CS/ECE 148 –

Data Science Fundamentals

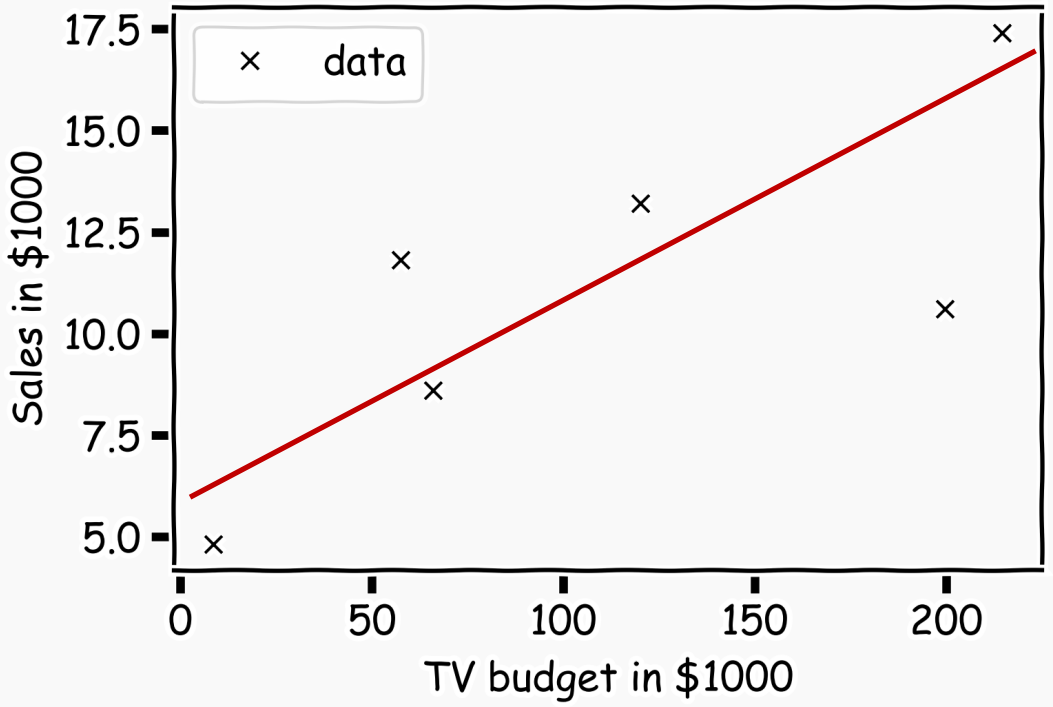
Multiple and Poly Linear Regression

UCLA Computer Science

Summary from last lecture

We **assume** a simple form of the statistical model f:

$$Y = f(X) + \epsilon = \beta_0 + \beta_1 X + \epsilon$$

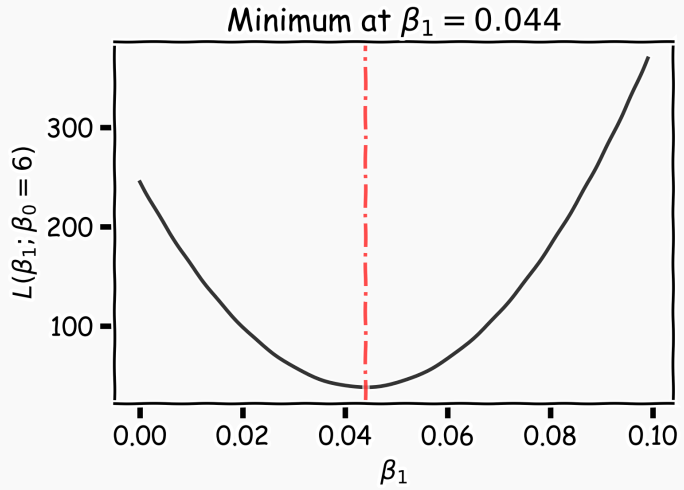


Summary from last lecture

We fit the model, i.e. estimate, $\hat{\beta}_0, \hat{\beta}_1$ that minimize the loss function, which we **assume** to be the MSE:

$$L_{MSE}(\beta_0, \beta_1) = \frac{1}{n}\sum_{n}[y_i - (\beta_0 + \beta_1 X)]^2$$

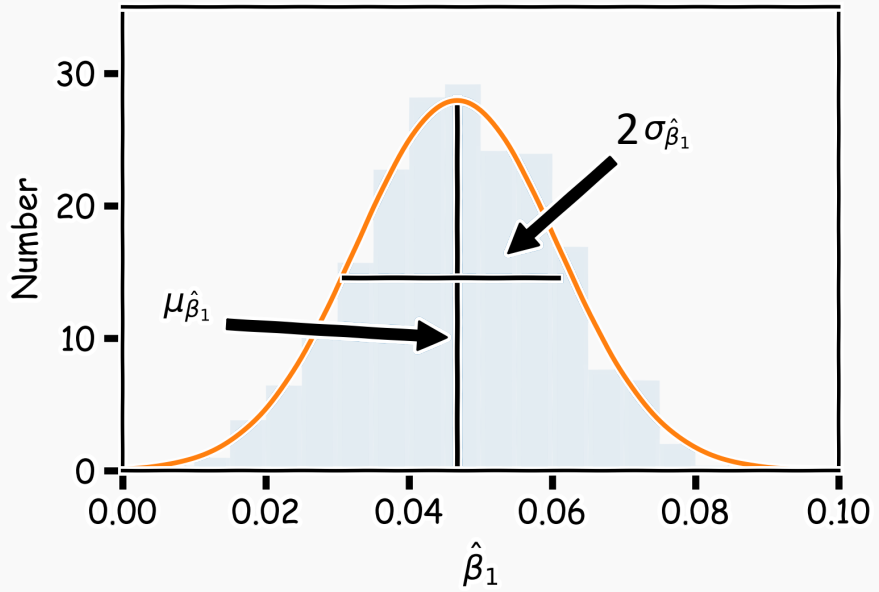
$$\widehat{\beta}_0, \widehat{\beta}_1 = \underset{\beta_0, \beta_1}{\operatorname{argmin}} L(\beta_0, \beta_1).$$



