Week 2: Linear Regression

DSAN 5300: Statistical Learning

Spring 2026, Georgetown University

Jeff Jacobs

jj1088@georgetown.edu

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Schedule

Today's Planned Schedule:

	Start	End	Topic
Lecture	6:30pm	7:10pm	Simple Linear Regression →
	7:10pm	7:30pm	Deriving the OLS Solution →
	7:30pm	8:00pm	Interpreting OLS Output →
Break!	8:00pm	8:10pm	
	8:10pm	8:30pm	Quiz Review →
	8:30pm	9:00pm	Quiz 2!

Linear Regression

- What happens to my **dependent variable** Y when my **independent variable** X increases by **1 unit**?
- Keep the **goal** in front of your mind:

> 🎯 **The Goal of Regression**
>
> **Find a line $\hat{y} = mx + b$ that best predicts Y for given values of X**

- *Sanity Note 1*: 🎯 $\Rightarrow$ measuring error via **vertical** distance from line
- *Sanity Note 2:* 🎯 $\Rightarrow$ modeling distribution of $\boxed{Y \mid X}$, not (X, Y)!
  - Predicting Y from X ***and*** X from Y $\Rightarrow$ **principal component line** $\neq$ **regression**!

How Do We Define "Best"?

- Intuitively, two different ways to measure **how well a line fits the data**:

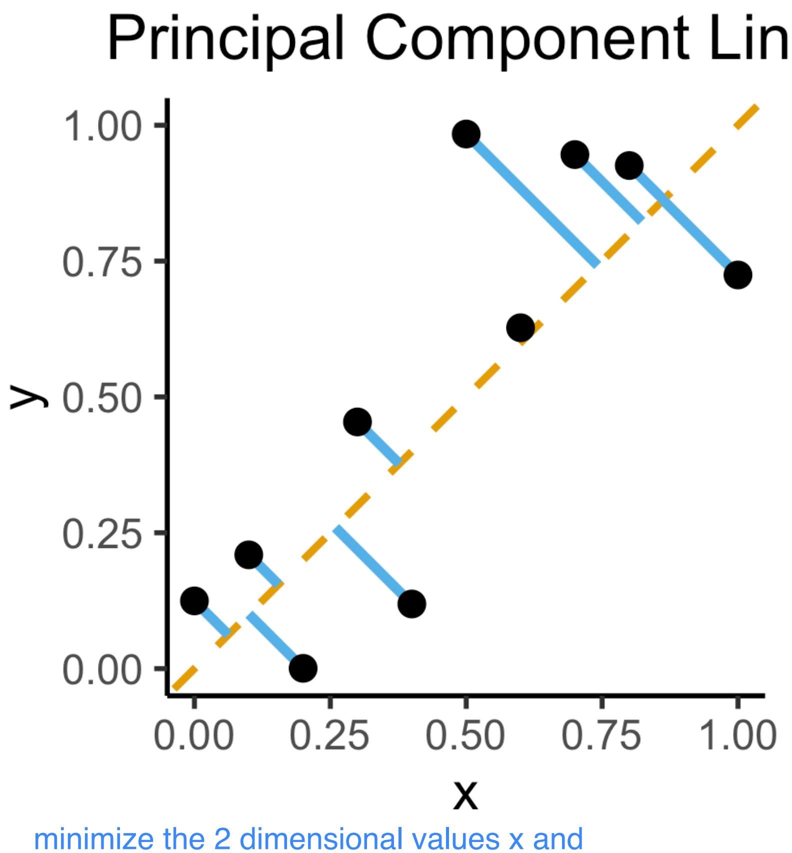


Figure 1: The line that minimizes blue distances does **not** predict Y as well as regression line, despite intuitive appeal!

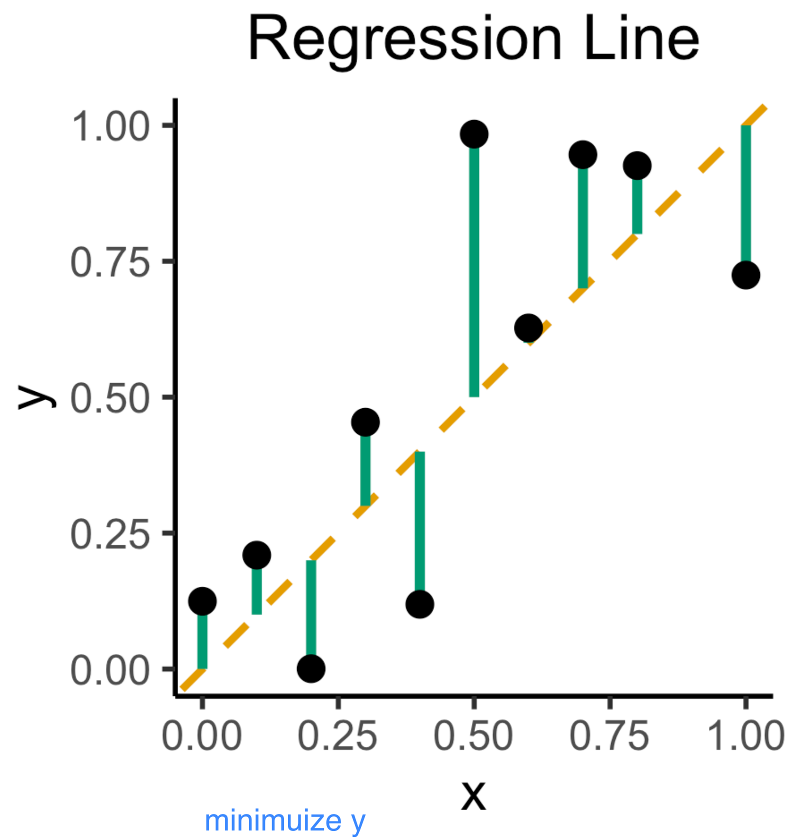
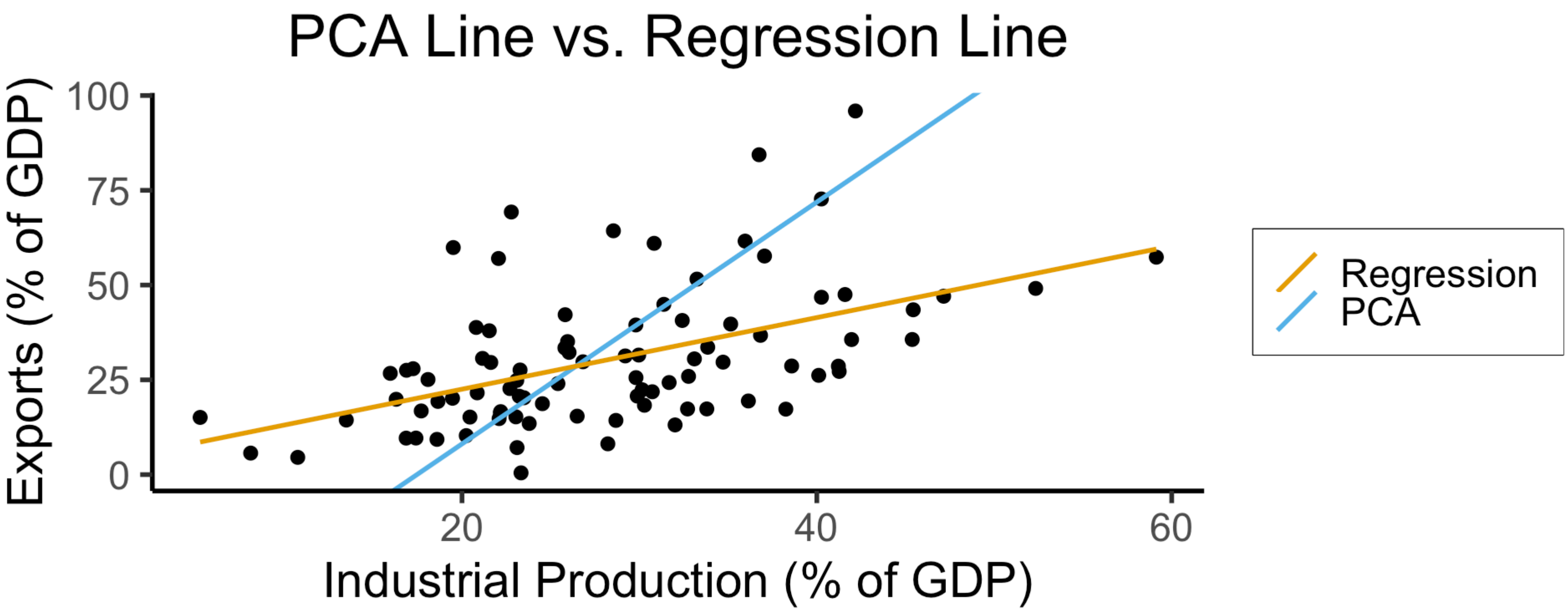


