## IMGD 2905

## Simple Linear Regression

## Chapter 10



## Motivation

- Have data (sample, x's. e.g., playtime)
- Want to know likely value of next observation (A)
A. Compute mean $y$-value (with confidence interval)
$\rightarrow$ Predict A
- But what if have additional information?

E.g., playtime versus skins owned
$\rightarrow$ Better prediction!


## Motivation

- Have data (sample, x’s), based on X
E.g., playtime versus skins owned
- Want to know likely value of next observation (Y)
- A - reasonable to compute mean $y$-value (with confidence interval)
- B - could do same, but there appears to be relationship between X and Y !
$\rightarrow$ Predict B (here, use X data
 to predict Y )
e.g., "trendline" (regression)


## Overview

Broadly, two types of prediction techniques:

1. Regression - mathematical equation to model, then use model for predictions

- We'll discuss simple linear regression

2. Machine learning - branch of AI, use computer algorithms to determine relationships (predictions)

- CS 4342 Machine Learning



## Types of Regression Models



- Explanatory variable explains dependent variable
- Variable X (e.g., skill level) explains Y (e.g., KDA)
- Can have 1 (simple) or 2+ (multiple)
- Linear if coefficients added, else Non-linear


## Outline

- Introduction
- Simple Linear Regression
- Linear relationship
- Residual analysis
- Fitting parameters
- Measures of Variation
- Misc


## Simple Linear Regression

- Goal - find a linear (line) relationship between two values
- E.g., travel time and car speed, KDA and skill,
- First, make sure relationship is linear! How?
$\rightarrow$ Scatterplot
(c) no clear relationship
(b) not a linear relationship
(a) linear relationship - proceed with linear regression





## Linear Relationship

- From algebra: line in form

$$
Y=m X+b
$$

$-m$ is slope, $b$ is $y$-intercept

- Slope (m) is amount $Y$ increases when $X$ increases by 1 unit (specifying units important!)
- Intercept (b) is where line crosses y-axis, or where $y$-value when $x=0$



## Simple Linear Regression Example

- Size of house related to its market value.
$X=$ square footage
$Y=$ market value ( $\$$ )
- Scatter plot (42 homes)
- indicates linear trend

| , | A | B | C |
| :---: | :---: | :---: | :---: |
| 1 | Home Market Value |  |  |
| 2 |  |  |  |
| 3 | House Age | Square Feet | Market Value |
| 4 | 33 | 1.812 | \$90,000.00 |
| 5 | 32 | 1.914 | \$104,400.00 |
| 6 | 32 | 1,842 | \$93,300.00 |
| 7 | 33 | 1.812 | \$91,000.00 |
| 8 | 32 | 1,836 | \$101,900.00 |
| 9 | 33 | 2.028 | \$108,500.00 |
| 10 | 32 | 1.732 | \$87,600.00 |



## Simple Linear Regression Example

- Two possible lines shown below ( $A$ and $B$ )
- Want to determine best regression line
- Line A looks a better fit to data
- But how to know?

$$
Y=m X+b
$$



## Simple Linear Regression Example

- Two possible lines shown below (A and $B$ )
- Want to determine best regression line
- Line A looks a better fit to data - But how to know?

$$
Y=m X+b
$$

Line that gives best fit to data is one that minimizes prediction error
$\rightarrow$ Least squares line (more later)

Market Value


## Simple Linear Regression Example x 国 Chart

- Scatterplot
- Right click $\rightarrow$ Add Trendline




## Simple Linear Regression Example x 国 Formulas

$=$ SLOPE (C4:C45, B4:B45)
$\rightarrow$ Slope $=35.04$
=INTERCEPT(C4:C45,B4:B45)
$\rightarrow$ Intercept $=32,600$

| 4 | A | B | C |
| :---: | :---: | :---: | :---: |
| 1 | Home Market Value |  |  |
| 2 |  |  |  |
| 3 | House Age | Square Feet | Market Value |
| 4 | 33 | 1.812 | \$90,000.00 |
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Estimate $Y$ when $X=1800$ square feet

$$
Y=32,600+35.04 \times(1800)=\$ 95,672
$$

## Simple Linear Regression Example

 Market value $=32600+35.04 \times$ (square feet) Predicts market value better than just average

But before use, examine residuals

## Groupwork

## Simple Linear Regression

https://web.cs.wpi.edu/~imgd2905/d23/groupwork/11regression/handout.html

## Groupwork

1. In simple linear regression, the y-intercept (b) represents the:
a. predicted value of $Y$
b. change in $Y$ per unit change in $X$
c. predicted value of $Y$ when $X=0$
d. variation around the line

2. A simple linear regression model for predicting a player's points $(Y)$ is $6 \mathrm{X}+10$, where X is the player's level.

