Master of Science in Business Analytics

Machine Learning I
OPAN 6602

Week 1 Live Session

Instructor:
Tommy Jones, PhD

GEORGETOWN UNIVERSITY / McDONOUGH SCHOOL of BUSINESS

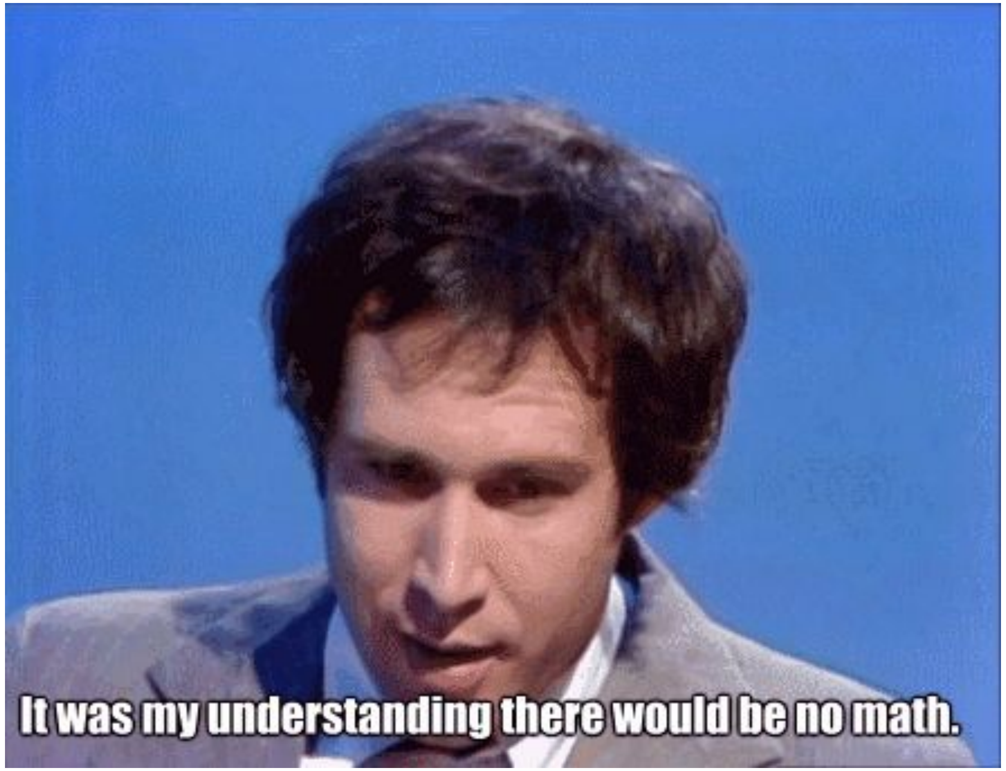
“All models are wrong. Some Models are useful.”

– George Box

“An approximate answer to the right question is worth far more than a precise answer to the wrong one.”

– John Tukey

Welcome to Foundations of Machine Learning I



Objectives:

- Know when to apply which model
- Know when a model is or is not working well
- Know how to run these models in Python

Week 1 Live Session Agenda

1. **Course Introduction**
2. Machine Learning Overview
3. Linear Regression Review
4. Coding Examples

October 30	Live Session 1: Linear Regression I
November 6	Live Session 2: Linear Regression II
November 12	*Project 1 Due*
November 13	Live Session 3: Logistic Regression
November 20	Live Session 4: Model Validation & Feature Engineering
December 3	*Project 2 Due*
December 4	Live Session 5: Biased Regression Models
December 11	Live Session 6: Decision Trees
December 18	*Final Project Due*

Course Introduction

- Machine Learning Concepts
  - Focus on supervised learning
- Tools: Python, Google Colab
- Assignments and Grades
  - Project 1: Multiple Linear Regression (Individual) 30%
  - Project 2: Logistic Regression (Individual) 30%
  - Project 3: (Group) 35% (25% report, 10% peer-evaluation)
  - Class participation (Individual) 5%

Office Hours

Me:

Mondays 4:30 - 6:00 PM Eastern, by appointment.
https://calendar.app.google/YGm3wdBi51mRBka5A

Manav (TA):

Sundays 1 - 2:30pm ET
Tuesdays 7:30 - 9pm ET
https://georgetown.zoom.us/my/manavarora

Tour of Course Canvas

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Defining Machine Learning

Machine Learning (from getting started video)
"A subfield of Artificial Intelligence where algorithms 'learn' patterns in data to solve problems."

Statistical Learning (from ISL pp. 16-17)
"Statistical Learning [is] a set of approaches for estimating f" where f defines the relationship between variable(s), Y, and variable(s), X, with some error, ϵ as in the equation below.

$$Y = f(X) + \epsilon$$

Types of Machine Learning

Supervised
We want to learn patterns in the data **based on a known outcome** we are trying to predict.