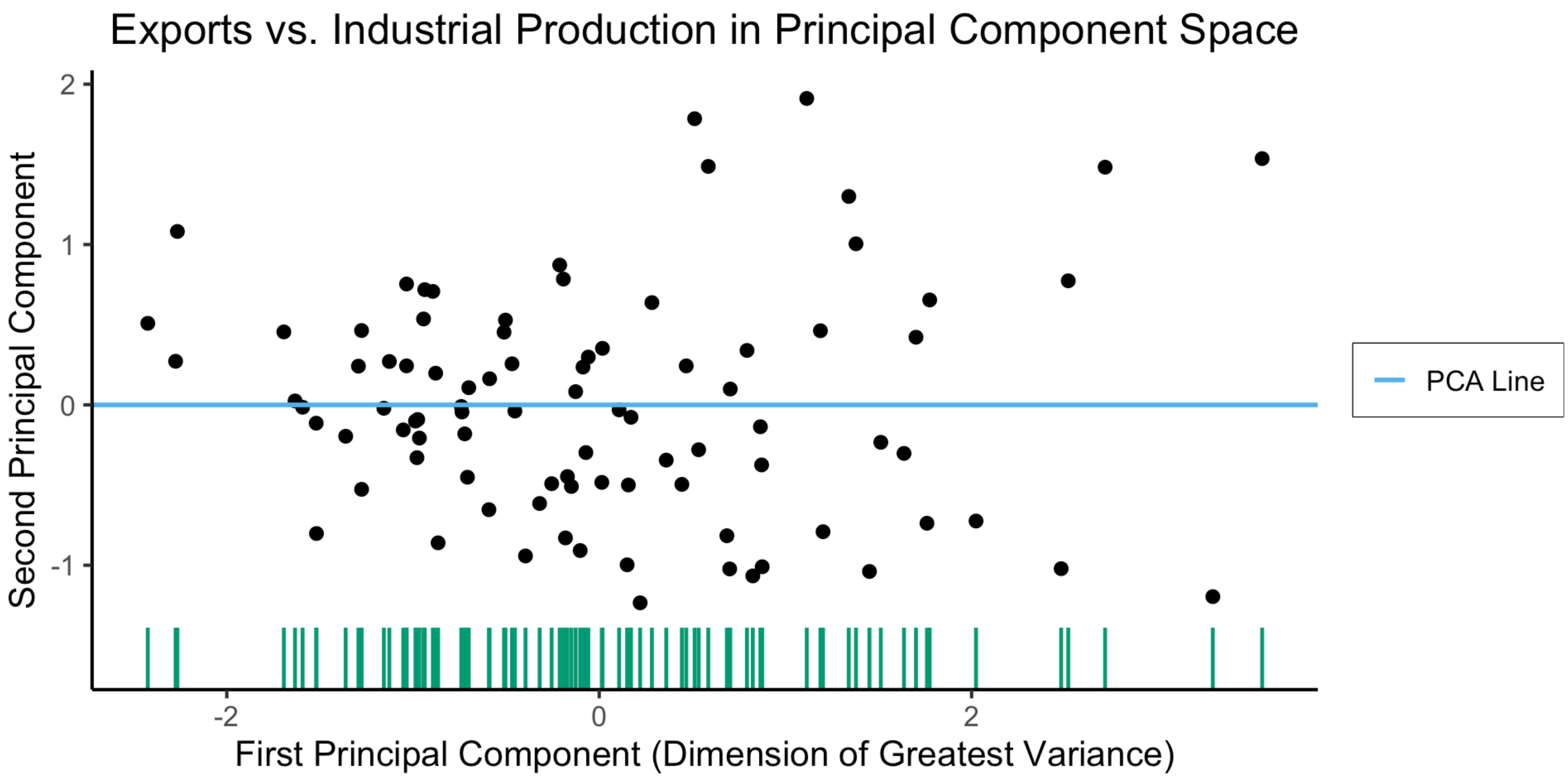
Figure 2: The line that minimizes green distances **optimally** predicts Y from X, in a mathematically-provable sense!

Principal Component Analysis

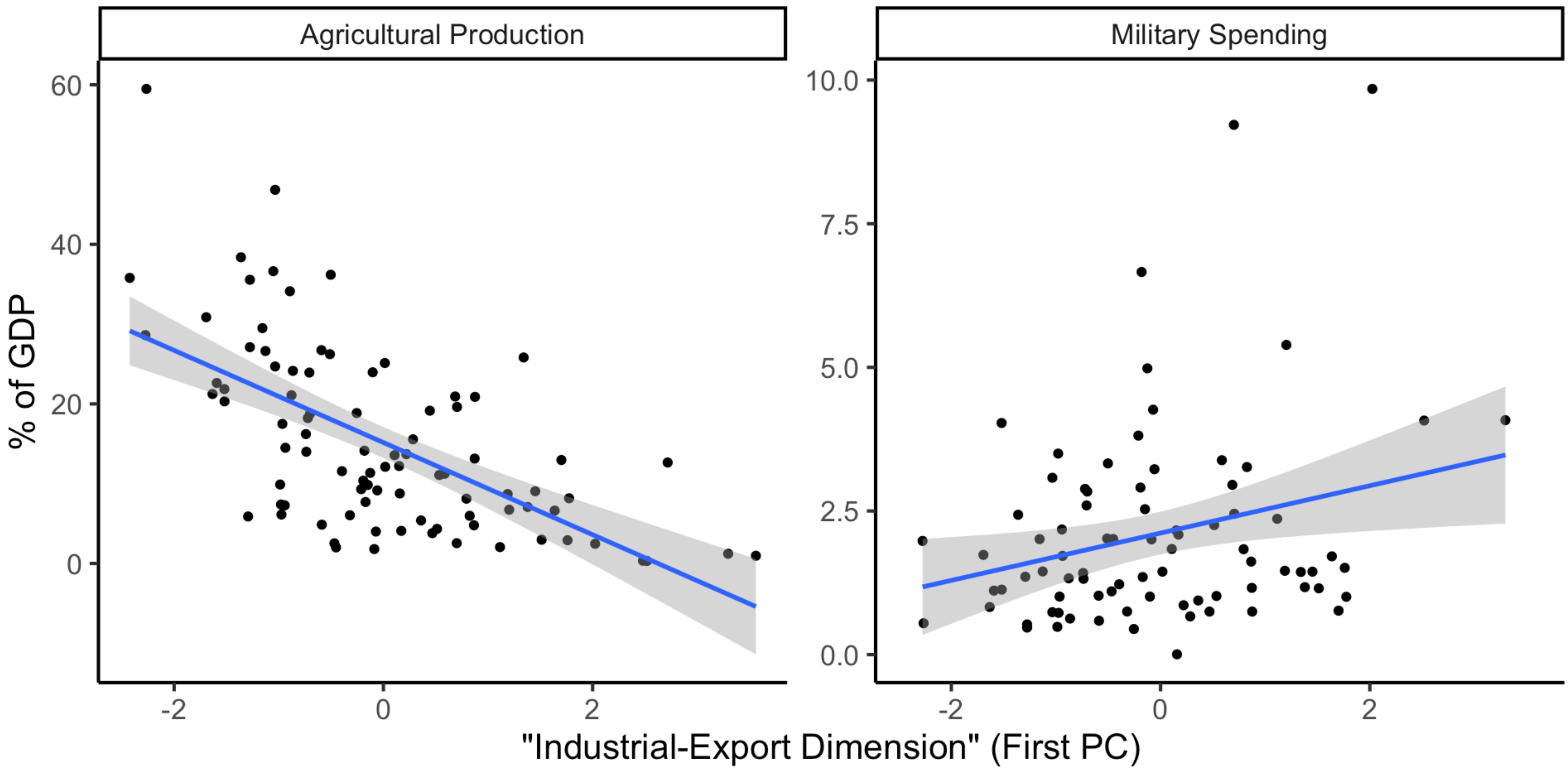
- **Principal Component Line** can be used to **project** the data onto its **dimension of highest variance** (recap from 5000!)
- More simply: PCA can **discover** meaningful axes in data (**unsupervised** learning / **exploratory** data analysis settings)



Create Your Own Dimension!



...And Use It for EDA



But in Our Case...

- x and y dimensions **already have meaning**, and we have a **hypothesis** about effect of x on y!

The Regression Hypothesis $\mathcal{H}_{\text{reg}}$

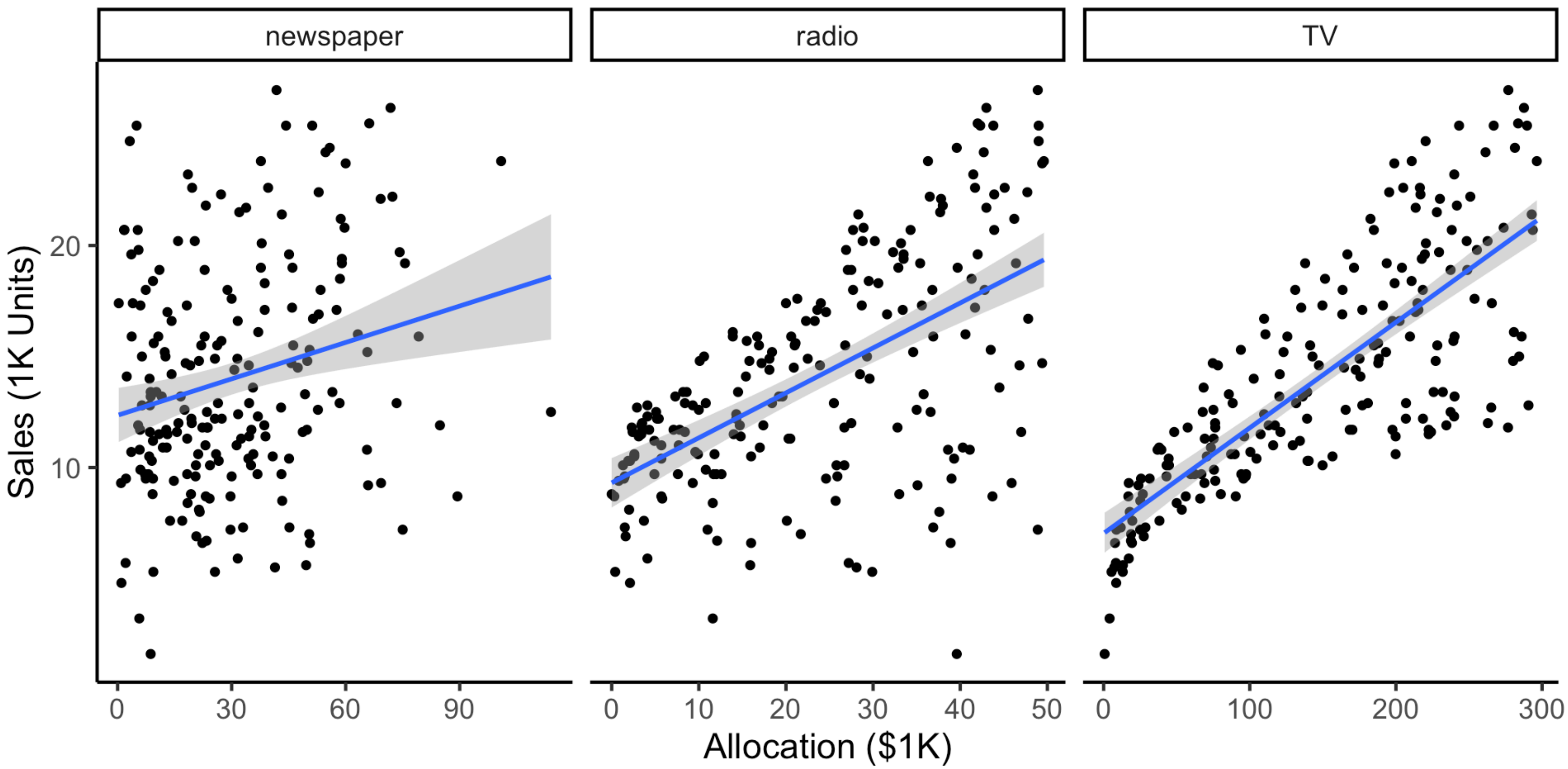
Given data (X, Y), we estimate $\hat{y} = \widehat{\beta}_0 + \widehat{\beta}_1 x$, hypothesizing that:

- Starting from $y = \underbrace{\widehat{\beta}_0}_{\text{Intercept}}$ when $x = 0$,
- An **increase** of x by **1 unit** is associated with an **increase** of y by $\underbrace{\widehat{\beta}_1}_{\text{Coefficient}}$ **units**

- We want to measure **how well** our line predicts y for any given x value $\implies$ **vertical distance** from regression line

Example: Advertising Effects

- **Independent variable**: $ put into advertisements; **Dependent variable**: Sales
- **Goal 1**: *Predict* sales for a given allocation
- **Goal 2**: *Infer* best allocation for a given advertising budget (more simply: a new $1K appears! Where should we invest it?)