- How many more points can a player expect to get when they level up?
- How many points can a level 10 player expect to get?


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## Residual Analysis

- Before predicting, confirm that linear regression assumptions hold
- Variation around line is normally distributed
- Variation equal for all $X$
- Variation independent for all $X$
- How? Compute residuals (error in prediction)



## Residual Analysis

https://www.qualtrics.com/support/stats-iq/analyses/regression-guides/interpreting-residual-plots-improve-regression/


Note that we've colored in a few dots in orange so you can get the sense of how this transformation works.

Variation around line normally distributed ? Variation equal for all $X$ Variation independent for all X?

## Residual Analysis - Good



## Residual Analysis - Bad



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(done)
(done)
(next)


## Linear Regression Model



Random error associated with each observation (Residual)

## Fitting the Best Line

- Plot all $\left(X_{i}, Y_{i}\right)$ Pairs



## Fitting the Best Line

- Plot all $\left(X_{i}, Y_{i}\right)$ Pairs
- Draw a line. But how do we know it is best?



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## Linear Regression Model

- Relationship between variables is linear function



## Least Squares Line

- Want to minimize difference between actual y and predicted $\hat{y}$
- Add up $\varepsilon_{i}$ for all observed y's
- But positive differences offset negative ones!
- (remember when this happened for variance?)
$\rightarrow$ Square the errors! Then, minimize (using Calculus)


$$
\begin{aligned}
& \text { Minimize: } \\
& \sum_{i=1}^{n}\left(Y_{i}-b_{0}-b_{1} X_{i}\right)^{2}
\end{aligned}
$$

Take derivative
Set to 0 and solve

## Least Squares (LS) Line Graphically

LS minimizes $\sum_{i=1}^{n} \hat{\varepsilon}_{i}^{2}=\hat{\varepsilon}_{1}^{2}+\hat{\varepsilon}_{2}^{2}+\hat{\varepsilon}_{3}^{2}+\hat{\varepsilon}_{4}^{2}$


## Least Squares Line Graphically Interactive Demo

Create new situations moving the green data points about the graph.

Line of Best Fit: Click the circle at the left to Show/Hide. Drag RED dots to position the line.

Residuals: Click the circle at the left to Show/Hide.

Squares: Click the circle at the left to Show/Hide.

- Least Squares Regression Line: Click the circle at the left to Show/Hide.

https://www.desmos.com/calculator/zvrc4lg3cr


## Outline

- Introduction
- Simple Linear Regression
- Measures of Variation
- Coefficient of Determination
- Correlation
- Misc


## Measures of Variation



- Several sources of variation in y
- Error in prediction (unexplained)
- Variation from model (explained)

Break this down (next)

## Sum of Squares of Error (SSE)



- Least squares regression selects line with lowest total sum of squared prediction errors
- Sum of Squares of Error, or SSE
- Measure of unexplained variation


## Sum of Squares Regression (SSR)



- Differences between prediction and population mean
- Gets at variation due to X \& Y
- Sum of Squares Regression, or SSR
- Measure of explained variation


## Sum of Squares Total

- Total Sum of Squares, or SST = SSR + SSE



## Coefficient of Determination

- Proportion of total variation (SST) explained by the regression (SSR) is known as the Coefficient of Determination ( $\mathrm{R}^{2}$ )

$$
R^{2}=\frac{S S R}{S S T}=1-\frac{S S E}{S S T}
$$

- Ranges from 0 to 1 (often said as a percent)

1 - regression explains all of variation
0 - regression explains none of variation

## Coefficient of Determination Visual Representation



## Coefficient of Determination Example



- How "good" is regression model? Roughly:

$$
0.8 \leq R^{2} \leq 1 \quad \text { strong }
$$

## Coefficient of Determination Example




- How "good" is regression model? Roughly:
$0.8 \leq R^{2} \leq 1$
$0 \leq R^{2}<0.5$
weak