Unsupervised
We want to learn patterns in the data **without or independent of a known outcome** we are trying to predict.

Reinforcement
Used primarily in robotics. An algorithm interacts with its environment within a structure of rewards and penalties.

Comprehension Check:
Is this supervised or unsupervised ML?

Competition: October 2006.

Using a training data set of 400,000 Netflix customers' ratings for 18,000 movies, participants were asked to build a model predicting customer ratings.

The test set was a set of 1 million customer-movie pairs that are missing in the training data,

Ratings ranged between 1 (terrible) and 5 (amazing).

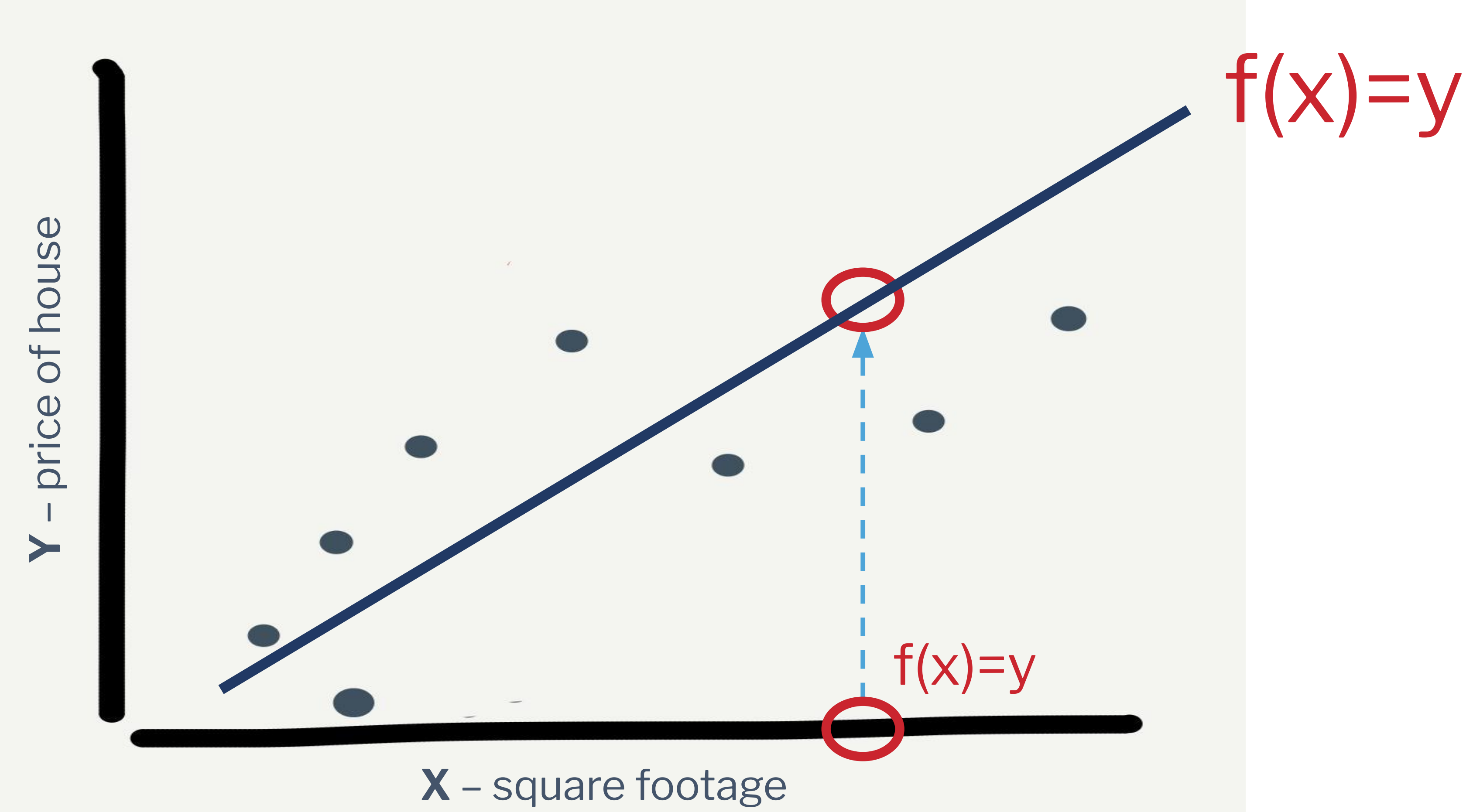
Netflix's original algorithm achieved a RMSE of 0.953. The first team to achieve a 10% improvement to Netflix's algorithm wins one million dollars.

Comprehension Check:
Is this supervised or unsupervised ML?

