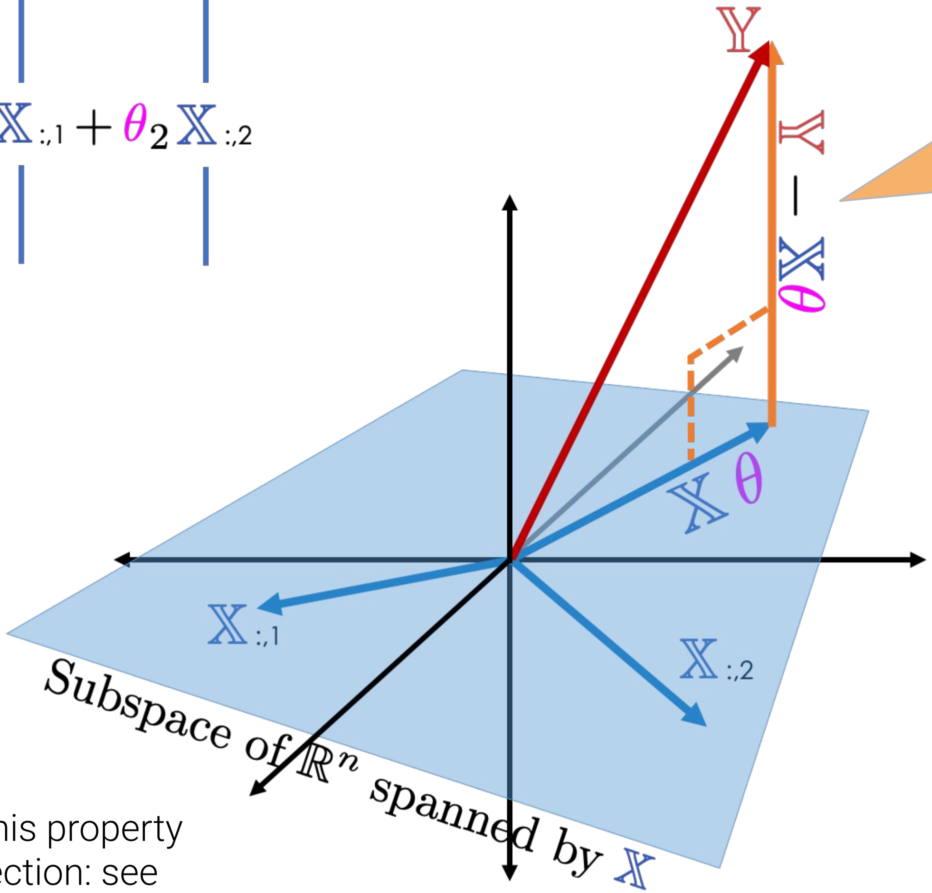
$$R(\theta) = \frac{1}{n}||\mathbb{Y} - \mathbb{X}\theta||_2^2$$

$$\begin{array}{c} \\ n \\ \\ \end{array}\begin{bmatrix} | \\ \hat{\mathbb{Y}} \\ | \end{bmatrix}_{1} = \theta_1 \begin{matrix} | \\ \mathbb{X}_{:,1} \\ | \end{matrix} + \theta_2 \begin{matrix} | \\ \mathbb{X}_{:,2} \\ | \end{matrix}$$



How do we minimize this distance – the norm of the residual vector (squared)?