## How "Good" is the Regression Model?



I DON'T TRUST LINEAR REGRESSIONS WHEN ITS HARDER TO GUESS THE DIRECTION OF THE CORRELATION FROM THE SCATTER PLOT THAN TO FIND NEW CONSTELLATIONS ON IT.
https://xkcd.com/1725/

## Relationships Between X \& Y



# Relationship Strength and Direction Correlation 

- Correlation measures strength and direction of linear relationship
-1 perfect neg. to +1 perfect pos.
- Sign is same as regression slope
- Denoted $R$. Why? Square $R=R^{2}$

$$
\begin{aligned}
& \text { Pearson's Correlation } \\
& \begin{aligned}
\text { Coefficient } \\
\mathrm{r}=\frac{\sum(X-\bar{X})(Y-\bar{Y})}{\sqrt{\sum(X-\bar{X})^{2}} \sqrt{(Y-\bar{Y})^{2}}} \leftarrow \quad \begin{array}{c}
\text { Vary } \\
\text { together } \\
\text { Vary }
\end{array} \\
\sqrt{\text { Separately }}
\end{aligned}
\end{aligned}
$$

Where, $\bar{X}$ = mean of X variable $\bar{Y}=$ mean of $Y$ variable

## Correlation Examples



## Groupwork

- Introduction
- Icebreaker: What game are you looking forward to playing this summer?
- Groupwork
- Think, discuss, write down - qualtrics
- Correlation
- Consider scatterplots
- Estimate correlation
https://web.cs.wpi.edu/~im
gd2905/d23/groupwork/12-
correlation/handout.html


## Correlation Examples


??


## Correlation Examples


??

??

## Correlation Examples



## Correlation Examples



## Correlation Examples





(Note, would want to use residual analysis before using predictions!)

## Correlation Examples



(Note, would want to use residual analysis before using predictions!)

Anscombe's Quartet
https://en.wikipedia.org/wiki/Anscombe\'s quartet



Summary stats: Mean $_{x} 9$
Mean $_{\mathrm{y}} 7.5$
Var $_{x} \quad 11$
Var $_{y} \quad 4.125$
Model: $\mathrm{y}=0.5 \mathrm{x}+3$
$R^{2}=0.69$

## Correlation Summary



## Correlation is not Causation



Buying sunglasses causes people to buy ice cream?

## Correlation is not Causation



Importing lemons causes fewer highway fatalities?

## Correlation is not Causation

https://science.sciencemag.org/content/sci/348/6238/980.2/F1.large.jpg?width=800\&height=600\&carousel=1


## Correlation is not Causation



SOUNDS LIKE THE CLASS HELPED.

https://xkcd.com/552/

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(done)
(done)
(done)
(next)


## Extrapolation versus Interpolation

- Prediction
- Interpolation within measured X-range
- Extrapolation outside measured X-range



## Be Careful When Extrapolating



## Prediction and Confidence Intervals (1 of 2)



# Prediction and Confidence Intervals (2 of 2) 

95\% Confidence Bands


95\% Prediction Bands


## Multiple Independent Variables

- Chronic heart disease (CHD) correlates with smoking

$$
-R^{2}=0.5
$$

- But what about other 50\%
- Correlation with exercise? Cholesterol?


## Cigarettes Exercise CHD Mortality Cholesterol

## Multiple Linear Regression



## Single Linear Regression $\rightarrow$ Multiple Linear Regression

- Use several independent variables to predict dependent variable


## Single predictor <br> $X \longrightarrow Y$

- Weights each predictor based on strength of relationship
- Makes adjustments for inter-relationships among predictors
- Gives overall fit ( $R^{2}$ )