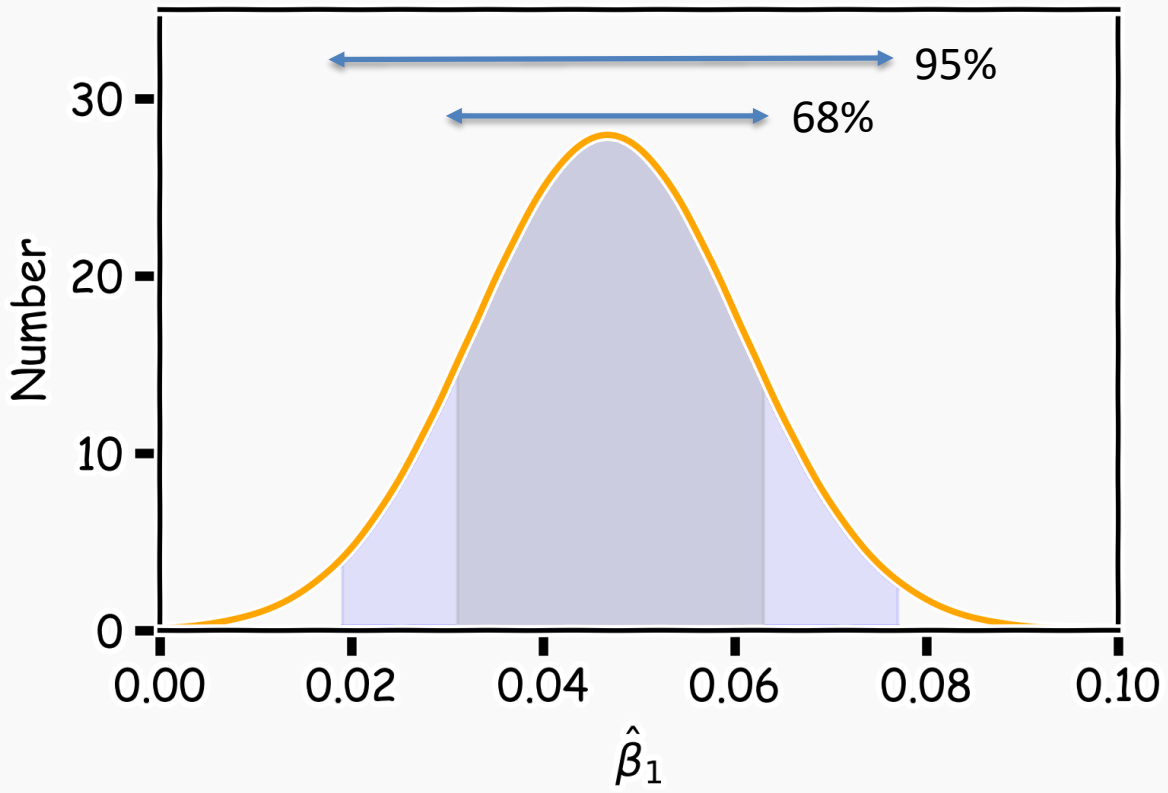
Summary from last lecture

We acknowledge that because there are errors in measurements and a limited sample, there is an inherent uncertainty in the estimation of $\hat{\beta}_0, \hat{\beta}_1$.

We used **bootstrap** to estimate the distributions of $\hat{\beta}_0, \hat{\beta}_1$



Summary from last lecture



Interpretation of Predictors

Question: What do you think a predictor coefficient means?

$$Sales = 7.5 + 0.04\,TV$$

What does 7.5 mean and what does 0.04 mean?

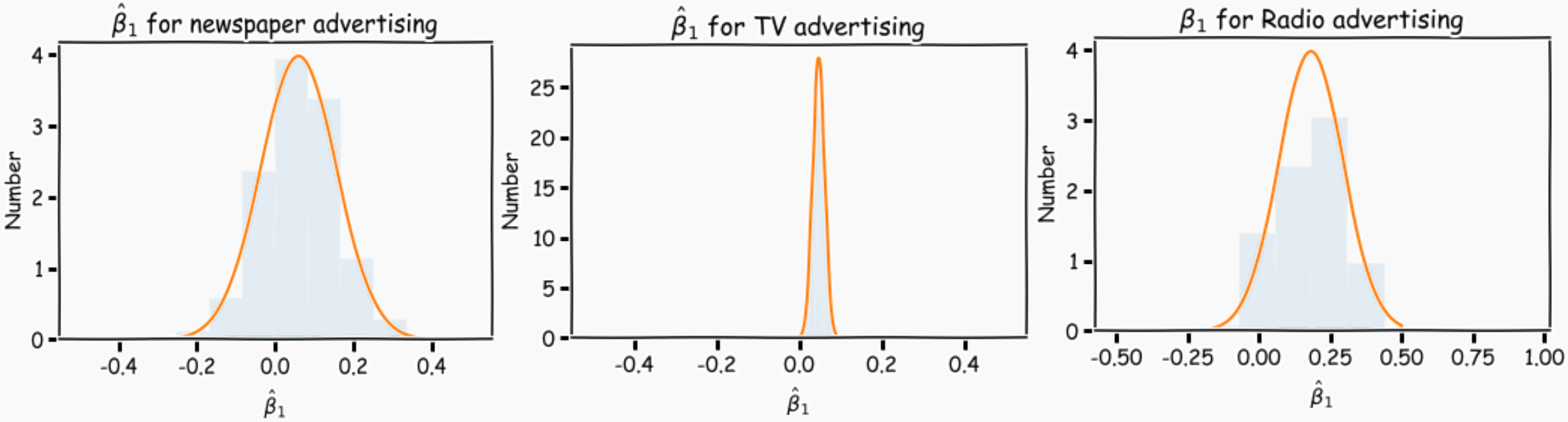
If we increase the TV by $1000, what would you expect the increase in sales to be?

What if? $Sales = 7.5 + 1.01\,TV$

The interpretation of the predictors depends on the values but decisions depend on how much we trust these values.

And also we can answer the question, 'how significant are the predictors?' Here we show the same analysis for all three predictors.

Question: Which ones are important?



Now we know how to generate these distributions we are ready to answer ***'how significant are the predictors?'***