Unsupervised ML

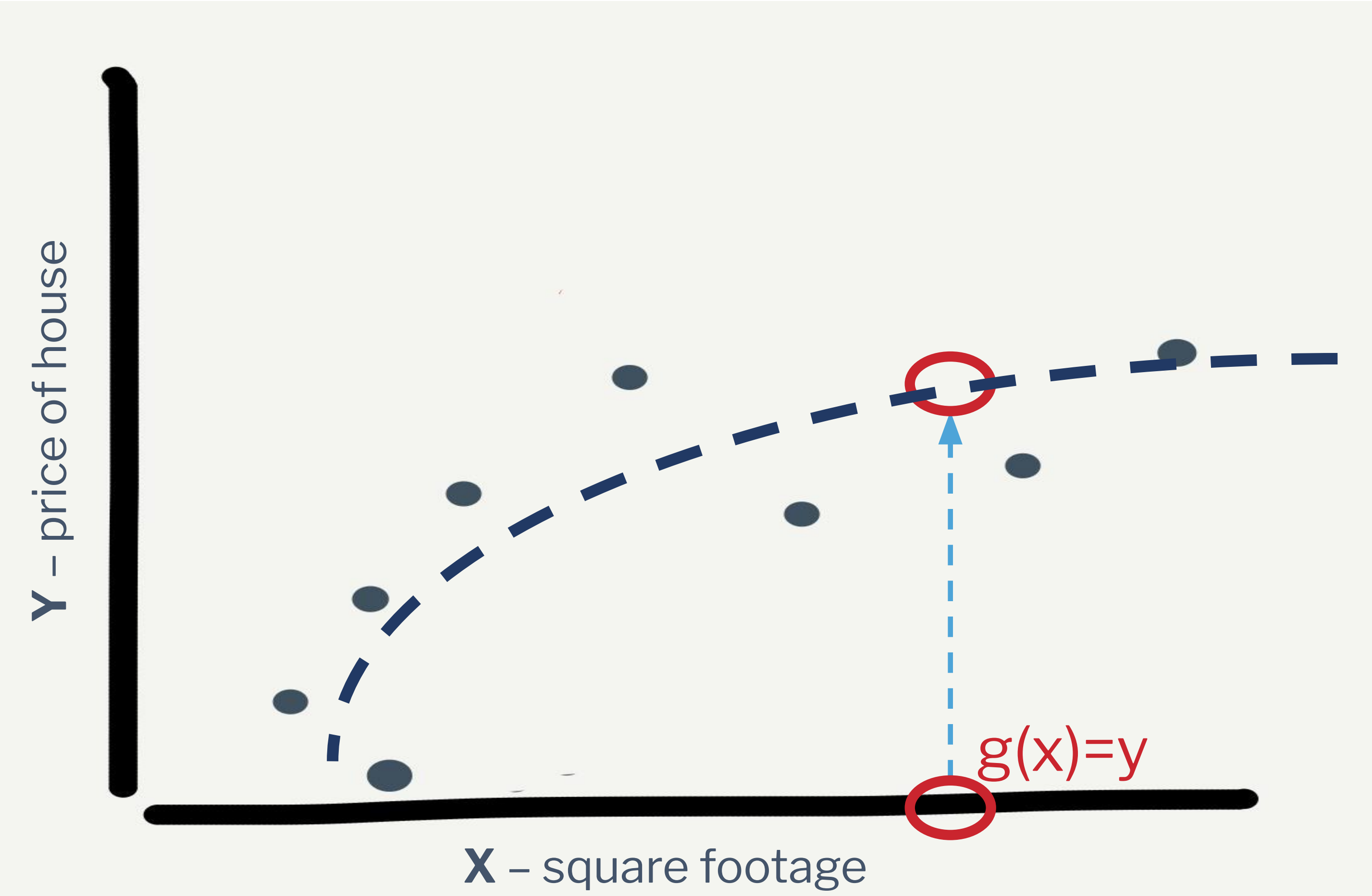
Supervised ML

Supervised Learning: Numeric Prediction (Regression)