$$\hat{\mathbb{Y}} = \theta_1 \mathbb{X}_{:,1} + \theta_2 \mathbb{X}_{:,2}$$

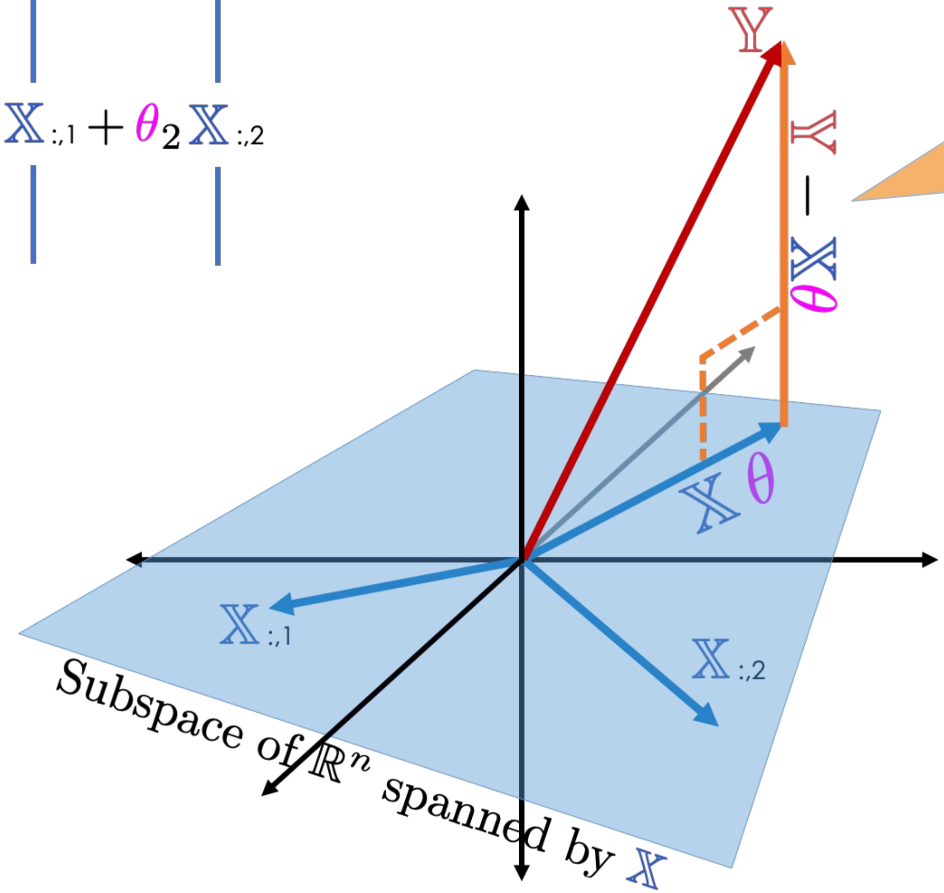


How do we minimize this distance – the norm of the residual vector (squared)?

The vector in span(X) that is closest to Y is the **orthogonal projection** of Y onto span(X).

We will not prove this property of orthogonal projection: see [Khan Academy](#).

$$\hat{\mathbb{Y}} = \theta_1 \mathbb{X}_{:,1} + \theta_2 \mathbb{X}_{:,2}$$



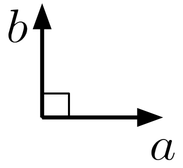
How do we minimize this distance – the norm of the residual vector (squared)?

The vector in span(X) that is closest to Y is the **orthogonal projection** of Y onto span(X).

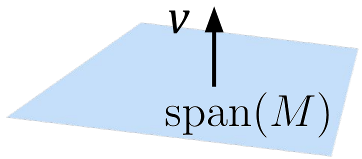
Thus, we should choose the θ that makes the residual vector **orthogonal** to span(X).

[Linear Algebra] Orthogonality

1. Vector a and Vector b are **orthogonal** if and only if their dot product is 0: $a^T b = 0$
This is a generalization of the notion of two vectors in 2D being perpendicular.



2. A vector v is **orthogonal** to $\text{span}(M)$, the span of the columns of a matrix M, if and only if v is orthogonal to **each column** in M.



Let's express **2** in matrix notation. Let $v \in \mathbb{R}^{n\times 1}$, $M \in \mathbb{R}^{n\times d}$ where $M = \begin{bmatrix} | & | & & | \\ m_1 & m_2 & \dots & m_d \\ | & | & & | \end{bmatrix}$:

$$\begin{aligned} m_1^T v &= 0 \\ m_2^T v &= 0 \\ &\vdots \\ m_d^T v &= 0 \end{aligned}$$

v is orthogonal to each column of M, $m_j \in \mathbb{R}^{n\times 1}$

$$\begin{bmatrix} m_1^T v \\ m_2^T v \\ \vdots \\ m_d^T v \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$$\boxed{\underbrace{M^T}_{M^T \in \mathbb{R}^{d\times n}} v = \underbrace{\vec{0}}_{\text{zero vector}}}$$

zero vector
(d-length vector full of 0s).