Simple Linear Regression

- For now, we treat **Newspaper**, **Radio**, **TV** advertising separately: how much do **sales** increase per \$1 into [medium]? (Later we'll consider them jointly: multiple regression)

Our model:

$$Y = \underbrace{\beta_0}_{\text{Intercept}} + \underbrace{\beta_1}_{\text{Slope}} X + \varepsilon$$

...Generates **predictions** via:

$$\hat{y} = \underbrace{\widehat{\beta}_0}_{\substack{\text{Estimated} \\ \text{intercept}}} + \underbrace{\widehat{\beta}_1}_{\substack{\text{Estimated} \\ \text{slope}}} \cdot x$$

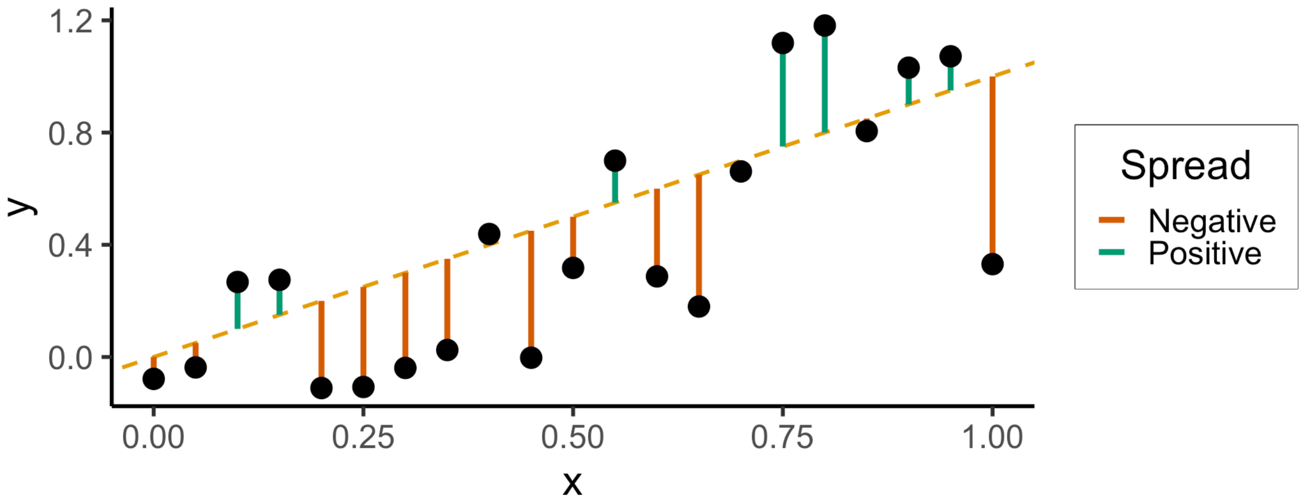
- Note how these predictions will be **wrong** (unless the data is perfectly linear)
- We've accounted for this in our model (by including ε term)!
- But, we'd like to find estimates $\widehat{\beta}_0$ and $\widehat{\beta}_1$ that produce the **"least wrong" predictions**: motivates focus on **residuals** $\hat{\varepsilon}_i$**...**

This is the residuals, which we don't want to use to measure the error
because the positive and negative cancel out each other

$$\hat{\varepsilon}_i = \underbrace{y_i}_{\substack{\text{Real} \\ \text{label}}} - \underbrace{\hat{y}_i}_{\substack{\text{Predicted} \\ \text{label}}} = \underbrace{y_i}_{\substack{\text{Real} \\ \text{label}}} - \underbrace{\left(\widehat{\beta}_0 + \widehat{\beta}_1 \cdot x\right)}_{\text{Predicted label}}$$

Least Squares: Minimizing Residuals

What can we **optimize** to ensure these residuals are as small as possible?



Sum?

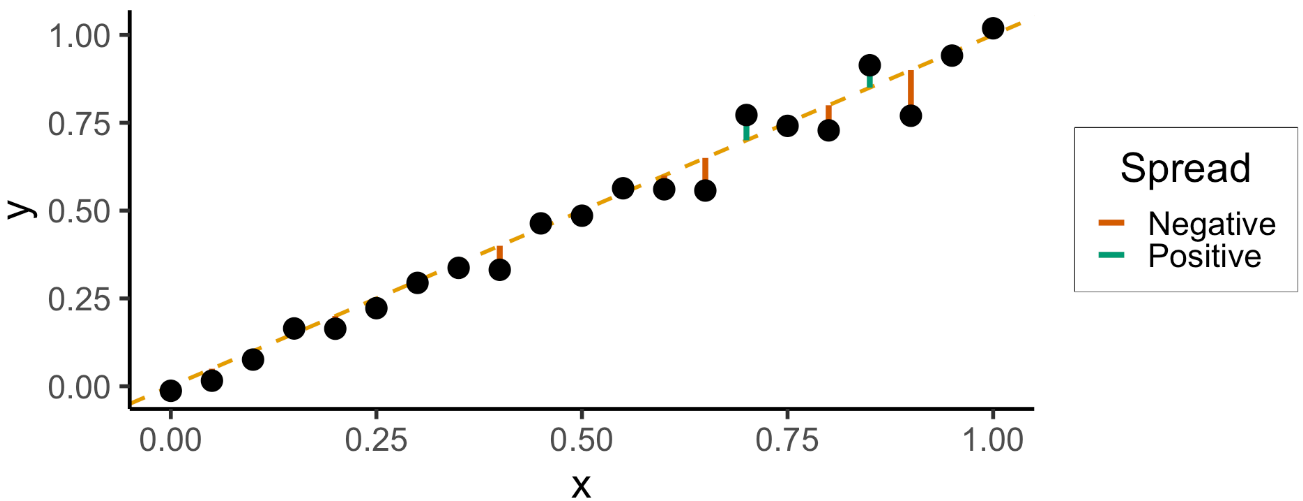
`0.0000000000`

Sum of Squares?

`3.8405017200`

Sum of absolute vals?

`7.6806094387`



Sum?

`0.0000000000`

Sum of Squares?

`1.9748635217`

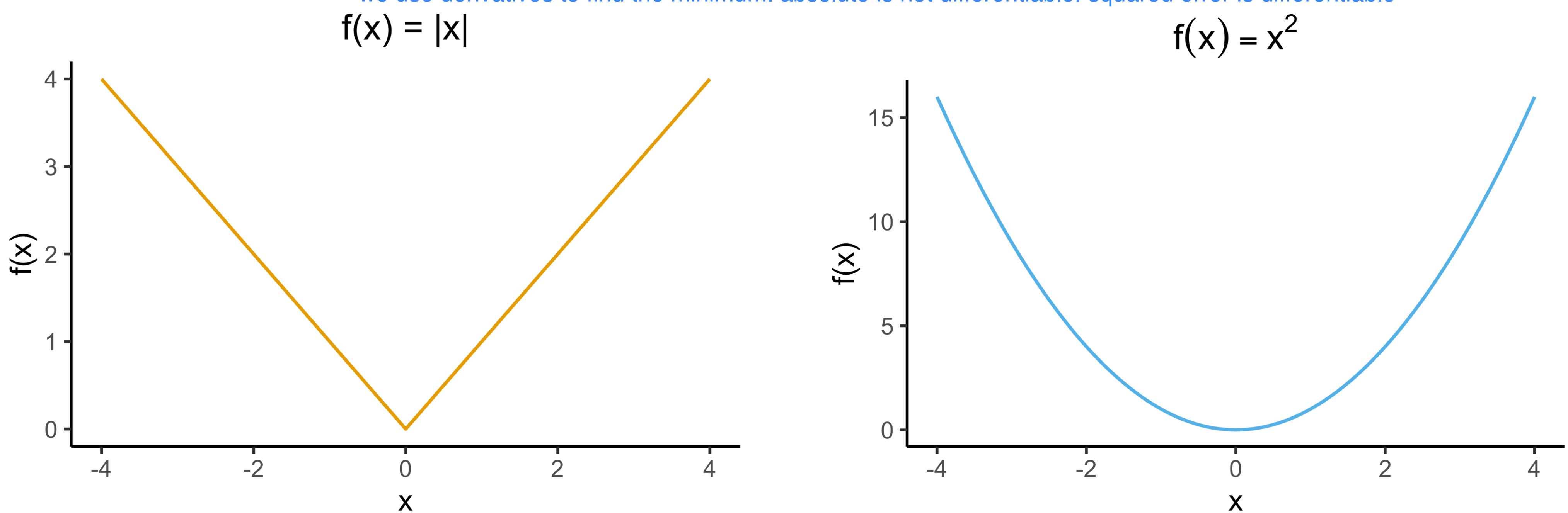
Sum of absolute vals?

`5.5149697440`

Why Not Absolute Value?

- Two feasible ways to prevent positive and negative residuals **cancelling out**:
  - **Absolute error** $\left|y - \hat{y}\right|$ or **squared error** $\left(y - \hat{y}\right)^2$
- But remember: we're aiming to **minimize** 👀 these residuals; ghost of calculus past 😱
- We *minimize* by taking *derivatives*… which one is **differentiable** everywhere?