X	Y
850	650,220
1,300	753,475
2,400	999,876
…	…

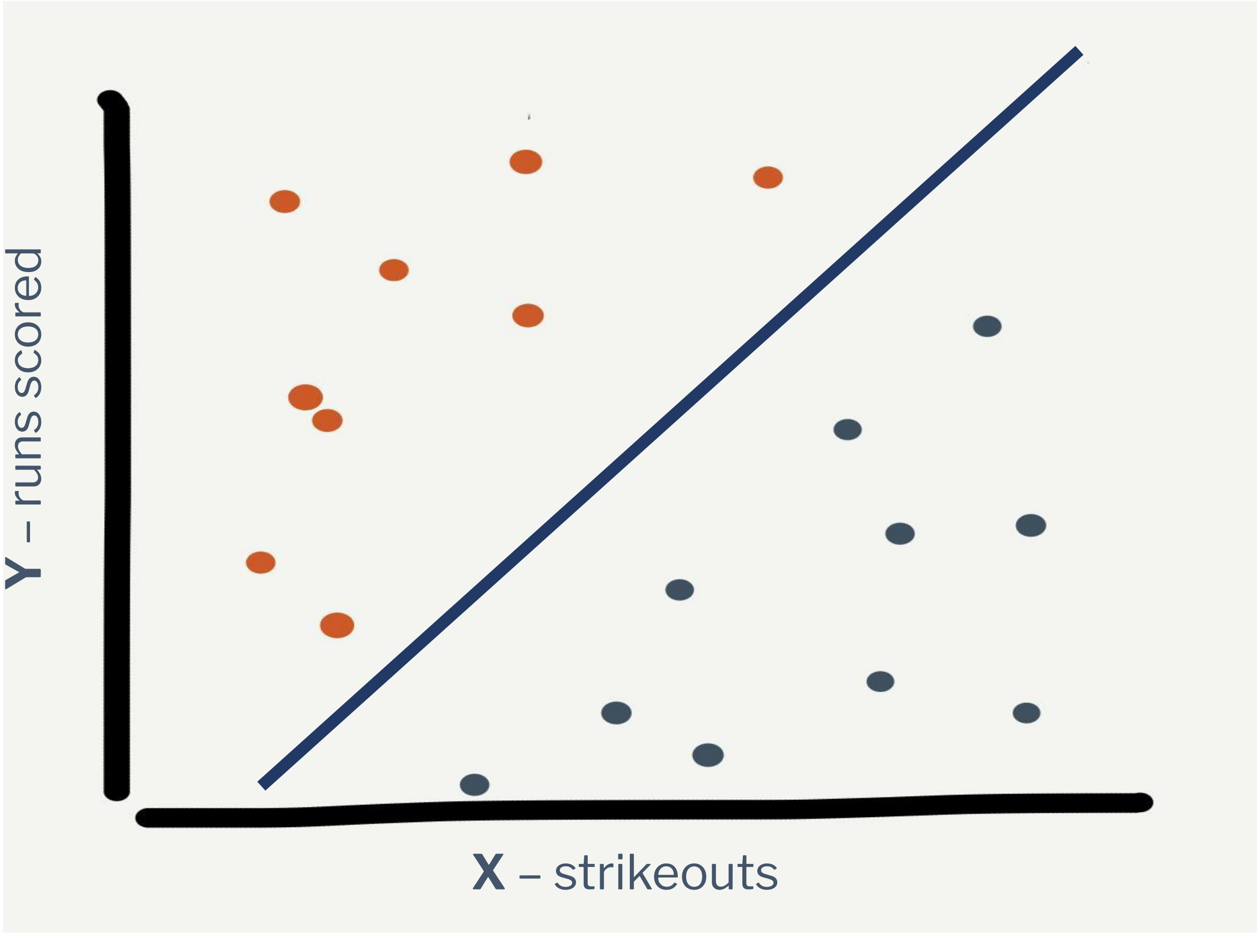
Supervised Learning: Numeric Prediction (Regression)