Ordinary Least Squares Proof

The **least squares estimate** $\hat{\theta}$ is the parameter θ that minimizes the objective function $R(\theta)$:

$$R(\theta) = \frac{1}{n}||\mathbb{Y} - \mathbb{X}\theta||_2^2$$

Equivalently, this is the $\hat{\theta}$ such that the residual vector $\mathbb{Y} - \mathbb{X}\hat{\theta}$ is orthogonal to $\text{span}(\mathbb{X})$.

Definition of orthogonality of $\mathbb{Y} - \mathbb{X}\hat{\theta}$ to $\text{span}(\mathbb{X})$ (0 is the $\vec{0}$ vector)

$$\mathbb{X}^T\left(\mathbb{Y} - \mathbb{X}\hat{\theta}\right) = 0$$

Rearrange terms

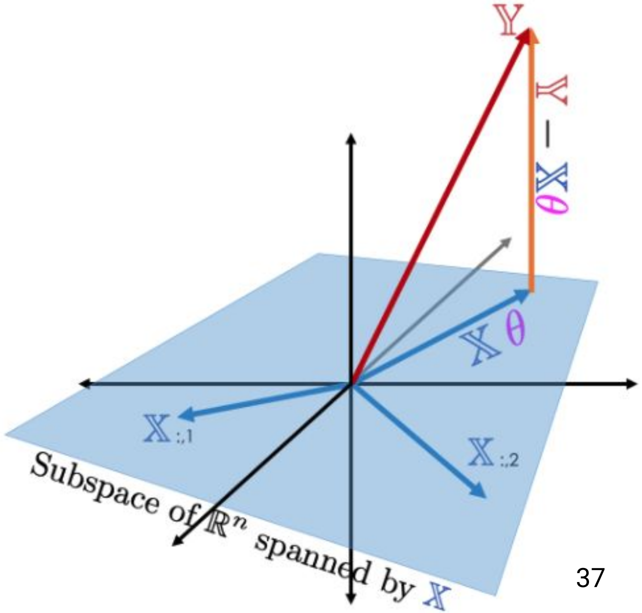
$$\mathbb{X}^T\mathbb{Y} - \mathbb{X}^T\mathbb{X}\hat{\theta} = 0$$

The **normal equation**

$$\mathbb{X}^T\mathbb{X}\hat{\theta} = \mathbb{X}^T\mathbb{Y}$$

If $\mathbb{X}^T\mathbb{X}$ is invertible

$$\boxed{\hat{\theta} = \left(\mathbb{X}^T\mathbb{X}\right)^{-1}\mathbb{X}^T\mathbb{Y}}$$



$$\hat{\theta} = (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbb{Y}$$

This result is so important that it deserves its own slide.

It is the **least squares estimate** and the solution to the normal equation $\mathbb{X}^T\mathbb{X}\hat{\theta} = \mathbb{X}^T\mathbb{Y}$.

$$\hat{\theta} = (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbb{Y}$$

This result is so important that it deserves its own slide.

It is the **least squares estimate** and the solution to the normal equation $\mathbb{X}^T\mathbb{X}\hat{\theta} = \mathbb{X}^T\mathbb{Y}$.

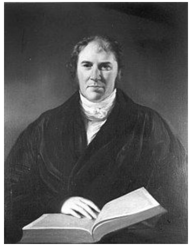
Least Squares Estimate

1. Choose a model	Multiple Linear Regression	$\hat{\mathbb{Y}} = \mathbb{X}\theta$
2. Choose a loss function	L2 Loss Mean Squared Error (MSE)	$R(\theta) = \frac{1}{n}\lvert\lvert\mathbb{Y} - \mathbb{X}\theta\rvert\rvert_2^2$
3. Fit the model ✅	Minimize average loss with ~~calculus~~ geometry	$\hat{\theta} = (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbb{Y}$
4. Evaluate model performance	Visualize, ~~Root MSE~~ Multiple R^2	

Interlude

1809, German mathematician Carl Freidrich Gauss

1805, French mathematician Adrien-Marie Legendre [mistaken portrait]



1809 Irish-American Robert Adrain

Within ten years of publication, OLS was standard in astronomy/geodesy in France/Italy/Prussia.

The "least squares method" is directly translated from the French “méthode des moindres carrés.”