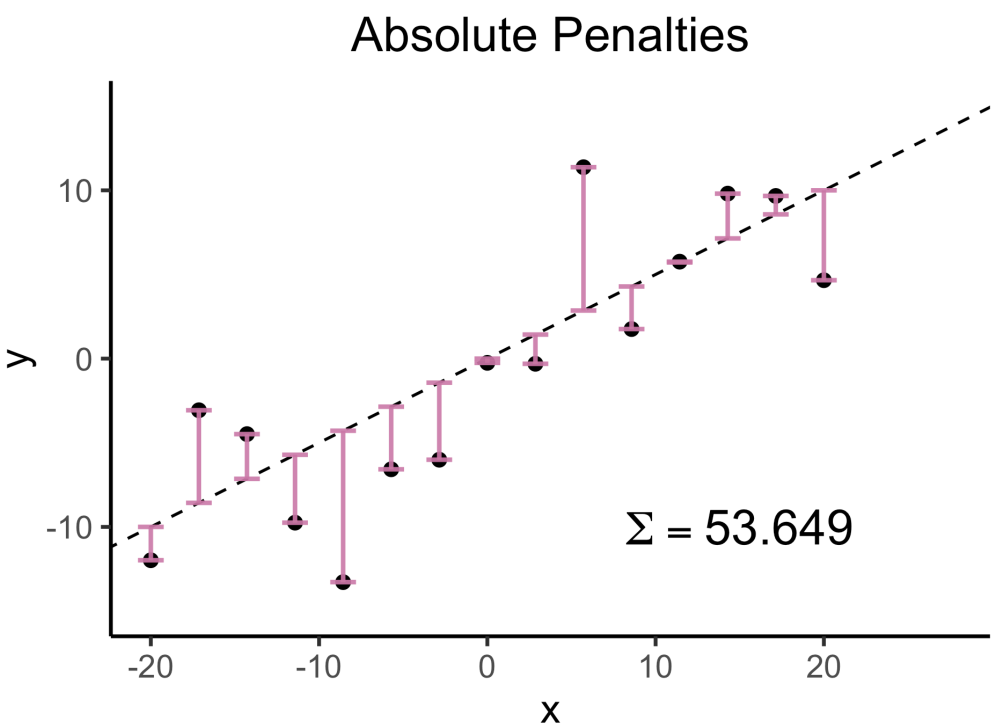
we use derivatives to find the minimum. absolute is not differentiable. squared error is differentiable

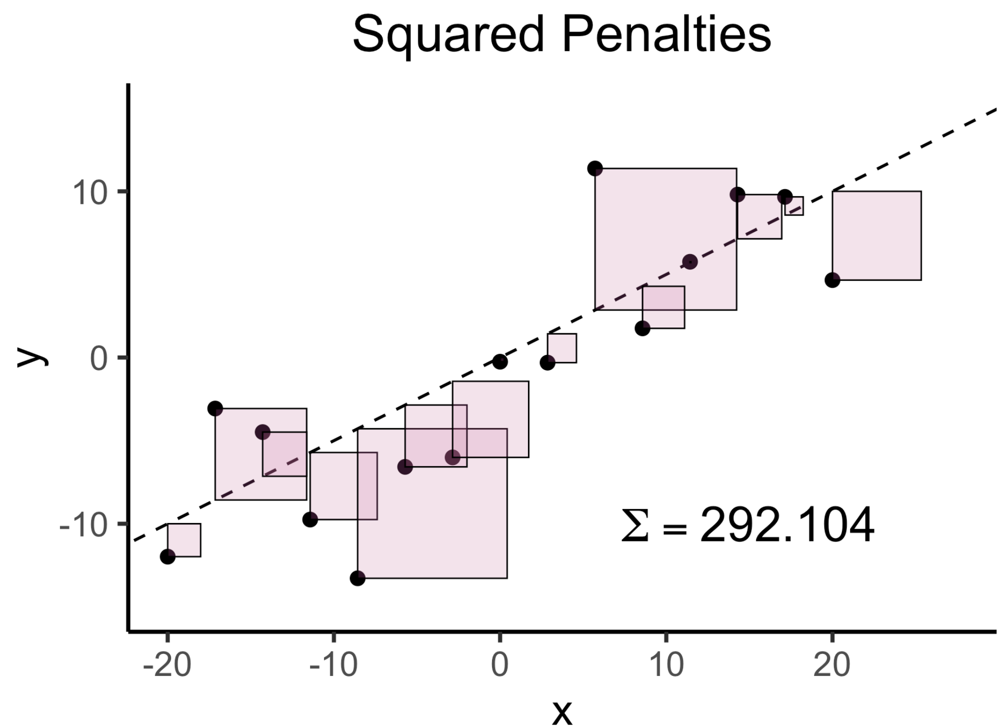


Outliers Penalized Quadratically

- May feel arbitrary at first (we're "forced" to use squared error because of calculus?)
- It also has **important consequences** for "learnability" via gradient descent!

think about type1 and type2 errors. squared penalizes errors more than absolute





Key Features of Regression Line

- Regression line is **BLUE**: **B**est **L**inear **U**nbiased **E**stimator
- What exactly is it the "best" linear estimator of?

$$\hat{y} = \underbrace{\widehat{\beta}_0}_{\substack{\text{Estimated} \\ \text{intercept}}} + \underbrace{\widehat{\beta}_1}_{\substack{\text{Estimated} \\ \text{slope}}} \cdot x$$

is chosen so that

$$\hat{\theta} = \left(\widehat{\beta}_0, \widehat{\beta}_1\right) = \underset{\beta_0, \beta_1}{\operatorname{argmin}} \left[\sum_{x_i \in X} \left(\overbrace{\hat{y}(x_i)}^{\text{Predicted } y} - \overbrace{\mathbb{E}[Y \mid X = x_i]}^{\text{Avg. } y \text{ when } x = x_i} \right)^2 \right]$$

Where Did That $\mathbb{E}[Y \mid X = x_i]$ Come From?

- From our assumption that the irreducible **errors** ε_i are **normally distributed** $\mathcal{N}(0, \sigma^2)$

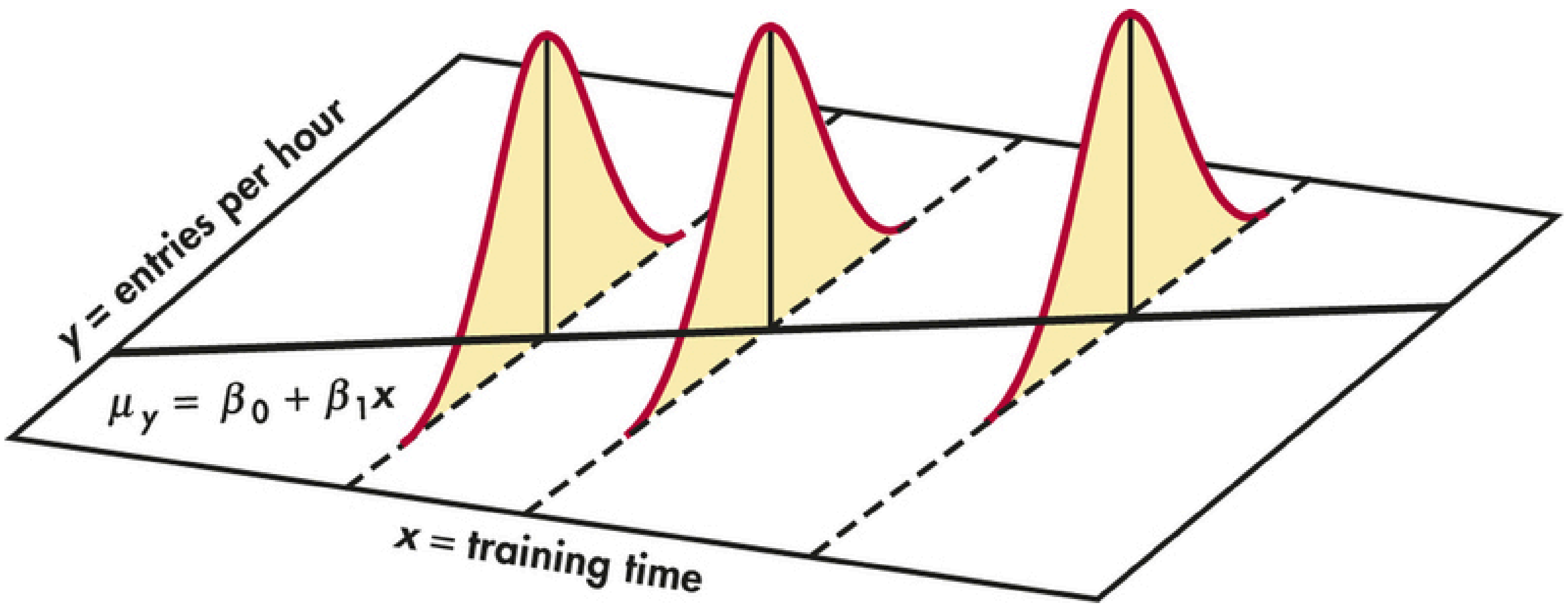


Image Source

- Kind of an immensely important point, since it **gives us a hint for checking whether model assumptions hold**: spread around the regression line should be $\mathcal{N}(0, \sigma^2)$

Heteroskedasticity

- If spread **increases** or **decreases** for larger x, for example, then $\varepsilon \not\sim \mathcal{N}(0, \sigma^2)$

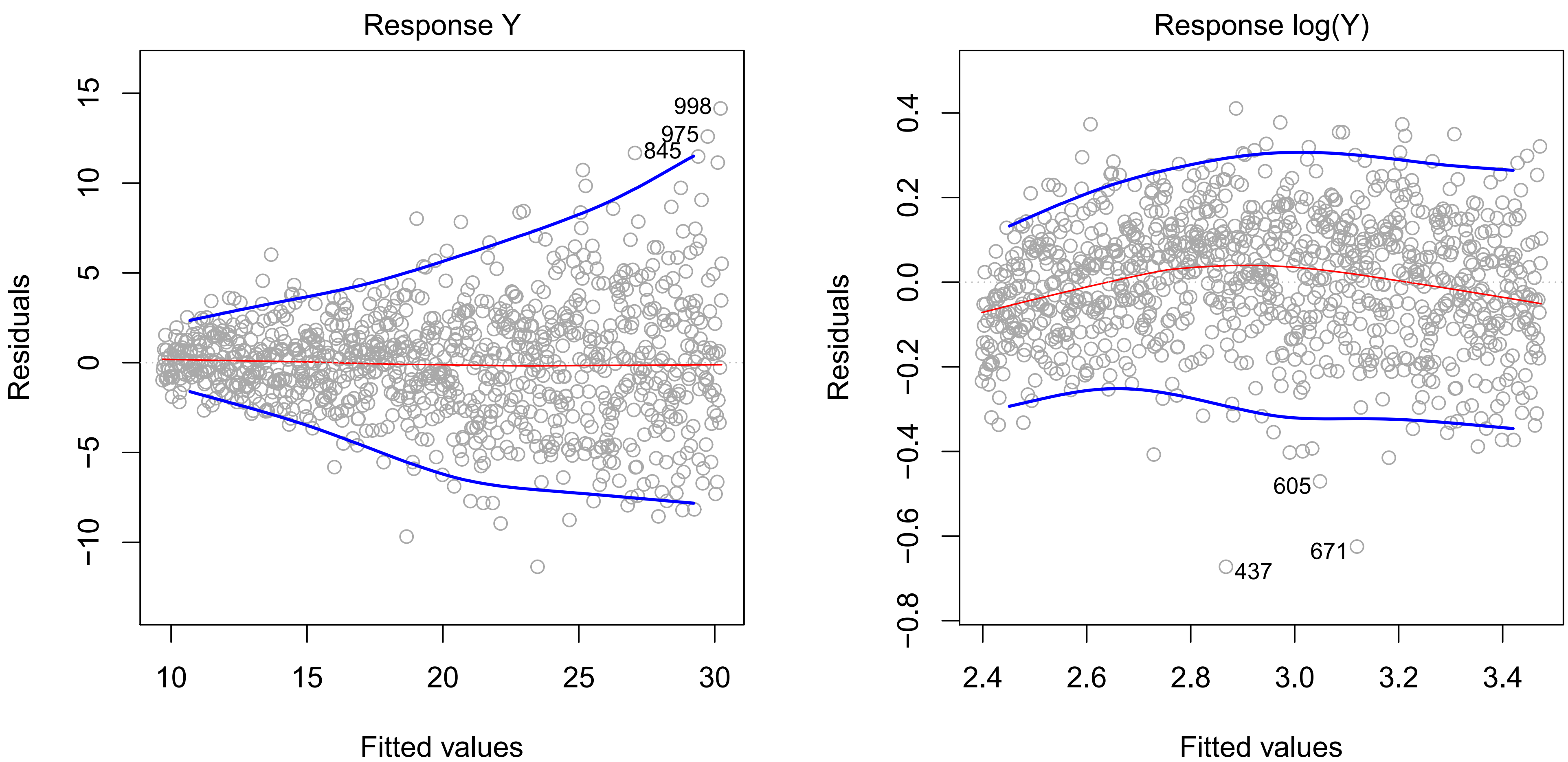


Figure 3.11 from James et al. (2023)

But... What About Other Types of Vars?