g(x)=y

X	Y
850	650,220
1,300	753,475
2,400	999,876
…	…

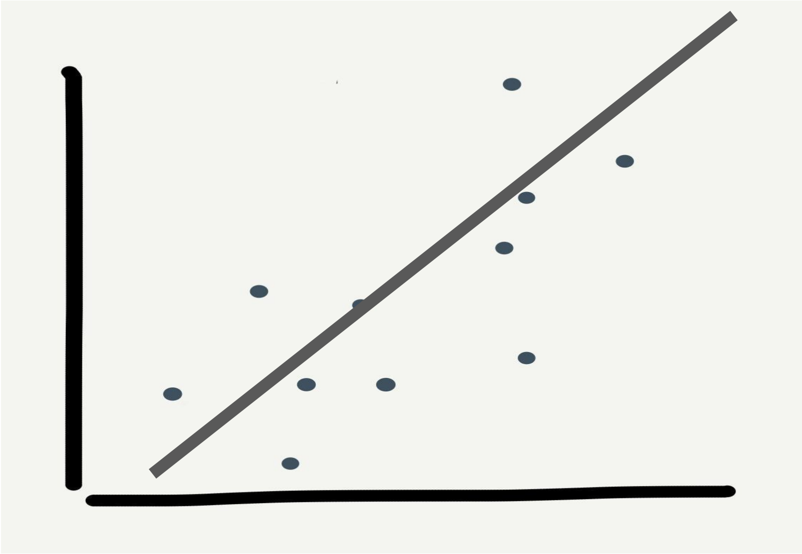
Supervised Learning: Classification



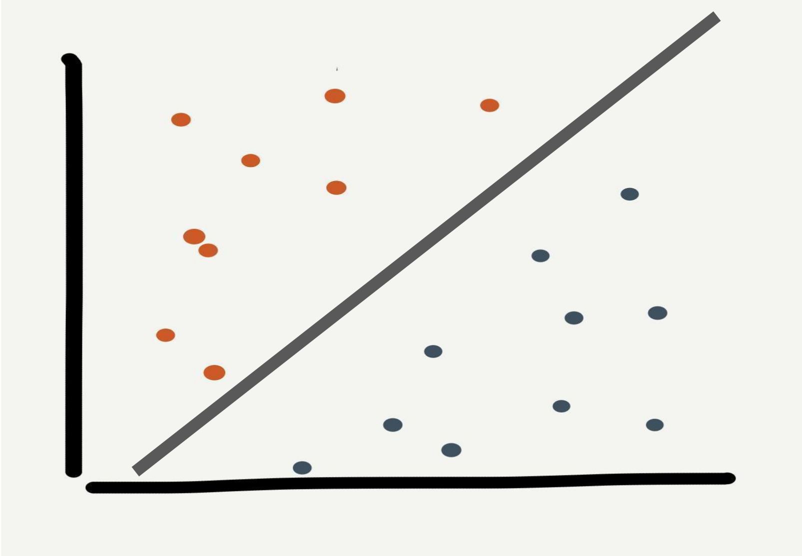
Win
Loss

X	Y	Class
0	5	Win
7	3	Loss
5	10	Win
…	…	…

Numeric Prediction



Classification



Unsupervised ML & Reinforcement Learning

Unsupervised

- Clustering (including embedding)
- Association Rules
- Anomaly Detection

Reinforcement

- An "agent" (the model) interacts with an environment and receives feedback in the form of rewards or penalties

Covered in later courses

Week 1 Live Session Agenda

1. Course Introduction
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3. **Linear Regression Review**
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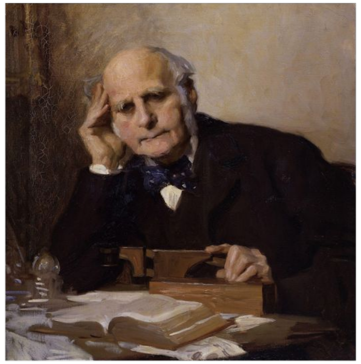
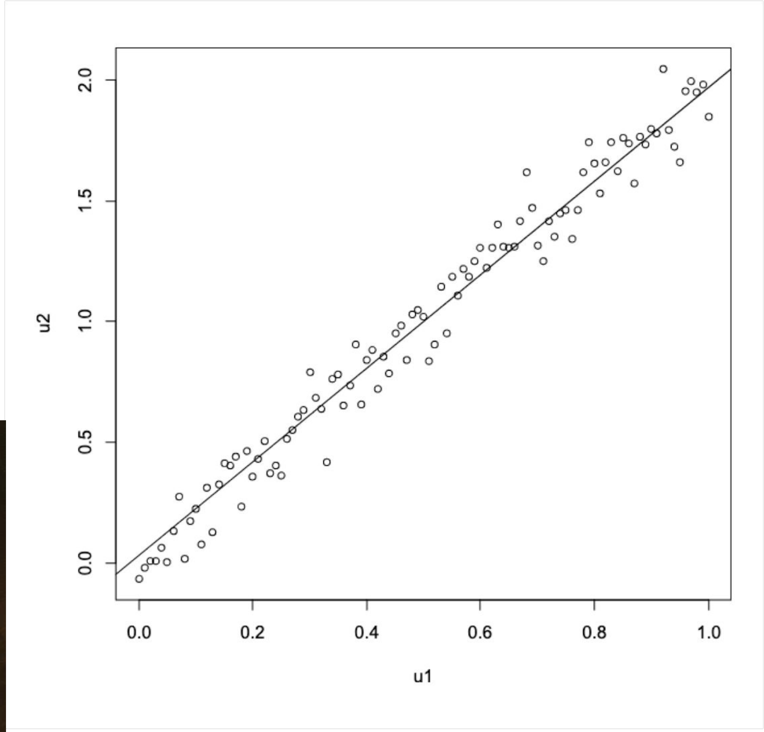
Linear Regression (OLS) - The Oldest ML Model?

By Christian Albrecht Jensen - Public Domain

By Julien-Léopold Boilly- Public Domain



By Charles Wellington Furse - Public Domain



Comprehension Check:
Which of the following is *not* an assumption of OLS?

1. Errors are distributed normally.

2. The relationship between Y and X is linear in the parameters.

3. The data set is representative of the population.

4. The errors have a mean of zero.

5. The errors have constant variance.

Comprehension Check:
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3. **The data set is representative of the population.**

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Linear Regression
AKA Ordinary Least Squares (OLS)

For linear regression model

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p + \epsilon$$

1. The relationship between *Y* and the *X*'s are linear in its parameters.
2. $\epsilon \sim N(0, \sigma)$*
3. σ is constant (homoskedasticity).*
4. Errors are i.i.d (implicitly, x_i and x_j are independent $\forall\ i, j$)*

If you ***only*** want to ***predict***, you only need this.

If you also want to ***explain***, you need these.

Prediction vs. Explanation

If prediction is your goal:

Only “linear in parameters” assumption really matters.
You can (mostly) go wild with transformations.
Still watch out for structural breaks (data drift).