In Gauss’s 1809 work on celestial bodies, “he claimed to have been in possession of the method of least squares since 1795. This naturally led to a priority dispute with Legendre.” [link]

Performance

Lecture 11, Data 100 Fall 2022

Linear Algebra Resources: Ed post

Least Squares Estimate

1. Choose a model	Multiple Linear Regression	$\hat{\mathbb{Y}} = \mathbb{X}\theta$
2. Choose a loss function	L2 Loss Mean Squared Error (MSE)	$R(\theta) = \frac{1}{n}\lvert\lvert\mathbb{Y} - \mathbb{X}\theta\rvert\rvert_2^2$
3. Fit the model	Minimize average loss with ~~calculus~~ geometry	$\hat{\theta} = (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbb{Y}$
4. Evaluate model performance	Visualize, ~~Root MSE~~ Multiple R^2	

Multiple Linear Regression

$$\hat{\mathbb{Y}} = \mathbb{X}\theta$$

Prediction vector $\mathbb{R}^n$

Design matrix $\mathbb{R}^{n \times (p+1)}$

Parameter vector $\mathbb{R}^{(p+1)}$

Note that our **true output** is also a vector:

$$\mathbb{Y} \in \mathbb{R}^n$$

$$R(\theta) = \frac{1}{n}||\mathbb{Y} - \mathbb{X}\theta||_2^2$$

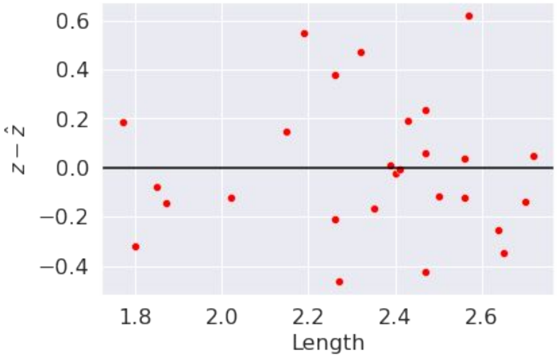
$$\hat{\theta} = (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbb{Y}$$

Demo

[Visualization] Residual Plots

Simple linear regression

Plot residuals vs
the single feature x.



Compare

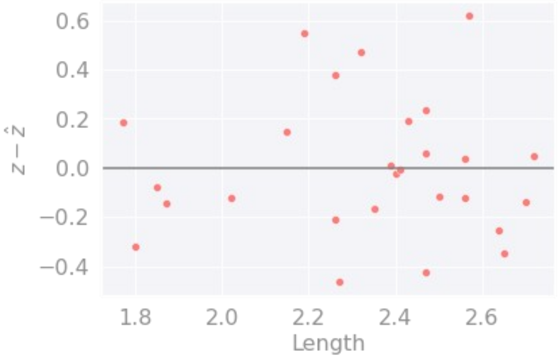
[Visualization] Residual Plots

Compare

See notebook

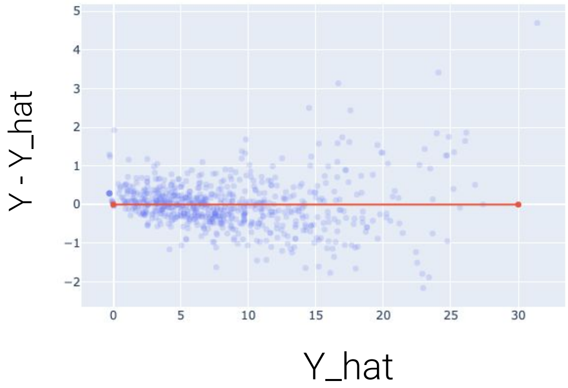
Simple linear regression

Plot residuals vs
the single feature x.



Multiple linear regression

Plot residuals vs
fitted (predicted) values $\hat{y}$.
Check distribution around



Same interpretation as before (Data 8 [textbook]):

- A good residual plot shows no pattern.
- A good residual plot also has a similar vertical spread throughout the entire plot. Else (heteroscedasticity), the accuracy of the predictions is not reliable.