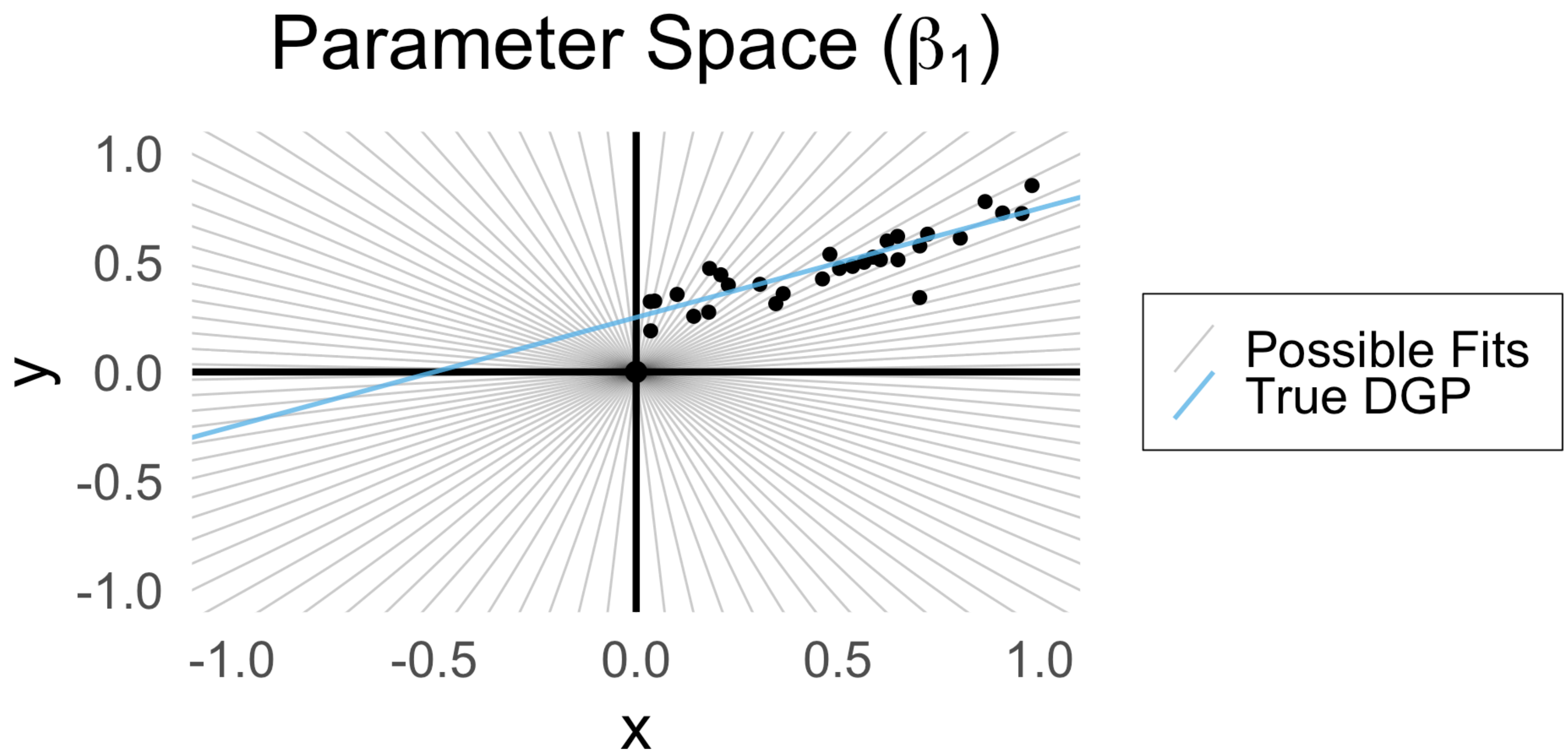
- 5000: you saw **nominal**, **ordinal**, **cardinal** vars
- 5100: you wrestled with **discrete** vs. **continuous** RVs
- Good News #1: Regression can handle **all** these types+more!
- Good News #2: Distinctions between **classification** and **regression** diminish as you learn fancier regression methods!
  - tldr: Predict continuous probabilities $\Pr(Y) \in [0, 1]$ (regression), then guess 1 if $\Pr(Y) > 0.5$ (classification)
- By end of 5300 you should have something on your toolbelt for handling most cases like *"I want to do [regression / classification], but my data is [not cardinal+continuous]"*

Deriving the Least Squares Estimate

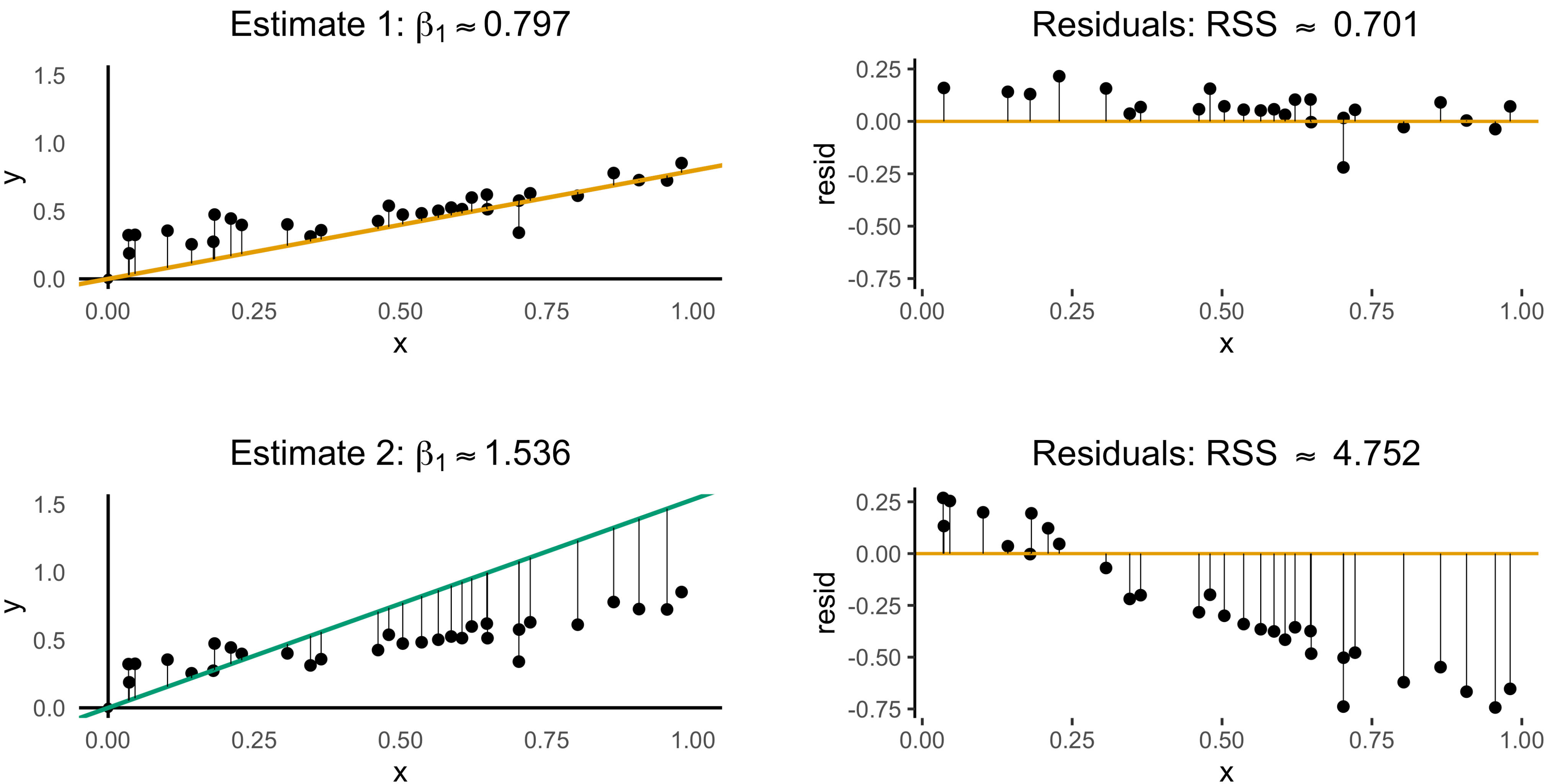
A Sketch (HW is the Full Thing)

- OLS for regression **without** intercept: Which $\boxed{\textbf{line through origin}}$ best predicts Y?
- (Good practice + reminder of how **restricted** linear models are!)

$$Y = \beta_1 X + \varepsilon$$



Evaluating with Residuals



Now the Math

$$\beta_1^* = \overbrace{\underset{\beta_1}{\text{argmin}}}^{\substack{\text{Find thing} \\ \text{that minimizes}}} \left[\sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \right] = \underset{\beta_1}{\text{argmin}} \left[\sum_{i=1}^{n} (y_i - \beta_1 x_i)^2 \right]$$

We can compute this derivative to obtain:

$$\frac{\partial}{\partial \beta_1} \left[\sum_{i=1}^{n} (\beta_1 x_i - y_i)^2 \right] = \sum_{i=1}^{n} \frac{\partial}{\partial \beta_1} (\beta_1 x_i - y_i)^2 = \sum_{i=1}^{n} 2(\beta_1 x_i - y_i) x_i$$