If explanation is your goal:

Statistical inference really matters → all assumptions apply.
Be careful with transformations that obscure explanation.
Sometimes it’s ok to trade good predictions for simplicity.

You can capture non linear relationships with OLS.

"Linear *in the parameters*" is key. Consider…

$$Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \epsilon$$

There is non-linear absolute relationship between *Y* and *X*.

But by including the quadratic of *X*, the relationship is *linear in the parameters*.

Marginal Effect

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + ... + \beta_p X_p + \epsilon$$

"A one unit change in X_1 leads to a β_1 unit change in Y."

Units of X and Y matter in interpretation, not mathematically.

e.g., if Y is in millions of dollars and X is in cents…Eek.

Working with transformed variables means you have to reverse transform to get marginal effects in human-interpretable units.

Marginal Effect → Take the Derivative

Things are more complicated with non-linear relationships.

$$Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \epsilon \qquad \frac{dY}{dX} = \beta_1 + 2\beta_2 X$$

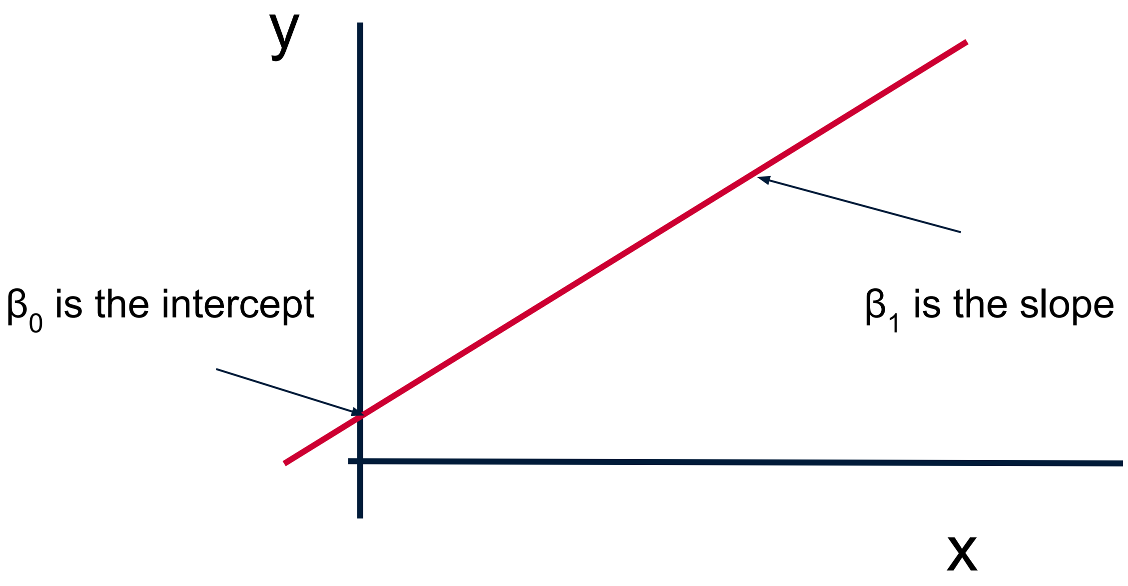
In this case, you can report the marginal effect different ways:

1. At a specific point (e.g, at the mean or median of *X*).
2. Averaged across the range of *X* in the training set.

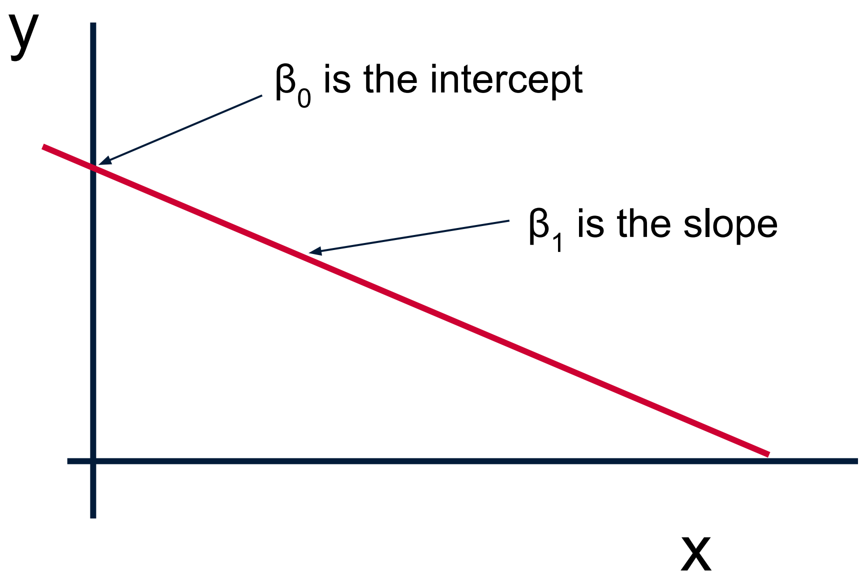
We have to do similar for logistic regression (week 3).