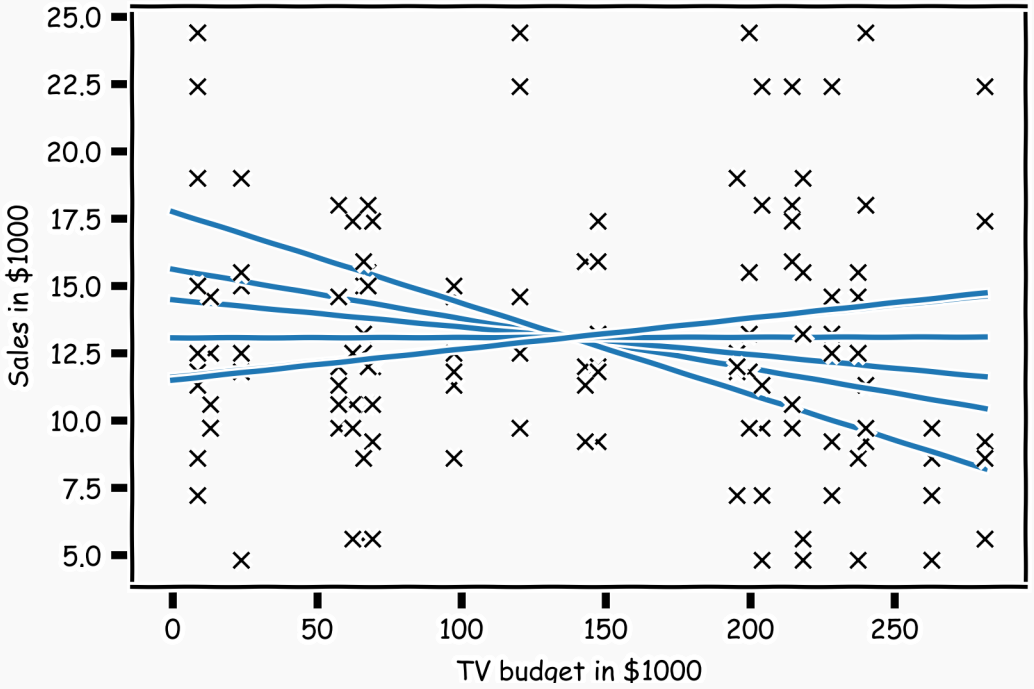
Hypothesis Testing

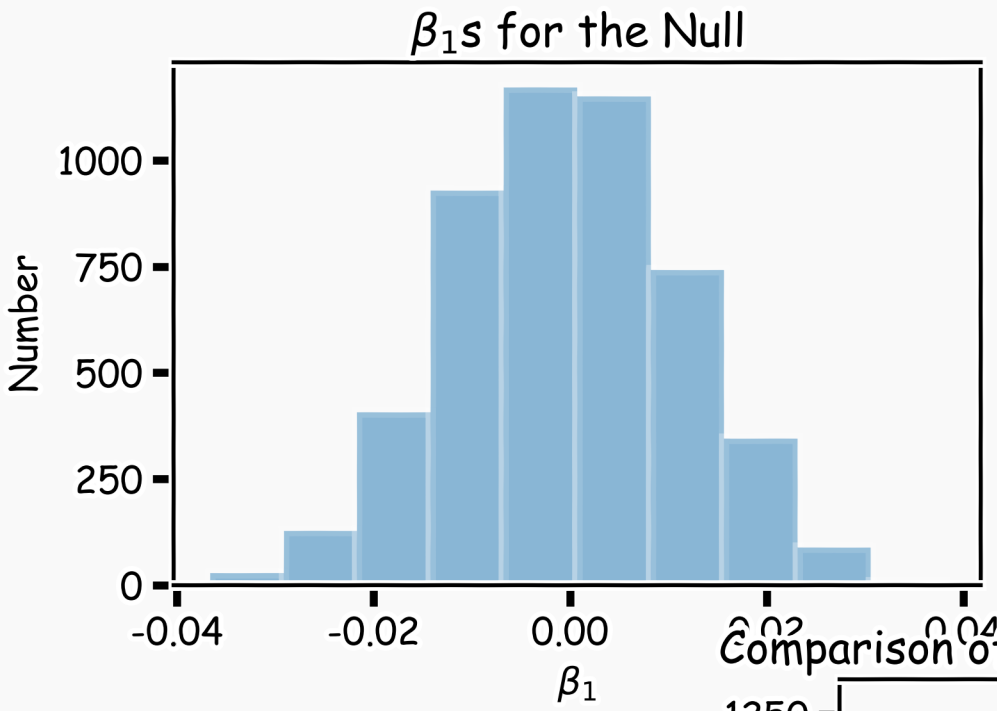
Hypothesis testing is a formal process through which we evaluate the validity of a statistical hypothesis by considering evidence **for** or **against** the hypothesis gathered by ***random sampling of the data***.

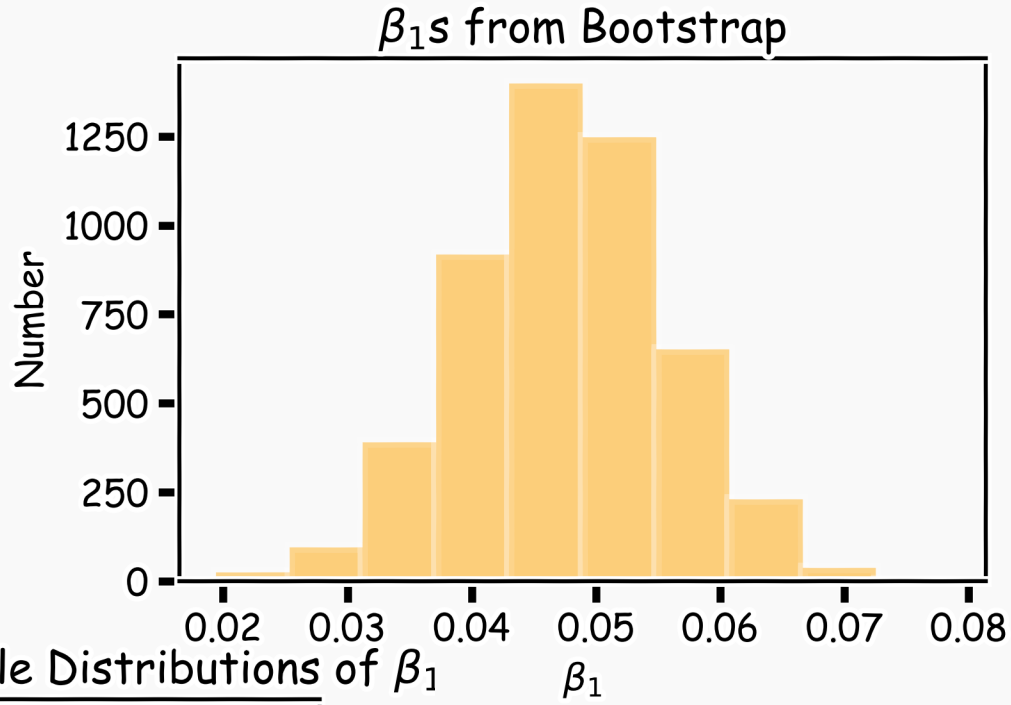
TV	sales
[illegible]	22.1
[illegible]	10.4
[illegible]	9.3
[illegible]	18.5
[illegible]	12.9
[illegible]	7.2
[illegible]	11.8
[illegible]	13.2
[illegible]	4.8
[illegible]	10.6
[illegible]	8.6
[illegible]	17.4
[illegible]	9.2
[illegible]	9.7
[illegible]	19.0
[illegible]	22.4
[illegible]	12.5
[illegible]	24.4