And our first-order condition means that:

$$\sum_{i=1}^{n} 2(\beta_1^* x_i - y_i) x_i = 0 \iff \beta_1^* \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i y_i \iff \boxed{\beta_1^* = \frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2}}$$

Doing Things With Regression

Regression: `R` vs. `statsmodels`

In (Base) R: `lm()`

Code

```r
lin_model <- lm(sales ~ TV, data=ad_df)
summary(lin_model)
```

```
Call:
lm(formula = sales ~ TV, data = ad_df)

Residuals:
    Min      1Q  Median      3Q     Max 
-8.3860 -1.9545 -0.1913  2.0671  7.2124 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept) 7.032594   0.457843   15.36   <2e-16 ***
TV          0.047537   0.002691   17.67   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 3.259 on 198 degrees of freedom
Multiple R-squared:  0.6119,	Adjusted R-squared:  0.6099 
F-statistic: 312.1 on 1 and 198 DF,  p-value: < 2.2e-16
```

General syntax:

```r
lm(
  dependent ~ independent + controls,
  data = my_df
)
```

In Python: `smf.ols()`

Code

```python
import statsmodels.formula.api as smf
results = smf.ols("sales ~ TV", data=ad_df).fit()
print(results.summary(slim=True))
```

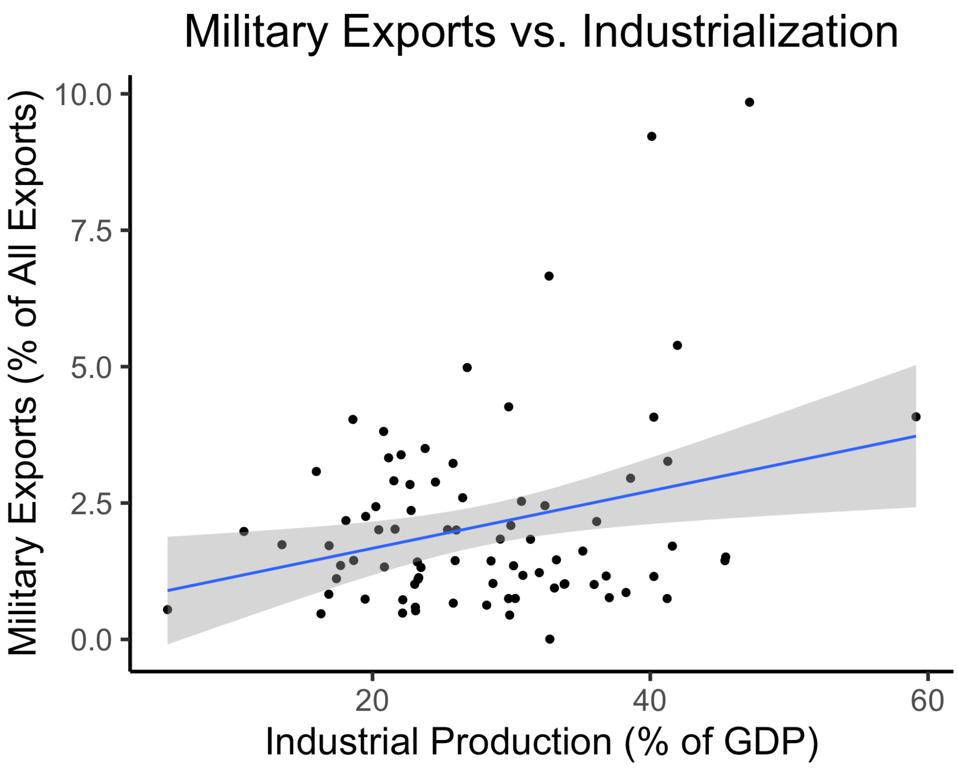
```
                            OLS Regression Results                            
==============================================================================
Dep. Variable:                  sales   R-squared:                       0.612
Model:                            OLS   Adj. R-squared:                  0.610
No. Observations:                 200   F-statistic:                     312.1
Covariance Type:            nonrobust   Prob (F-statistic):           1.47e-42
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Intercept      7.0326      0.458     15.360      0.000       6.130       7.935
TV             0.0475      0.003     17.668      0.000       0.042       0.053
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
```

General syntax:

```python
smf.ols(
  "dependent ~ independent + controls",
  data = my_df
)
```

Interpreting Output




```
Call:
lm(formula = military ~ industrial, data = gdp_df)

Residuals:
    Min      1Q  Median      3Q     Max
-2.3354 -1.0997 -0.3870  0.6081  6.7508

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  0.61969    0.59526   1.041   0.3010
industrial   0.05253    0.02019   2.602   0.0111 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.'
0.1 ' ' 1

Residual standard error: 1.671 on 79 degrees of
freedom
  (8 observations deleted due to missingness)
Multiple R-squared:  0.07895,   Adjusted R-squared:
```

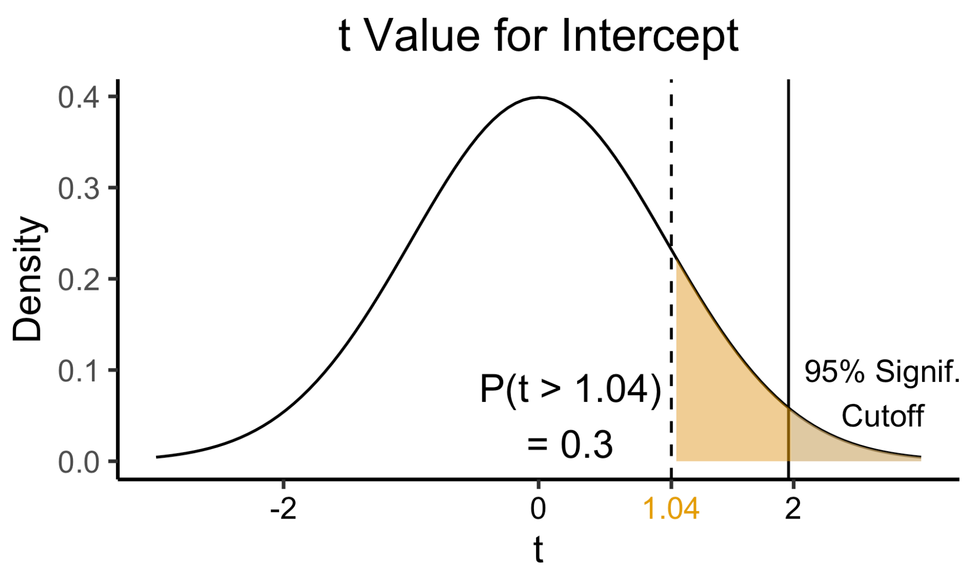
Zooming In: Coefficients

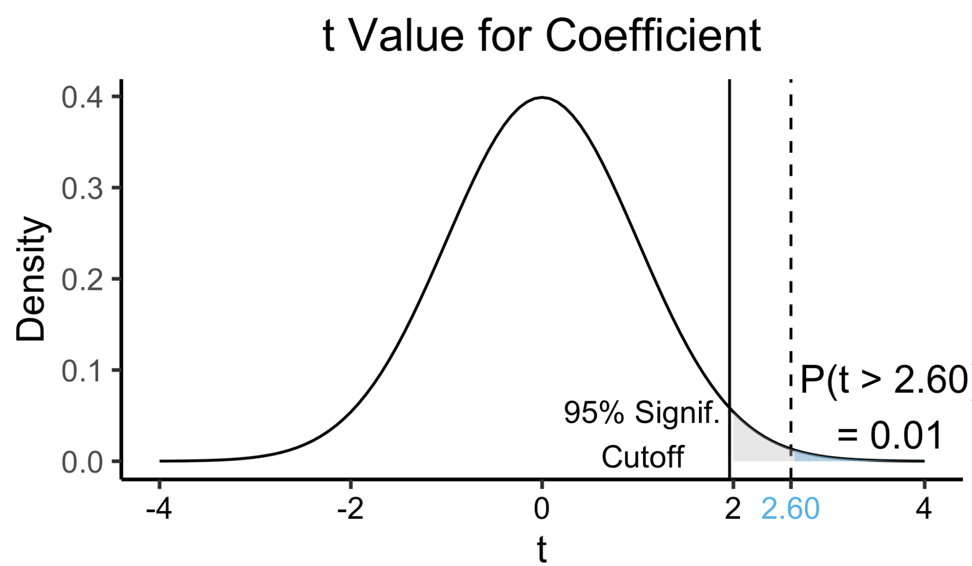
	Estimate	Std. Error	t value	Pr(>|t|)	
(Intercept)	0.61969	0.59526	1.041	0.3010	
industrial	0.05253	0.02019	2.602	0.0111	*
	$\widehat{\beta}$	Uncertainty	Test stat t	How extreme is t?	Signif. Level

$$\hat{y} \approx \underbrace{\overset{\beta_0}{\mathbf{0.620}}}_{\pm 0.595} + \underbrace{\overset{\beta_1}{\mathbf{0.053}}}_{\pm 0.020} \cdot x$$

Zooming In: Significance

	Estimate	Std. Error	t value	Pr(>|t|)	
(Intercept)	0.61969	0.59526	1.041	0.3010	
industrial	0.05253	0.02019	2.602	0.0111	*
	$\widehat{\beta}$	Uncertainty	Test stat t	How extreme is t?	Signif. Level





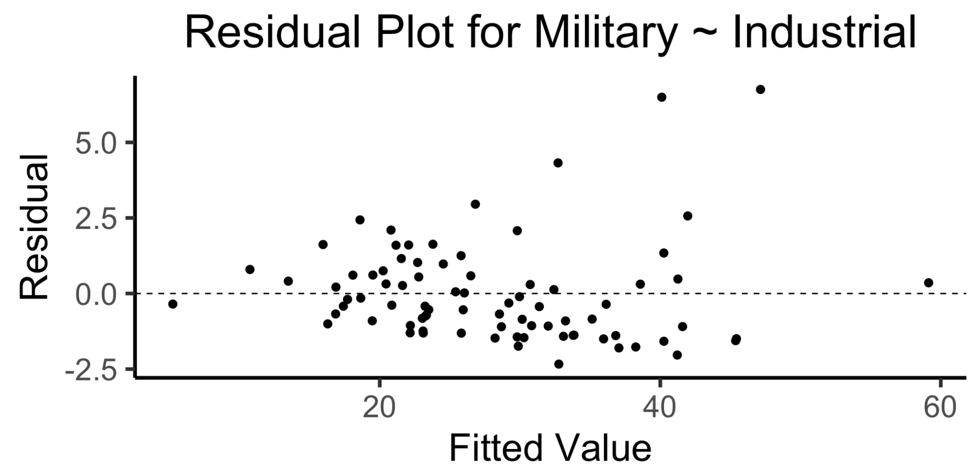
The Residual Plot

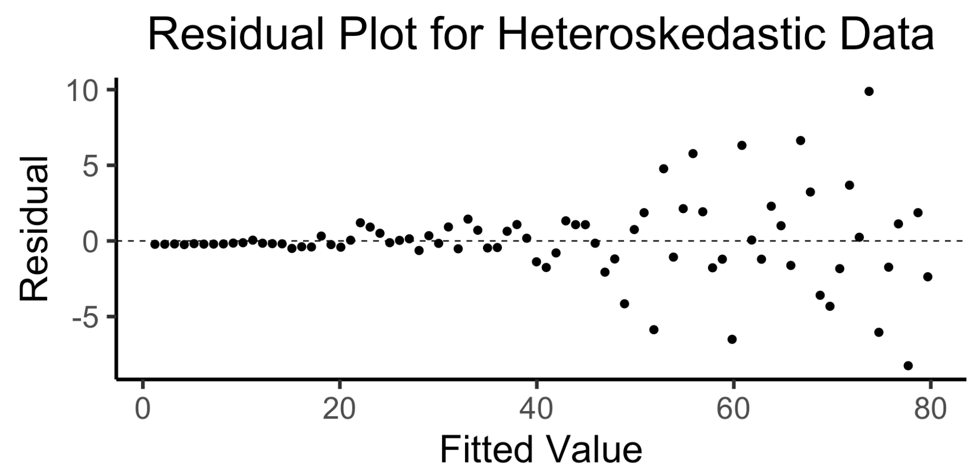
Recall **homoskedasticity** assumption: Given our model