Marginal Effects: Linear Parameters & "Constant Returns"

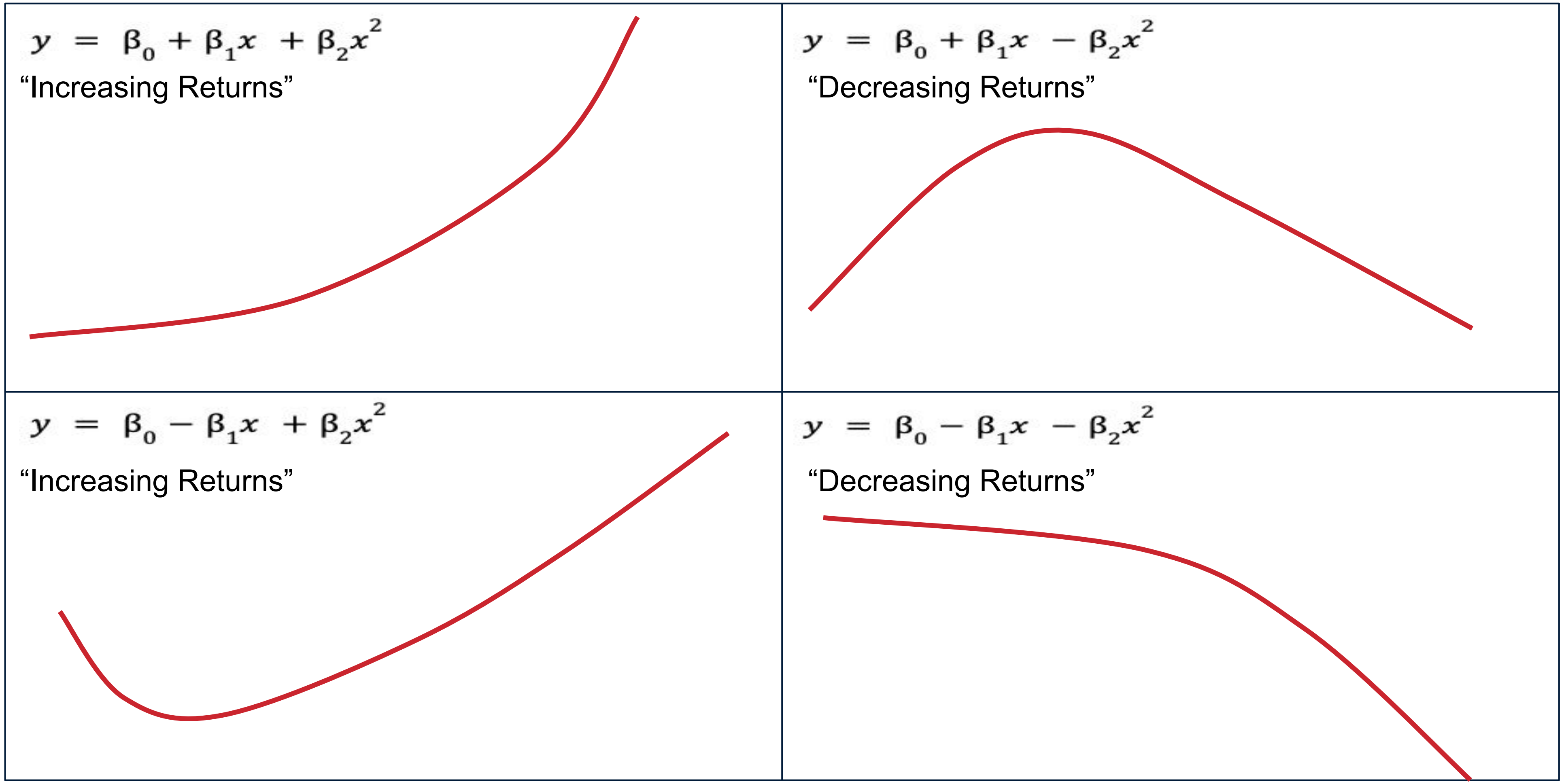
$y = \beta_0 + \beta_1 x$



$y = \beta_0 - \beta_1 x$



Marginal Effects: Using Quadratics



Coefficients in same direction → Acceleration (hockey stick)