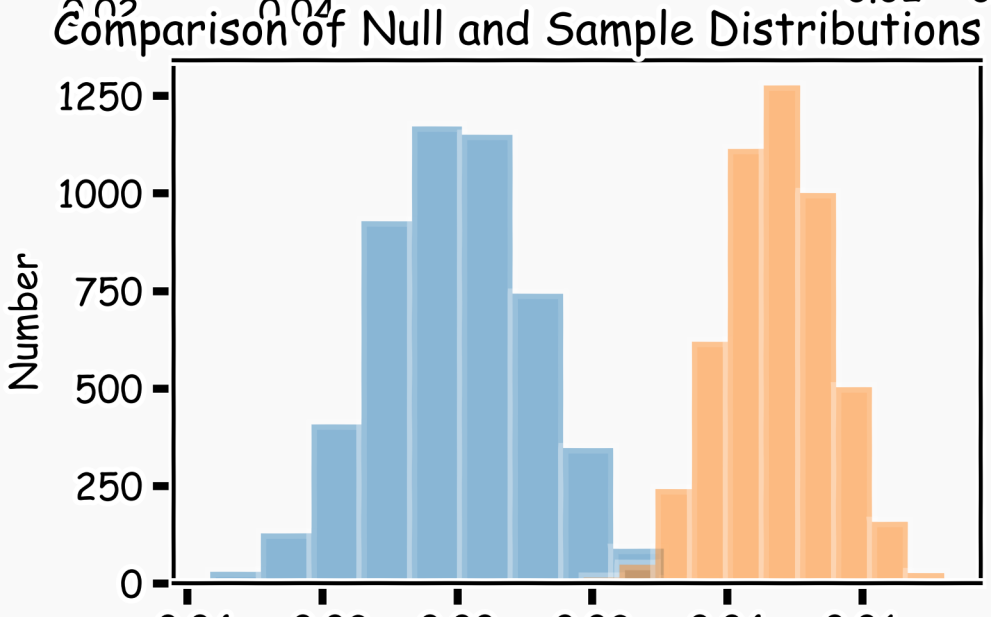
Random sampling of the data

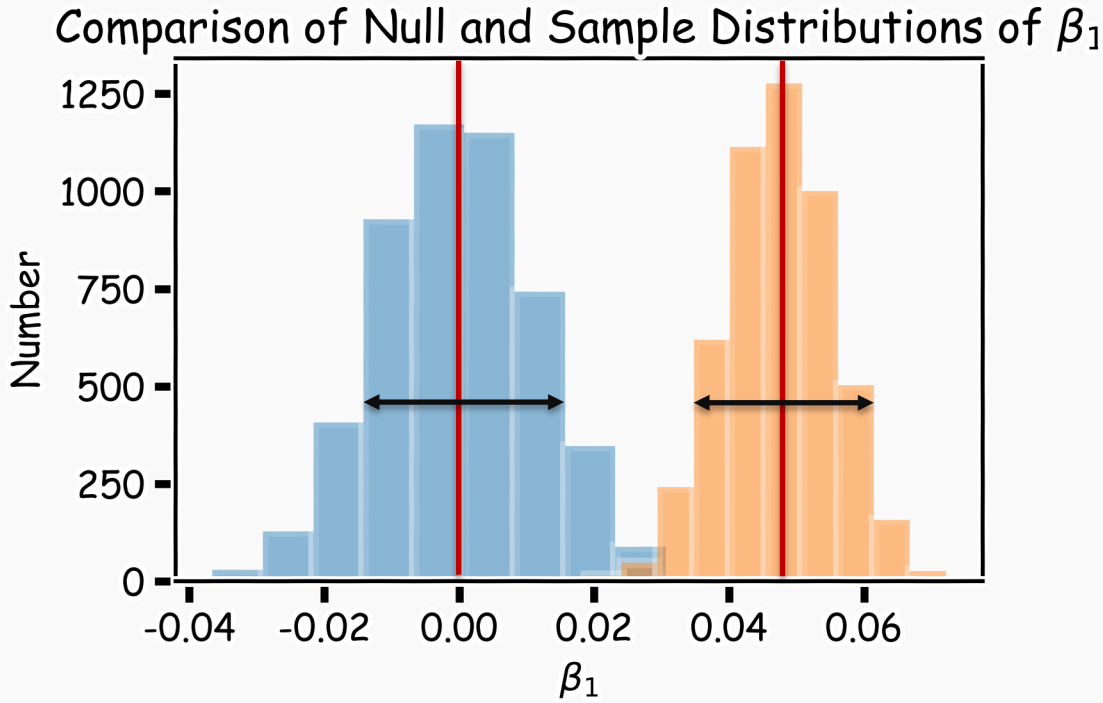
Shuffle the values of the predictor variable




β_1s for the Null
Number
1000
750
500
250
0
-0.04
-0.02
0.00
0.02
0.04
β_1


β_1s from Bootstrap
Number
1250
1000
750
500
250
0
0.02
0.03
0.04
0.05
0.06
0.07
0.08
β_1


Comparison of Null and Sample Distributions of β_1
Number
1250
1000
750
500
250
0



$\mu_{Null} = 0$

$\mu_{\hat{\beta}} = \mu_{boot}$

$\sigma_{\hat{\beta}} = SE(\hat{\beta}) = \sigma_{boot}$

$\sigma_{Null} \approx \sigma_{\hat{\beta}}$

Translate this to the significance. Let's look at the distance of the estimated value of the coefficient in units of SE($\hat{\beta}_1$) = $\sigma_{\hat{\beta}_1}$.

$$D = \frac{\mu_{\hat{\beta}} - \mu_{Null}}{\sigma_{\hat{\beta}}}$$

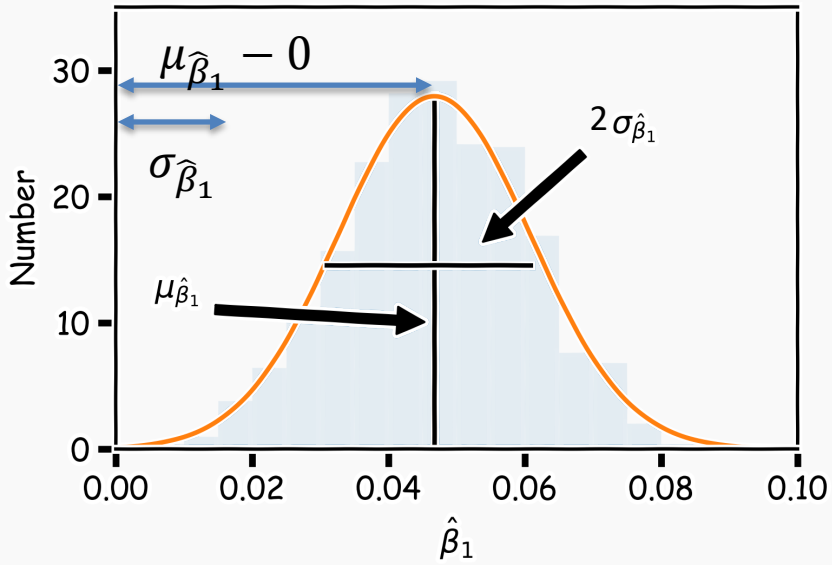
Importance of predictors

In practice, we do not need the distribution for Null.

Define a test statistic, which we we call t-test statistic

$$t = \frac{\mu_{\hat{\beta}_1}}{\sigma_{\hat{\beta}_1}}$$

Which measures the distance from zero in units of standard deviation.



We evaluate how often a particular value of *t* can occur by accident. We expect that *t* will have a *t-distribution with n-2 degrees* of freedom.

To compute the probability of observing any value equal to $|t|$ or larger, assuming $\hat{\beta}_1 = 0$ is easy. We call this probability the **p-value**.

a small p-value (<0.05) indicates that it is unlikely to observe such a substantial association between the predictor and the response due to chance.

Hypothesis Testing

Hypothesis testing is a formal process through which we evaluate the validity of a statistical hypothesis by considering evidence for or against the hypothesis gathered by **random sampling** of the data.

1. State the hypotheses, typically a **null hypothesis**, H_0 and an **alternative hypothesis**, H_1, that is the negation of the former.
2. Choose a type of analysis, i.e. how to use sample data to evaluate the null hypothesis. Typically this involves choosing a single test statistic.
3. **Sample** data and compute the test statistic.
4. Use the value of the test statistic to either reject or not reject the null hypothesis.

Hypothesis testing

3. **Sample**:

   Using bootstrap we can estimate $\hat{\beta}_1$, and therefore $\mu_{\hat{\beta}_1}$ and $\sigma_{\hat{\beta}_1}$ (similar for $\hat{\beta}_0$).

4. **Reject or not reject the hypothesis:**

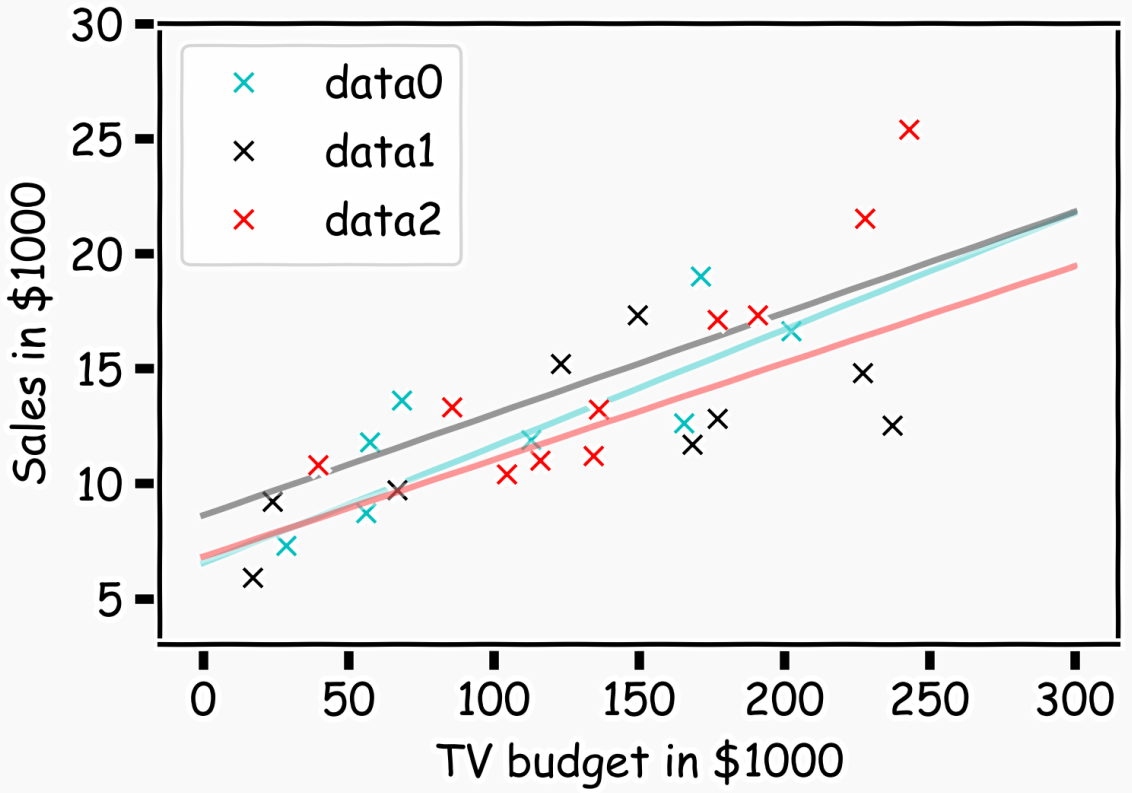
   If there is really no relationship between *X* and *Y* , then we expect that will have a *t-distribution with n-2 degrees* of freedom.