[Metrics] Multiple R^2

Compare

Simple linear regression

Error
RMSE

$$\sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

Linearity
Correlation coefficient, r

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

Multiple linear regression

Error
RMSE

$$\sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

Linearity
Multiple R^2, also called the **coefficient of determination**

$$R^2 = \frac{\text{variance of fitted values}}{\text{variance of } y} = \frac{\sigma_{\hat{y}}^2}{\sigma_y^2}$$

Compare

[Metrics] Multiple R^2

We define the **multiple R²** value as the **proportion of variance** or our **fitted values** (predictions) $\hat{y}$ to our true values y .

$$R^2 = \frac{\text{variance of fitted values}}{\text{variance of } y} = \frac{\sigma_{\hat{y}}^2}{\sigma_y^2}$$

Also called the **correlation of determination**.

R^2 ranges from 0 to 1 and is effectively
"the proportion of variance that the **model explains**."

For OLS with an intercept term (e.g. $\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_p x_p$),
$R^2 = [r(y, \hat{y})]^2$ is equal to the square of correlation between y, $\hat{y}$.

- For SLR, $R^2 = r^2$, the correlation between x, y.
- The proof of these last two properties is on the next hw

[Metrics] Multiple R^2

$$\text{predicted PTS} = 3.98 + 2.4 \cdot \text{AST}$$

R^2 = 0.457

$$\text{predicted PTS} = 2.163 + 1.64 \cdot \text{AST} + 1.26 \cdot \text{3PA}$$

R^2 = 0.609

Compare

Simple linear regression

Error
RMSE

$$\sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

Linearity
Correlation coefficient, r

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

Multiple linear regression

Error
RMSE

$$\sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

Linearity
Multiple R^2, also called the **coefficient of determination**

$$R^2 = \frac{\text{variance of fitted values}}{\text{variance of } y} = \frac{\sigma_{\hat{y}}^2}{\sigma_y^2}$$

As we add more features, our fitted values tend to become closer and closer to our actual y values. Thus, R^2 increases.

- The SLR **model** (AST only) explains 45.7% of the variance in the true y.
- The AST & 3PA **model** explains 60.9%.

Adding more features doesn't always mean our model is better, though!
We are a few weeks away from understanding why.

These slides were not covered in lecture 2/22 but will be useful when you explore properties of OLS in homework.

(Supplemental video: https://youtu.be/dhG8GiZcyUE)

OLS Properties

Lecture 11, Data 100 Fall 2022

OLS Problem Formulation

- Multiple Linear Regression Model
- Mean Squared Error

Geometric Derivation

- Lin Alg Review: Orthogonality, Span
- Least Squares Estimate Proof

Performance: Residuals, Multiple R^2

OLS Properties

- Residuals
- The Intercept Term
- Existence of a Unique Solution

Linear Algebra Resources: Ed post

Residual Properties

When using the optimal parameter vector, our residuals $e = \mathbb{Y} - \mathbb{X}\hat{\theta}$ are orthogonal to $\textbf{span}(\mathbb{X})$.

$$\mathbb{X}^T e = 0$$

<u>Proof</u> First line of our OLS estimate proof (slide).

For all linear models:

Since our predicted response $\hat{\mathbb{Y}}$ is in $\textbf{span}(\mathbb{X})$ by definition, it is orthogonal to the residuals.

$\hat{\mathbb{Y}} = \theta_0 \mathbb{X}_{:,0} + \theta_1 \mathbb{X}_{:,1} + \dots + \dots$

$$\hat{\mathbb{Y}}^T e = 0$$

For all linear models with an **intercept term**, the **sum of residuals is zero**.

$$\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_p x_p$$

$$\sum_{i=1}^{n} e_i = 0$$

$$\mathbb{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1p} \\ 1 & x_{21} & x_{22} & \dots & x_{2p} \\ 1 & x_{31} & x_{32} & \dots & x_{3p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{np} \end{bmatrix}$$

You will prove both properties in homework.

(Proof hint) $\mathbb{1}^T e = 0$

Properties when our model has an intercept term

For all linear models with an **intercept term**, the **sum of residuals is zero**.

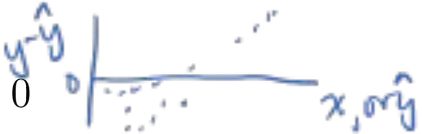
$$\sum_{i=1}^{n} e_i = 0$$

(previous slide)

1

- This is the real reason why we don't directly use residuals as loss.

$$R(\theta) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i) = \frac{1}{n}\sum_{i=1}^{n} e_i = 0$$



2

- This is also why positive and negative residuals will cancel out in any residual plot where the (linear) model contains an intercept term, even if the model is terrible.