- Note: Need independent variables not highly related to each other

$$
Y=b_{0}+b_{1} X_{1}+b_{2} X_{2}+b_{3} X_{3} . . b_{n} X_{n}
$$

## Multiple Linear Regression

Example: hours studied and pre-tests affect final score

$$
y=b 0+b 1^{*} \times 1+b 2 * x 2+E
$$



## Multiple Linear Regression Example (1 of 2)

- Hours studied and prep exams taken $\rightarrow$ exam score

|  | A | B | C |
| :---: | :---: | :---: | :---: |
| 1 | hours | prep_exams | score |
| 2 | 1 | 1 | 76 |
| 3 | 2 | 3 | 78 |
| 4 | 2 | 3 | 85 |
| 5 | 4 | 5 | 88 |
| 6 | 2 | 2 | 72 |
| 7 | 1 | 2 | 69 |
| 8 | 5 | 1 | 94 |
| 9 | 4 | 1 | 94 |

20 students


## Multiple Linear Regression Example (2 of 2)

- Independent variable
- Covers both independent variables



## Interpret

| SUMMARY OUTPUT |  | - $R^{2} 0.734$ |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  |  |  |
| Regression Statistics |  | - Overall significant ( $\mathrm{p}<0.05$ ) |  |  |  |  |
| Multiple R | $\begin{aligned} & 0.857 \\ & 0.734 \\ & \hline \end{aligned}$ | - Hours significant |  |  |  |  |
| R Square |  | - Prep exams not significant |  |  |  |  |
| Adjusted R Square | 0.703 |  |  |  |  |  |
| Standard Error | 5.366 | - Base score without prep 67.67 |  |  |  |  |
| Observations | 20 | - Each hour gains 5.56 percent |  |  |  |  |
| ANOVA |  |  |  |  |  |  |
|  | $d f$ | SS | MS | $F$ | Significance F |  |
| Regression | 2 | 1350.76 | 675.38 | 23.46 | 0. |  |
| Residual | 17 | 489.44 | 28.79 |  |  |  |
| Total | 19 | 1840.20 |  |  |  |  |
|  |  |  |  |  |  |  |
|  | Coefficients | Standard Error | $t$ Stat | $P$-value | Lower 95\% | Upper 95\% |
| Intercept | 67.67 | 2.82 | 24.03 | 0.00 | 61.73 | 73.61 |
| hours | 5.56 | ) 0.90 | 6.18 | 0.0 | 3.66 | 7.45 |
| prep_exams | -0.60 | 0.91 | -0.66 | 0.52 | -2.53 | 1.33 |

Score $=67.67+5.56 x$ hours $-0.60 \times$ prep_exams

## Beyond Linear Regression



- More complex models - beyond just linear

$$
Y=m X+b
$$

## More Complex Models


$y=12 x+9$

Complex

$y=18 x^{4}+13 x^{3}-9 x^{2}+3 x+20$

- Higher order polynomial model has less error
$\rightarrow$ A "perfect" fit (no error)
- How does a polynomial do this?


## Graphs of Polynomial Functions



Cubic Function (deg. $=3$ )
https://cdn-images-1.medium.com/max/2400/1*pjilpg20-MZds_3flVhf-Dw.jpeg


Linear Function (degree = 1)


Quartic Function (deg. $=4$ )


Quadratic Function
(degree = 2)


Quintic Function (deg. $=5$ )

Higher degree, more potential "wiggles"
But should you use?

## Underfit and Overfit


hups:/fistack.imgur.com/torit.png


Size
$\theta_{0}+\theta_{1} x+\theta_{2} x^{2}$
Just Right

$\theta_{0}+\theta_{1} x+\theta_{2} x^{2}+\theta_{3} x^{3}+\theta_{4} x^{4}$
Overfit

- Overfit analysis


## Test $\rightarrow$ Cross Validation

 be justified- Underfit analysis does not adequately match data since parameters are missing
$\rightarrow$ Both models fit well, but do not predict well (i.e., for non-observed values)
- Just right - fit data well "enough" with as few parameters as possible (parsimonious - desired level of prediction with as few terms as possible)


## Cross Validation (1 of 2)

Total number of examples

## Training Set <br> Test Set

Use to build model


## Cross Validation (2 of 2)

Repeat for different slices


- Overfit and Underfit will both have lower accuracy than "just right"



## Summary

- Can use regression to predict unmeasured values
- Before fit
- Visual relationship (scatter plot) and residual analysis
- Strength of fit - $\mathrm{R}^{2}$ and correlation (R)
- Beware
- Correlation is not causation
- Extrapolation
- Higher order, more complex models can fit better
- Beware of overfit $\rightarrow$ less predictive power