   To compute the probability of observing any value equal to $|t|$ or larger, assuming $\hat{\beta}_1 = 0$ is easy. We call this probability the p-value.

   a small p-value indicates that it is unlikely to observe such a substantial association between the predictor and the response due to chance

How well do we know $\hat{f}$?

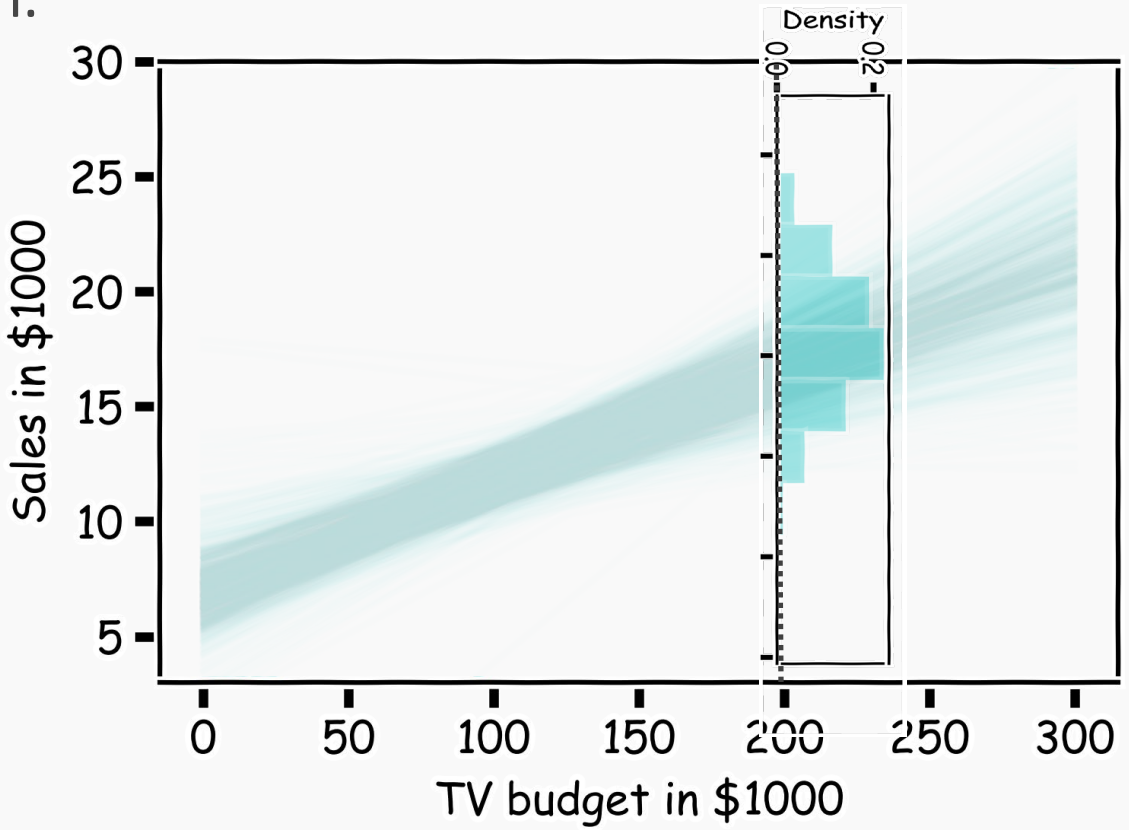
There is one such regression line for every bootstrapped sample.



How well do we know $\hat{f}$?

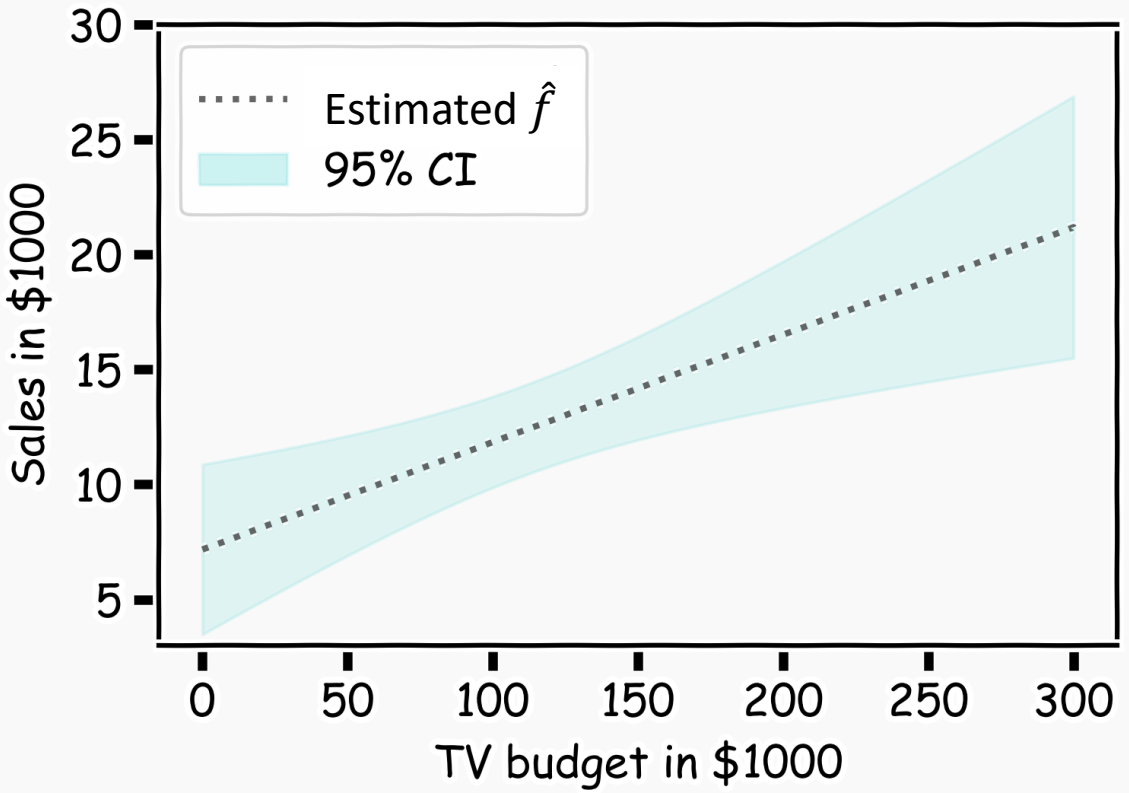
Below we show all regression lines for a thousand of such bootstrapped samples.