Coefficients in opposite direction → Deceleration and Critical points

Critical points are where slope changes direction

A Marginal Effects Helper Table

Transform	Model	Marginal Effect of x on y
None	$y = \beta_0 \pm \beta_1 x$	$\pm \beta_1$
Square/quadratic	$y = \beta_0 \pm \beta_1 \pm \beta_2 x^2$	$\pm \beta_1 \pm 2\beta_2 x$
Square root	$y = \beta_0 \pm \beta_1 x \pm \beta_2 \sqrt{x}$	$\pm\beta_1 \pm \frac{1}{2}\beta_2 \frac{1}{\sqrt{x}}$
Cube root	$y = \beta_0 \pm \beta_1 x \pm \beta_2 x^{1/3}$	$\pm\beta_1 \pm \frac{1}{3}\beta_2 \frac{1}{x^{1/3}}$
Standardization	$y = \beta_0 \pm \beta_1 x \pm \beta_2 \frac{x - \mu_x}{\sigma_x}$	$\pm\beta_1 \pm \frac{\beta_2}{\sigma_x}$
Normalization/MinMax	$y = \beta_0 \pm \beta_1 x \pm \beta_2 \frac{x - min_x}{max_x - min_x}$	$\pm\beta_1 \pm \frac{\beta_2}{max_x - min_x}$

Focus just on these for now.

Comprehension Check:
Which of the following is true?

1. Backward elimination begins with no X variables—an empty model.

2. "Stepwise selection" is a combination of both forward and backward selection techniques.

3. P-values are not typically used to test the significance at each step.

4. Forward selection starts with all variables in the model and deletes the worst variables one at a time.

Comprehension Check:
Which of the following is true?

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Automated Model Selection

Forward Selection, Backward Selection, Stepwise Selection

Be careful if explanation is your goal. In all cases:
- Biases in coefficients, predictions, standard errors
- Biases degrees of freedom of model (multiple testing)
- Biases p-values towards significance

If only prediction is your goal, you can mostly go wild..

Goodness of Fit Metrics: Numeric Prediction

MSE (minimize) - squared units of Y -

$$\frac{1}{n}\sum_{i=1}^{n}(\hat{f}(X) - Y)^2$$

RMSE (minimize) - units of Y -

$$\sqrt{\frac{1}{n}\sum_{i=1}^{n}(\hat{f}(X) - Y)^2}$$

MAE (minimize) - units of Y -

$$\frac{1}{n}\sum_{i=1}^{n}|\hat{f}(X) - Y|$$

R-squared (maximize) - prop. of var. -

$$1 - \frac{\sum_{i=1}^{n}(Y - \hat{f}(X))^2}{\sum_{i=1}^{n}(Y - E[Y])^2}$$

Adjusted R^2

All else constant, R^2 increases by adding predictor variables.

This can lead to overly-complex models and over fit.

Adjusted R^2 adds a penalizing factor for the number of predictor variables.

$$R^2_{adj.} = 1 - \frac{(1 - R^2)(n-1)}{n-p-1}$$

Modeling Process

Generalizes to all supervised learning methods.

1. Data pre-processing
2. Partition: train/test
3. Data exploration
4. Feature engineering
5. Feature & model selection
6. Model evaluation
7. Predictions & conclusions

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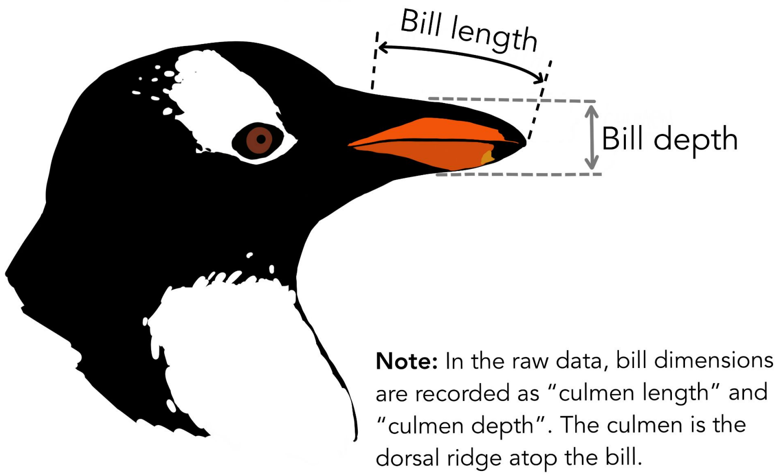
Code: Introducing the Palmer Penguins Data Set

https://allisonhorst.github.io/palmerpenguins/

Data were collected and made available by Dr. Kristen Gorman and the Palmer Station, Antarctica LTER, a member of the Long Term Ecological Research Network.



Note on Python Packages: statsmodels & sklearn

scikit-learn (sklearn)

- **Standard ML library in Python**; works seamlessly with tools like mlxtend for model selection.
- Geared toward **prediction tasks**: focus on training/test workflows, cross-validation, pipelines.
- Outputs coefficients and intercept, but no rich inference (no p-values, confidence intervals by default).
- Default choice for most machine learning models in this course.

statsmodels

- Built for **statistical inference and explanation**.
- Provides rich output: standard errors, p-values, confidence intervals, R^2, adjusted R^2, etc.
- Preferred **when the goal is to explain relationships or test hypotheses**, not just predict.
- Common in econometrics and social sciences, where interpretability is critical.

Demo: Regression on Penguins Data

Exercise: Regression on Penguins Data

End