3

It follows from the property above that for linear models with intercepts, the average predicted y value is equal to the average true y value.

$$\bar{y} = \bar{\hat{y}}$$

These properties are true when there is an intercept term, and not necessarily when there isn't.

You will prove these properties in homework.

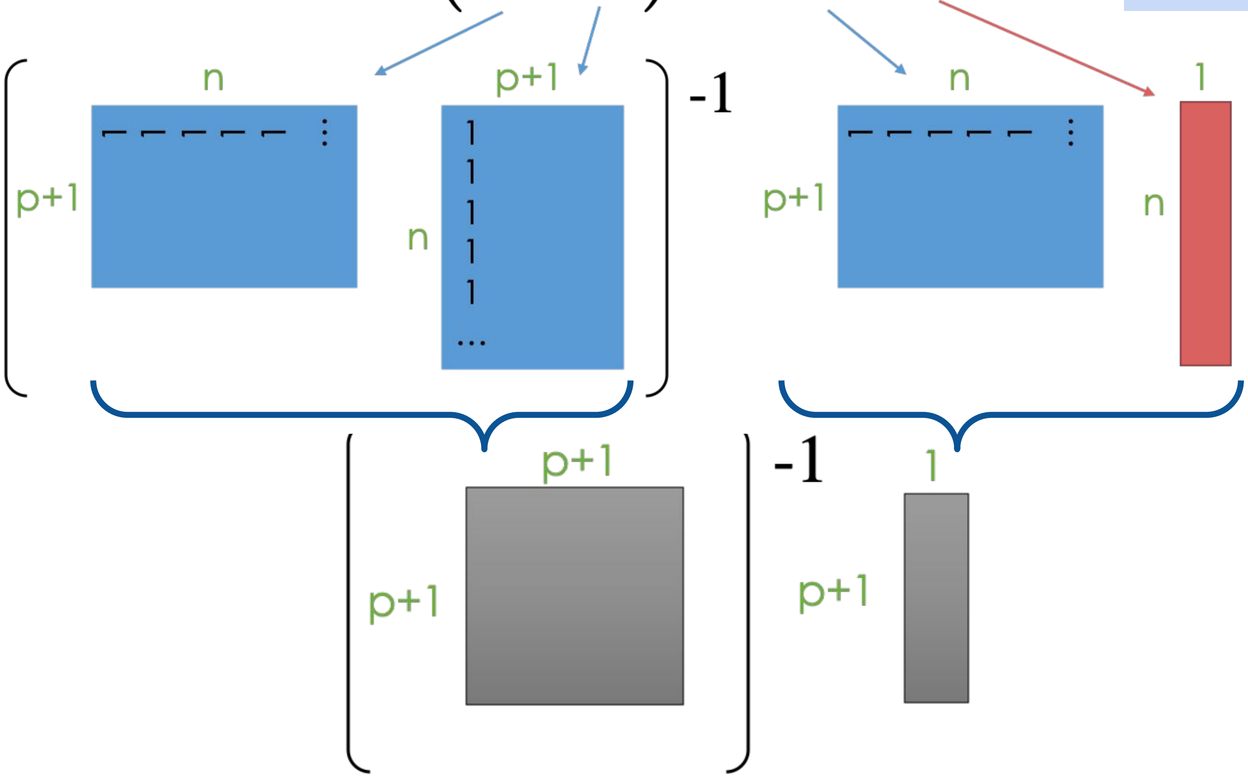
Does a unique solution always exist?

	Model	Estimate	Unique?
Constant Model + MSE	$\hat{y} = \theta$	$\hat{\theta} = \textbf{mean}(y)$	**Yes**. Any set of values has a unique mean.
Constant Model + MAE	$\hat{y} = \theta$	$\hat{\theta} = \textbf{median}(y)$	**Yes**, if odd. **No**, if even. Return average of middle 2 values.
Simple Linear Regression + MSE	$\hat{y} = a + bx$	$\hat{a} = \bar{y} - \hat{b}\bar{x}$ $\hat{b} = r\frac{\sigma_y}{\sigma_x}$	**Yes**. Any set of non-constant* values has a unique mean, SD, and correlation coefficient.
Ordinary Least Squares (Linear Model + MSE)	$\hat{\mathbb{Y}} = \mathbb{X}\theta$	$\hat{\theta} = (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbb{Y}$	???