For a given x, we examine the distribution of $\hat{f}$, and determine the mean and standard deviation.



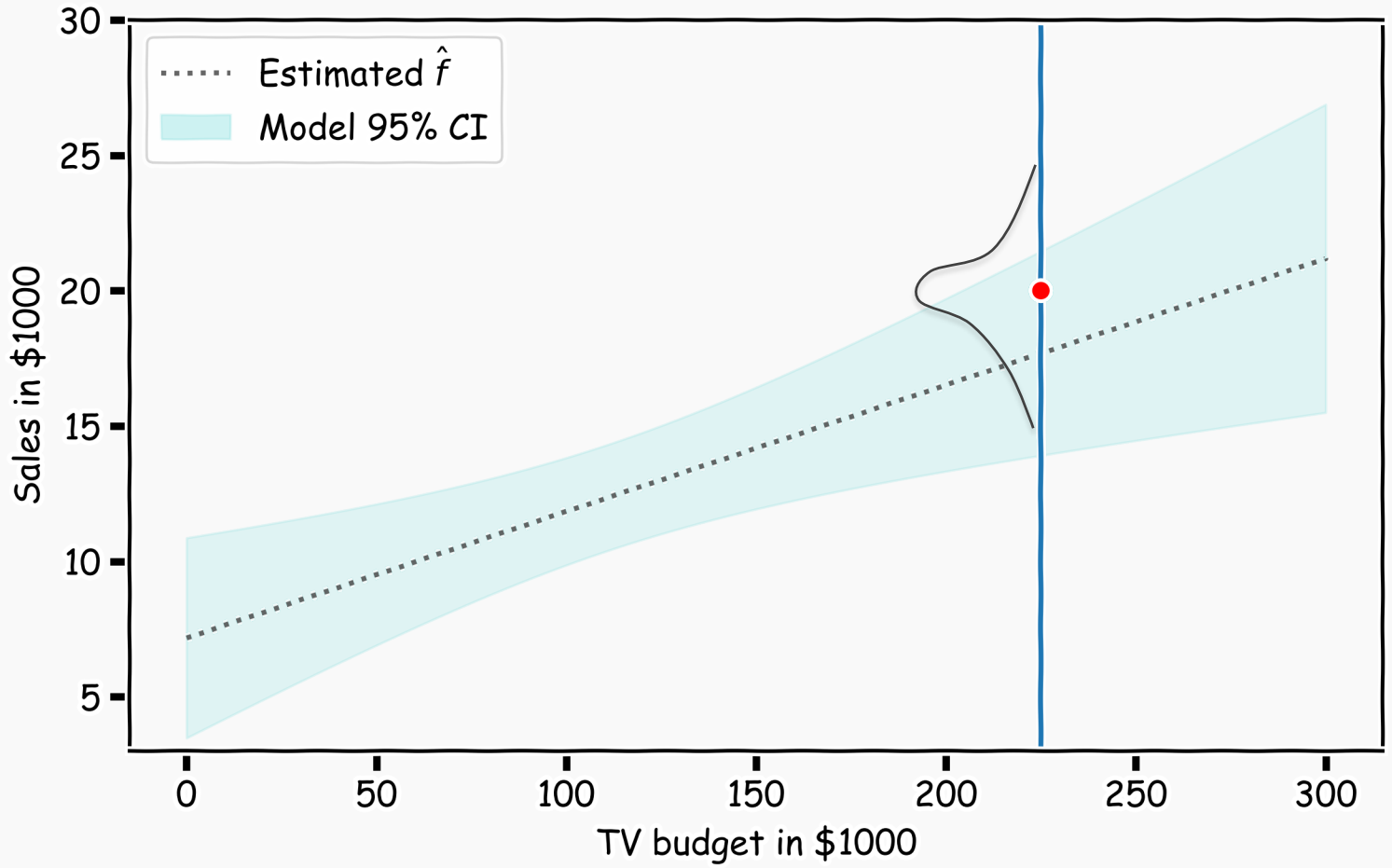
How well do we know $\hat{f}$?

For every x, we calculate the mean of the models, $\hat{f}$ (shown with dotted line) and the 95% CI of those models (shaded area).



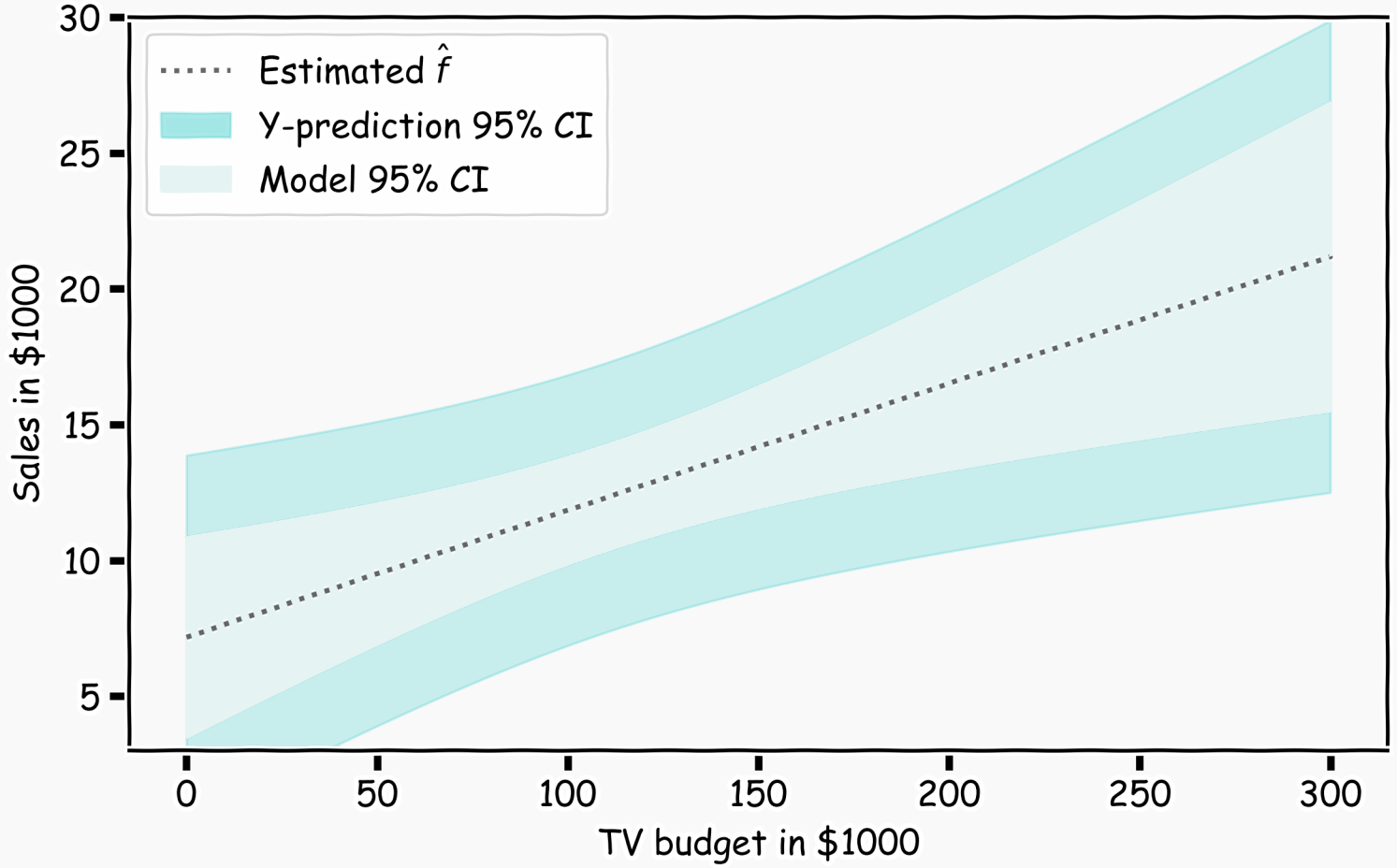
Confidence in predicting $\hat{y}$

- for a given x, we have a distribution of models $f(x)$
- for each of these $f(x)$, the prediction for $y \sim N(f, \sigma_\epsilon)$