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$$

the errors ε_i **should not vary systematically with** i

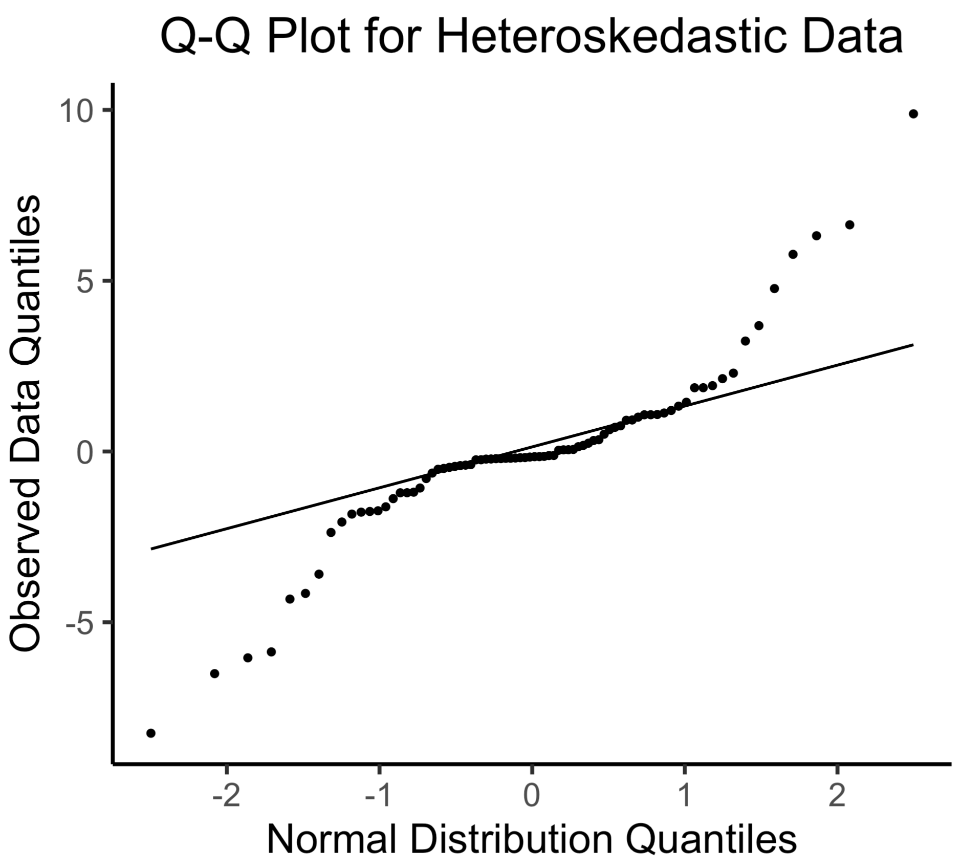
Formally: $\forall i \left[\mathrm{Var}[\varepsilon_i] = \sigma^2 \right]$

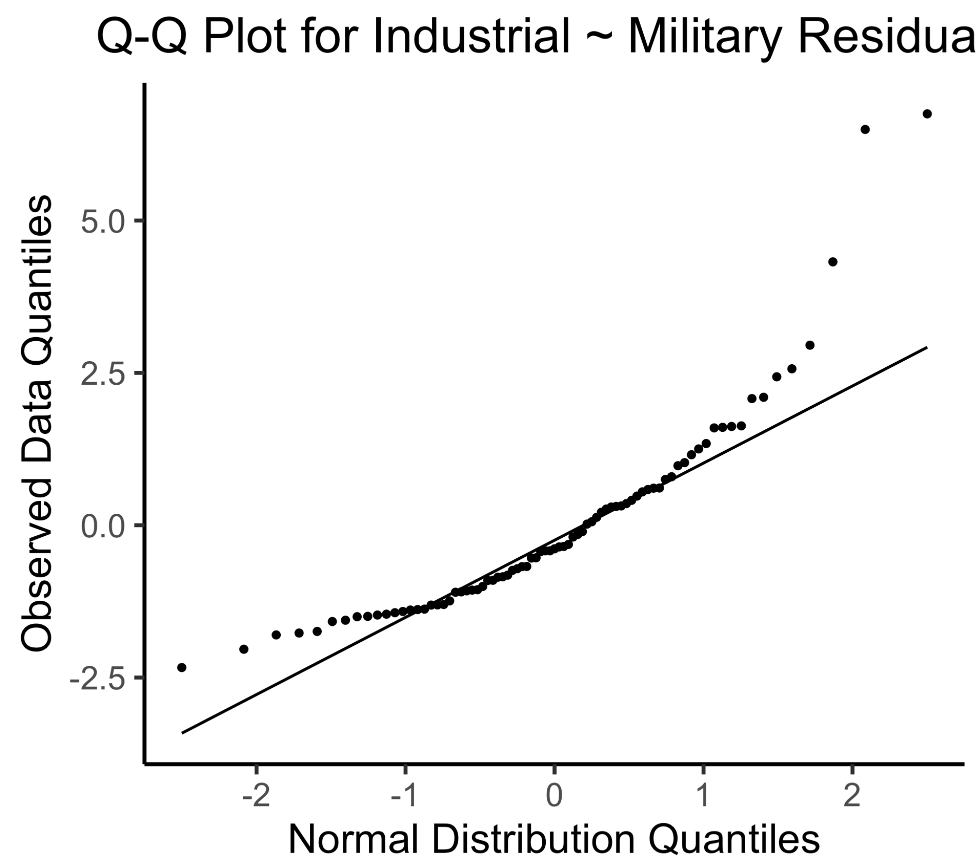




Q-Q Plot

- If $(\hat{y} - y) \sim \mathcal{N}(0, \sigma^2)$, points would lie on 45° line:





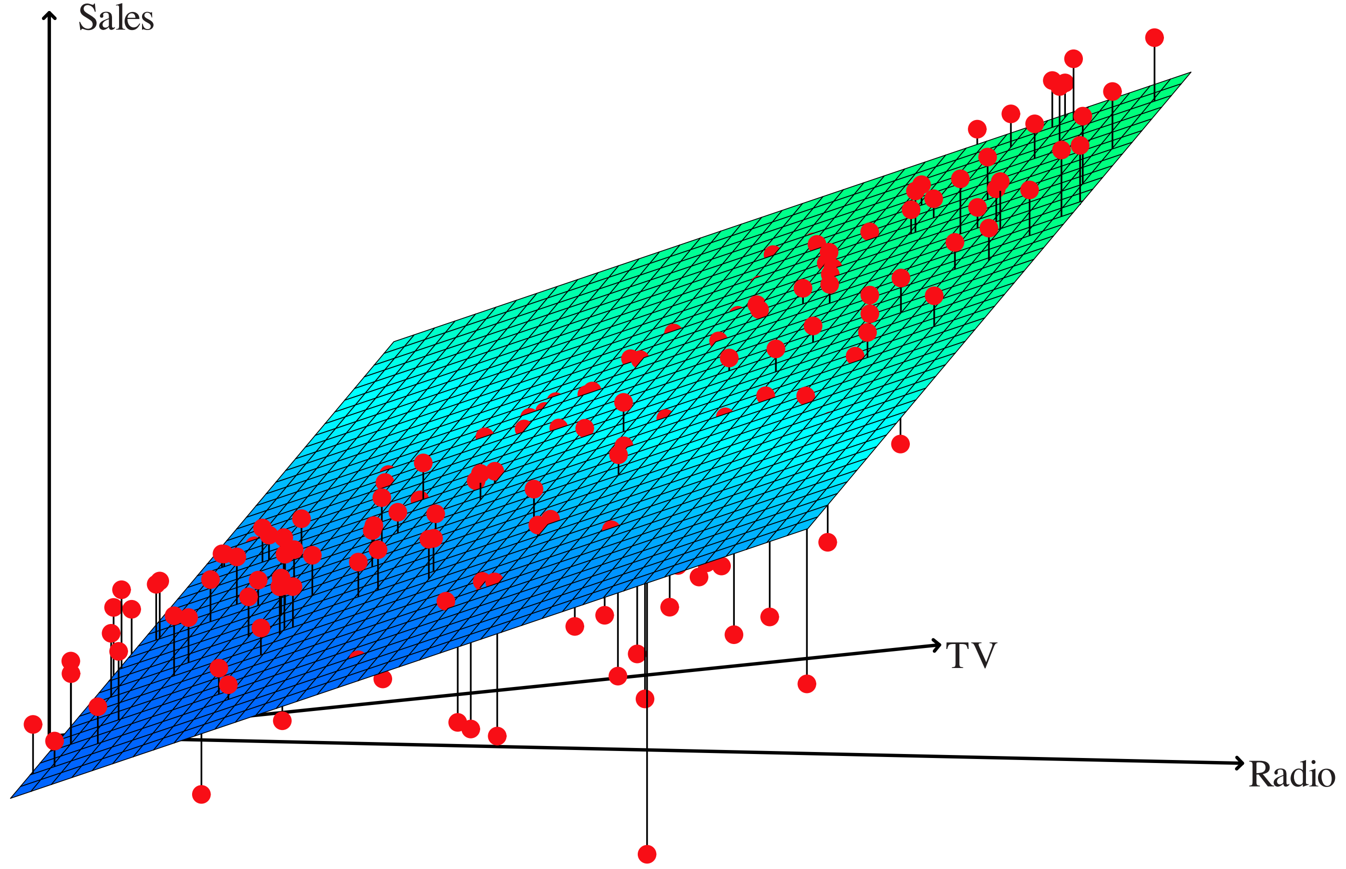
Multiple Linear Regression

- Notation: $x_{i,j}$ = value of independent variable j for person/observation i
- M = total number of independent variables

$$\hat{y}_i = \beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} + \cdots + \beta_M x_{i,M}$$