Understanding the solution matrices

$$\hat{\theta} = (\mathbb{X}^T \mathbb{X})^{-1} \mathbb{X}^T \mathbb{Y}$$

In most settings,
 # observations **N** **>>** **# features** **p**



Understanding the solution matrices

In practice, instead of directly inverting matrices, we can use more efficient numerical solvers to directly solve a system of linear equations.

The **Normal Equation**:

$$\mathbb{X}^T \mathbb{X} \hat{\theta} = \mathbb{X}^T \mathbb{Y}$$

$$\left[\begin{array}{cc} & p+1 \\ p+1 & \boxed{A} \end{array} \right] \hat{\theta} = \begin{array}{cc} & 1 \\ p+1 & \boxed{b} \end{array}$$

Note that at least one solution always exists:

Intuitively, we can always draw a line of best fit for a given set of data, but there may be multiple lines that are "equally good". (Formal proof is beyond this course.)

Uniqueness of a solution: Proof

Claim

The Least Squares estimate $\hat{\theta}$ is **unique** if and only if $\mathbb{X}$ is **full column rank**.

Proof

- The solution to the normal equation $\mathbb{X}^T\mathbb{X}\hat{\theta} = \mathbb{X}^T\mathbb{Y}$ is the least square estimate $\hat{\theta}$.

- $\hat{\theta}$ has a **unique** solution if and only if the square matrix $\mathbb{X}^T\mathbb{X}$ is **invertible**, which happens if and only if $\mathbb{X}^T\mathbb{X}$ is full (column) rank.
    - The **rank** of a matrix is the max **# of linearly independent columns (or rows)** it contains.
    - $\mathbb{X}^T\mathbb{X}$ has shape (p +1) x (p + 1), and therefore has max rank p + 1.

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

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

- $\mathbb{X}^T\mathbb{X}$ and $\mathbb{X}$ **have the same rank** (proof out of scope).

- Therefore $\mathbb{X}^T\mathbb{X}$ has rank p + 1 if and only if $\mathbb{X}$ has rank p + 1 (full column rank).

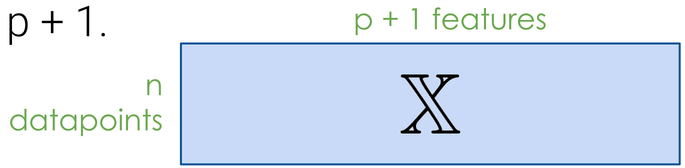
Uniqueness of a solution: Interpretation

Claim:

The Least Squares estimate $\hat{\theta}$ is **unique** if and only if $\mathbb{X}$ is **full column rank**.

When would we **not** have unique estimates?

1. If our design matrix $\mathbb{X}$ is "**wide**":
   - (property of rank) If n < p, rank of $\mathbb{X}$ = min(n, p + 1) **<** p + 1.
   - In other words, if we have way more features than observations, then $\hat{\theta}$ is not unique.
   - Typically we have n >> p so this is less of an issue.



2. If we our design matrix $\mathbb{X}$ has features that are **linear combinations of other features**.
   - By definition, rank of $\mathbb{X}$ is number of linearly independent columns in $\mathbb{X}$.
   - Example: If "Width", "Height", and "Perimeter" are all columns,
     - Perimeter = 2 * Width + 2 * Height → $\mathbb{X}$ is not full rank.
   - Important with one-hot encoding (to discuss in later).

$$\mathbb{X} = \begin{bmatrix} | & | & | & | \\ 1 & w & h & 2h+2w \\ | & | & | & | \end{bmatrix}$$

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Ordinary Least Squares (Linear Model + MSE)	$\hat{\mathbb{Y}} = \mathbb{X}\theta$	$\hat{\theta} = (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbb{Y}$	**Yes**, if $\mathbb{X}$ is full col rank (all cols lin independent, # datapts >> # feats)

LECTURE 11

Ordinary Least Squares

Content credit: Lisa Yan, Ani Adhikari, Deborah Nolan, Joseph Gonzalez