Confidence in predicting $\hat{y}$

- for a given x, we have a distribution of models $f(x)$
- for each of these $f(x)$, the prediction for $y \sim N(f, \sigma_\epsilon)$
- The prediction confidence intervals are then



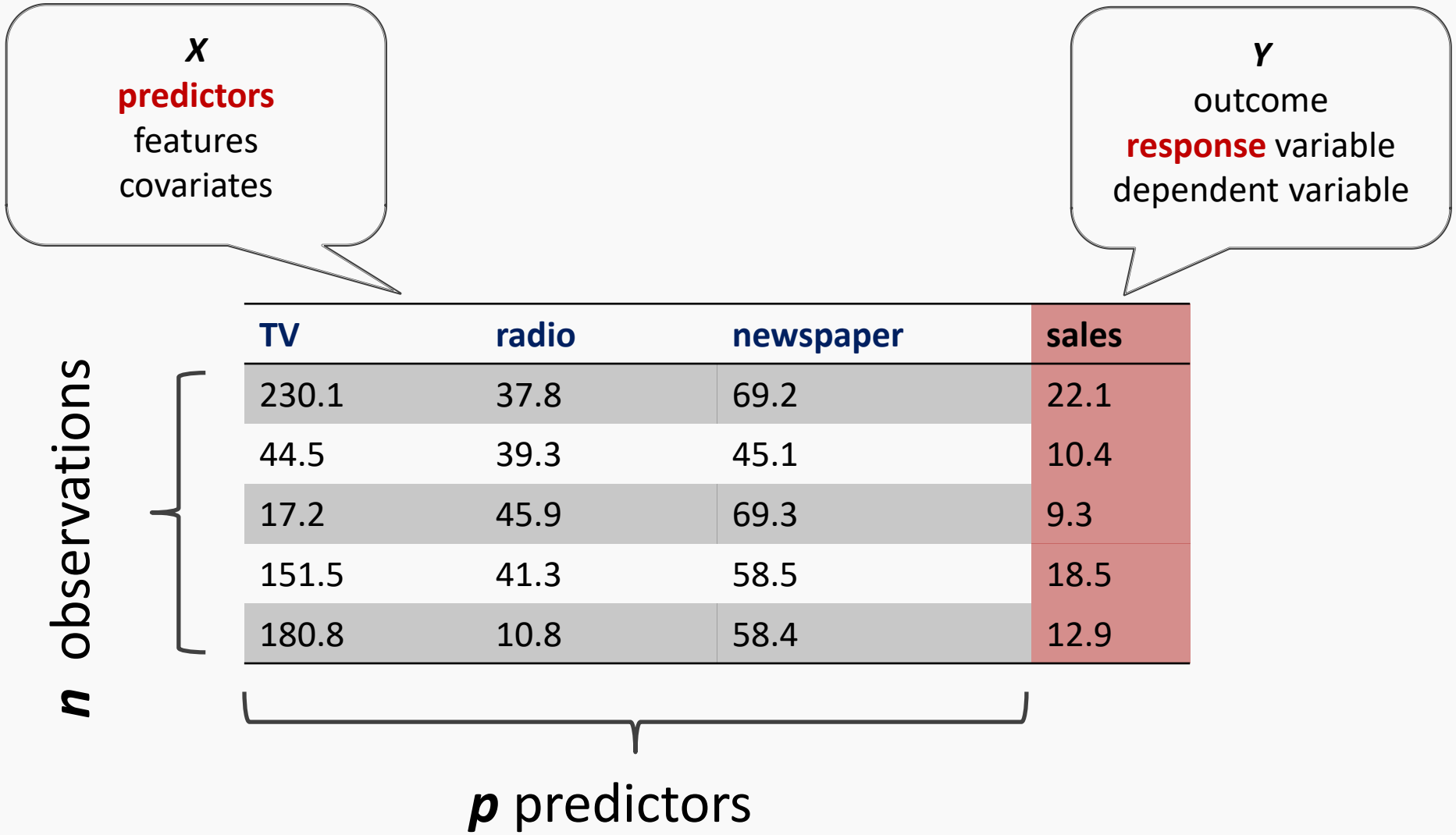
Multiple Linear Regression

If you have to guess someone's height, would you rather be told

- Their weight, only
- Their weight and gender
- Their weight, gender, and income
- Their weight, gender, income, and favorite number

Of course, you'd always want as much data about a person as possible. Even though height and favorite number may not be strongly related, at worst you could just ignore the information on favorite number. We want our models to be able to take in lots of data as they make their predictions.

Response vs. Predictor Variables



Multilinear Models

In practice, it is unlikely that any response variable Y depends solely on one predictor *x*. Rather, we expect that is a function of multiple predictors $f(X_1, \dots, X_J)$. Using the notation we introduced in last lecture,

$$Y = y_1, \dots, y_n, \quad X = X_1, \dots, X_J \text{ and } X_j = x_{1j}, \dots, x_{ij}, \dots, x_{nj}$$

In this case, we can still assume a simple form for f -a multilinear form:

$$Y = f(X_1, \dots, X_J) + \epsilon = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_J X_J + \epsilon$$

Hence, $\hat{f}$, has the form

$$\hat{Y} = \hat{f}(X_1, \dots, X_J) + \epsilon = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 + \dots + \hat{\beta}_J X_J + \epsilon$$

Multiple Linear Regression

Again, to fit this model means to compute $\hat{\beta}_0, \ldots, \hat{\beta}_J$ or to minimize a loss function; we will again choose the **MSE** as our loss function.