- β_j interpretation: a one-unit increase in $x_{i,j}$ is associated with a β_j unit increase in y_i, **holding all other independent variables constant**

Visualizing Multiple Linear Regression



(ISLR Fig 3.5): *A pronounced non-linear relationship. Positive residuals (visible above the surface) tend to lie along the 45° line, where budgets are split evenly. Negative residuals (most not visible) tend to be away from this line, where budgets are more lopsided.*

Interpreting MLR

```
Call:
lm(formula = sales ~ TV + radio + newspaper, data =
ad_df)

Residuals:
    Min      1Q  Median      3Q     Max
-8.8277 -0.8908  0.2418  1.1893  2.8292

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)  2.938889   0.311908   9.422   <2e-16 ***
TV           0.045765   0.001395  32.809   <2e-16 ***
radio        0.188530   0.008611  21.893   <2e-16 ***
newspaper   -0.001037   0.005871  -0.177     0.86
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1
' ' 1
```

Holding `radio` and `newspaper` spending constant…

- An **increase of $1K** in spending on TV ads is associated with…
- An **increase in sales of 46 units**

Holding `TV` and `newspaper` spending constant…

- An **increase of $1K** in spending on `radio` ads is associated with…
- An **increase in sales of 189 units**

But Wait...

$$\texttt{sales} = \overset{*}{\beta_0} + \overset{*}{\beta_1}\texttt{newspaper}$$

```
             Estimate Std. Error t value  Pr(>|t|)
(Intercept) 12.351407   0.621420 19.8761 < 2.2e-16 ***
newspaper    0.054693   0.016576  3.2996  0.001148 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.'
0.1 ' ' 1
```

$$\texttt{sales} = \overset{*}{\beta_0} + \overset{*}{\beta_1}\texttt{TV} + \overset{*}{\beta_2}\texttt{radio} + \overset{(\ )}{\beta_3}\texttt{paper}$$

```
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  2.9388894  0.3119082  9.4223   <2e-16 ***
TV           0.0457646  0.0013949 32.8086   <2e-16 ***
radio        0.1885300  0.0086112 21.8935   <2e-16 ***
newspaper   -0.0010375  0.0058710 -0.1767   0.8599
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.'
0.1 ' ' 1
```

- `newspaper` $\overset{*}{\rightarrow}$ `sales` in SLR, but `newspaper` $\overset{*}{\nrightarrow}$ `sales` in MLR?
- **Correlations** $\Rightarrow$ MLR results can be **drastically different** from SLR results
- This is a good thing! It's how we're able to **control for** confounding vars!

Correlations Among Features

▶ Code

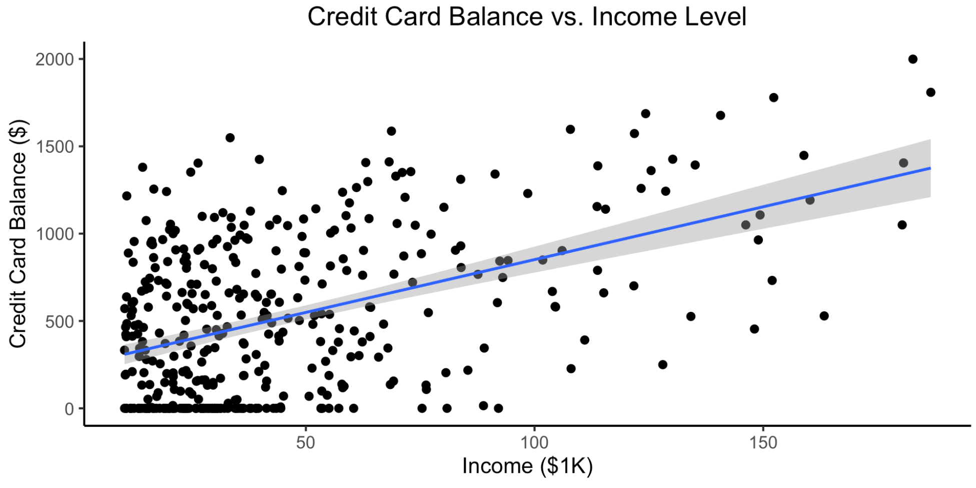
```
                 TV      radio  newspaper     sales
TV        1.00000000 0.05480866 0.05664787 0.7822244
radio     0.05480866 1.00000000 0.35410375 0.5762226
newspaper 0.05664787 0.35410375 1.00000000 0.2282990
sales     0.78222442 0.57622257 0.22829903 1.0000000
```

- Observe how $\text{cor}(\texttt{radio}, \texttt{newspaper}) \approx 0.35$ (highest feat-feat correlation)
- In markets where we spend more on `radio` our sales will tend to be higher…
- Corr matrix $\implies$ we spend more on `newspaper` in those same markets…
- In SLR which only examines `sales` vs. `newspaper`, we (**correctly!**) observe that higher values of `newspaper` are associated with higher values of `sales`…
- In essence, `newspaper` advertising is a **surrogate** for `radio` advertising $\implies$ in our SLR, `newspaper` "gets credit" for the association between `radio` and `sales`

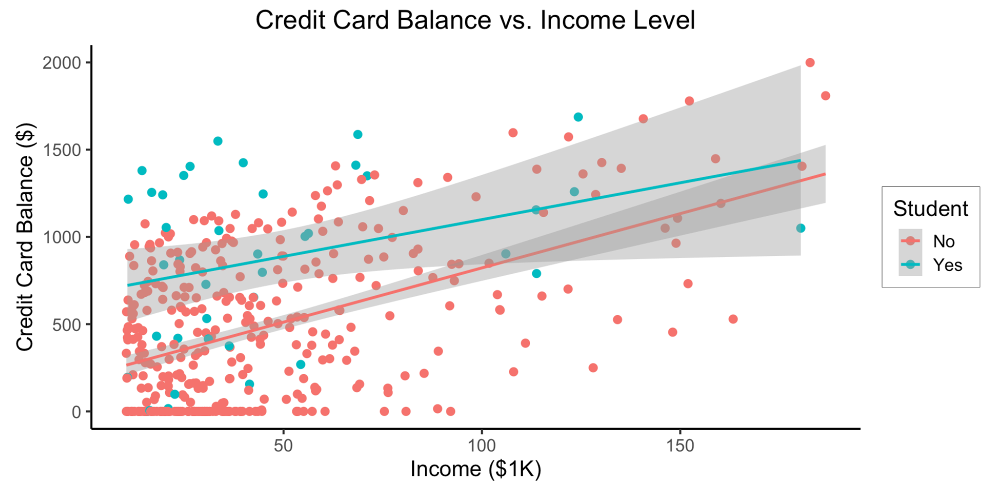
Regression Superpower: Incorporating Categorical Vars

(Preview for next week)

$$Y = \beta_0 + \beta_1 \times \texttt{income}$$



$$\begin{aligned} Y = &\beta_0 + \beta_1 \times \texttt{income} + \beta_2 \times \texttt{Student} \\ &+ \beta_3 \times (\texttt{Student} \times \texttt{Income}) \end{aligned}$$



- How does the $\texttt{Student} \times \texttt{Income}$ term help?
- Understanding this setup will open up a **vast** array of possibilities for regression 😎

Quiz Review

Objective Functions

"Fitting" a statistical model to data means **minimizing** some **loss function** that measures "how bad" our predictions are:

Optimization Problems: General Form

Find x^*, the solution to

$$
\begin{aligned}
\min_x \; & f(x) & \text{(Objective function)} \\
\text{s.t.} \; & g(x) = 0 & \text{(Constraints)}
\end{aligned}
$$

- Earlier we were able to write $x^* = \operatorname{argmax}_x f(x)$, since there were no constraints. Is there a way to write a formula like this *with* constraints?
- Answer: Yes! Thx Giuseppe-Luigi Lagrangia = Joseph-Louis **Lagrange**:

$$
x^* = \operatorname*{argmax}_{x,\,\lambda} f(x) - \lambda[g(x)]
$$

Example Problem

Example 1: Unconstrained Optimization

Find x^*, the solution to

$$\min_x \; f(x) = 3x^2 - x \\ \text{s.t.} \;\; \varnothing$$

Our Plan

- Compute the derivative $f'(x) = \frac{\partial}{\partial x} f(x)$,
- Set it equal to zero: $f'(x) = 0$, and
- Solve this equality for x, i.e., find values x^* satisfying $f'(x^*) = 0$

Computing the derivative:

$$f'(x) = \frac{\partial}{\partial x} f(x) = \frac{\partial}{\partial x}\left[3x^2 - x\right] = 6x - 1,$$

Solving for x^*, the value(s) satisfying $\frac{\partial}{\partial x} f'(x^*) = 0$ for just-derived $f'(x)$:

$$f'(x^*) = 0 \iff 6x^* - 1 = 0 \iff x^* = \frac{1}{6}.$$

Derivative Cheatsheet

Type of Thing	Thing	Change in Thing when x Changes by Tiny Amount
Polynomial	$f(x) = x^n$	$f'(x) = \frac{\partial}{\partial x} f(x) = nx^{n-1}$
Fraction	$f(x) = \frac{1}{x}$	Use Polynomial rule (since $\frac{1}{x} = x^{-1}$) to get $f'(x) = -\frac{1}{x^2}$
Logarithm	$f(x) = \ln(x)$	$f'(x) = \frac{\partial}{\partial x} = \frac{1}{x}$
Exponential	$f(x) = e^x$	$f'(x) = \frac{\partial}{\partial x} e^x = e^x$ (🧐❗)
Multiplication	$f(x) = g(x)h(x)$	$f'(x) = g'(x)h(x) + g(x)h'(x)$
Division	$f(x) = \frac{g(x)}{h(x)}$	Too hard to memorize... turn it into Multiplication, as $f(x) = g(x)(h(x))^{-1}$
Composition (Chain Rule)	$f(x) = g(h(x))$	$f'(x) = g'(h(x))h'(x)$
Fancy Logarithm	$f(x) = \ln(g(x))$	$f'(x) = \frac{g'(x)}{g(x)}$ by Chain Rule
Fancy Exponential	$f(x) = e^{g(x)}$	$f'(x) = g'(x)e^{g(x)}$ by Chain Rule

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