Given a set of observations,

$$\{(x_{1,1}, \ldots, x_{1,J}, y_1), \ldots (x_{n,1}, \ldots, x_{n,J}, y_n)\},$$

the data and the model can be expressed in vector/matrix notation,

$$\mathbf{Y} = \begin{pmatrix} y_1 \\ \vdots \\ y_y \end{pmatrix}, \qquad \mathbf{X} = \begin{pmatrix} 1 & x_{1,1} & \ldots & x_{1,J} \\ 1 & x_{2,1} & \ldots & x_{2,J} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n,1} & \ldots & x_{n,J} \end{pmatrix}, \qquad \boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_J \end{pmatrix},$$

Multilinear Model, example

For our data

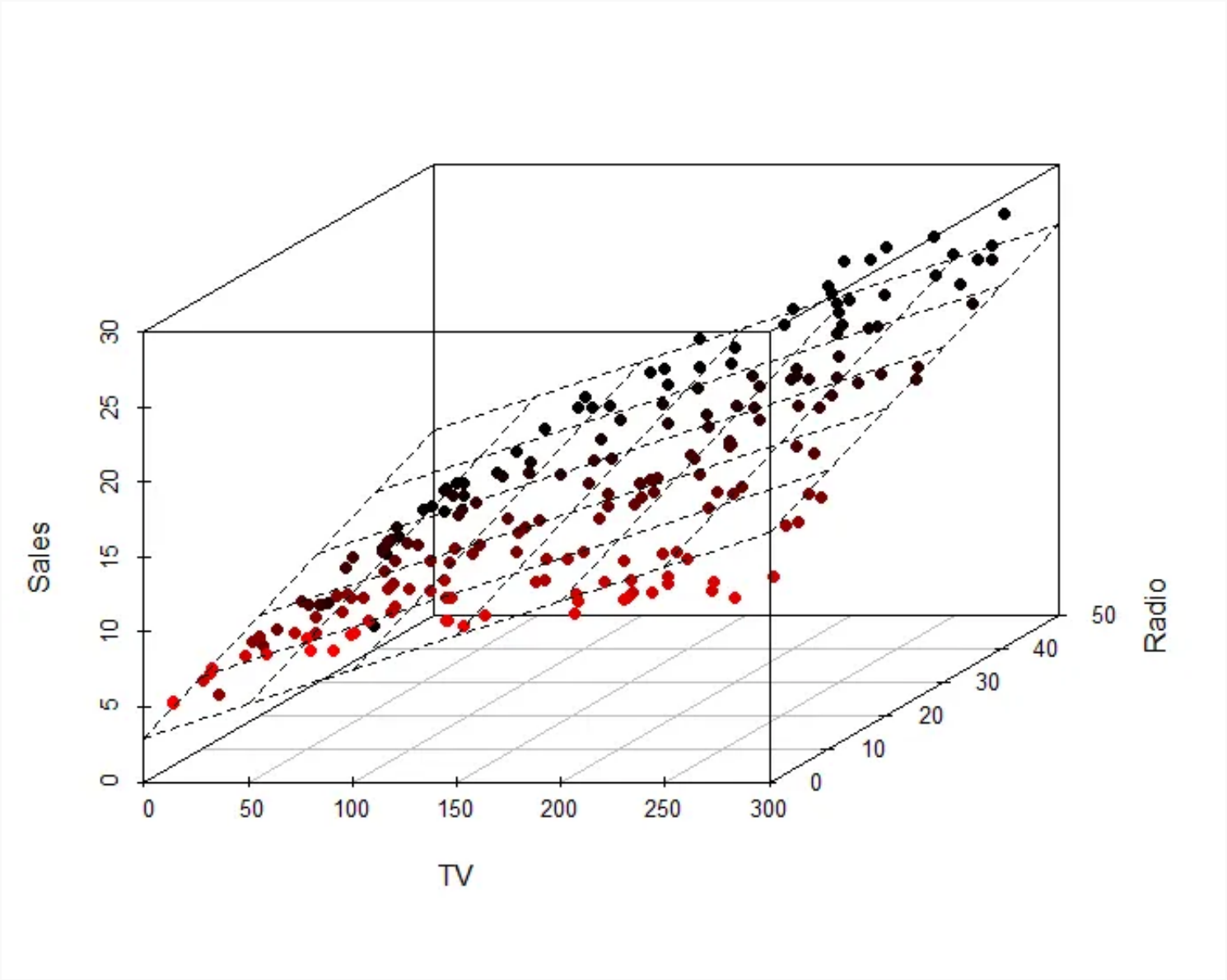
$$\text{Sales} = \beta_0 + \beta_1 \times TV + \beta_2 \times Radio + \beta_3 \times Newspaper + \epsilon$$

In linear algebra notation

$$\boldsymbol{Y} = \begin{pmatrix} Sales_1 \\ \vdots \\ Sales_n \end{pmatrix}, \boldsymbol{X} = \begin{pmatrix} 1 & TV_1 & Radio_1 & News_1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & TV_n. & Radio_n & News_n \end{pmatrix}, \boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \vdots \\ \beta_3 \end{pmatrix}$$

$$\begin{pmatrix} Sales_1 \end{pmatrix} = \begin{pmatrix} 1 & TV_1 & Radio_1 & News_1 \end{pmatrix} \times \begin{pmatrix} \beta_0 \\ \vdots \\ \beta_3 \end{pmatrix}$$

Multilinear Model, example



Multiple Linear Regression

The model takes a simple algebraic form:

$$\mathbf{Y} = \mathbf{X}\beta + \epsilon$$

Thus, the MSE can be expressed in vector notation as

$$\mathrm{MSE}(\beta) = \frac{1}{\mathrm{n}} \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}\|^2$$

Minimizing the MSE using vector calculus yields,

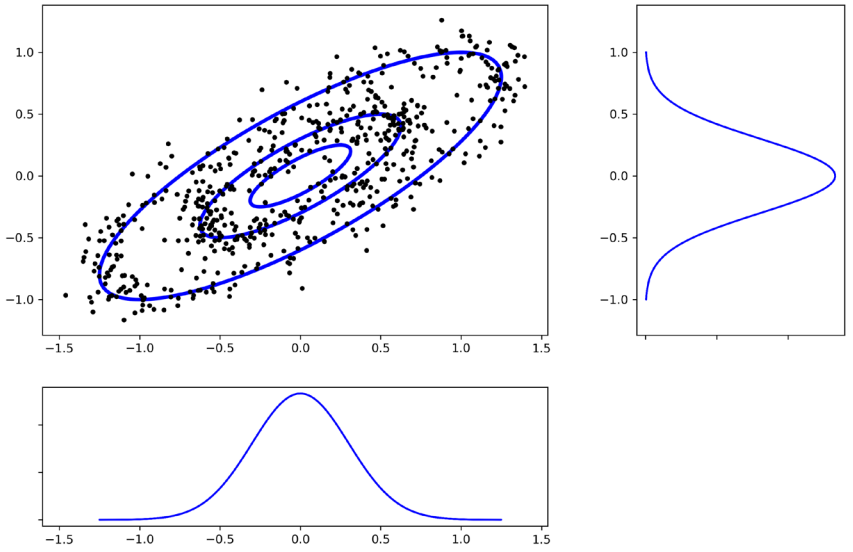
$$\widehat{\boldsymbol{\beta}} = \left(\mathbf{X}^\top \mathbf{X}\right)^{-1} \mathbf{X}^\top \mathbf{Y} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}}\, \mathrm{MSE}(\boldsymbol{\beta}).$$

Standard Errors for Multiple Linear Regression

As with the simple linear regression, the standard errors can be calculated either using statistical modeling

$$SE(\beta)^2 = \sigma^2(X^T X)^{-1}$$

Or **bootstrap**



Collinearity

Collinearity refers to the case in which two or more predictors are correlated (related).

We will re-visit collinearity in the next lecture when we address **overfitting**, but for now we want to examine how does collinearity affects our confidence on the coefficients and consequently on the importance of those coefficients.

Collinearity

Three individual models

TV

Coef.	Std.Err.	t	P>|t|	[0.025	0.975]
6.679	0.478	13.957	2.804e-31	5.735	7.622
0.048	0.0027	17.303	1.802e-41	0.042	0.053

RADIO

Coef.	Std.Err.	t	P>|t|	[0.025	0.975]
9.567	0.553	17.279	2.133e-41	8.475	10.659
0.195	0.020	9.429	1.134e-17	0.154	0.236

NEWS

Coef.	Std.Err.	t	P>|t|	[0.025	0.975]
11.55	0.576	20.036	1.628e-49	10.414	12.688
0.074	0.014	5.134	6.734e-07	0.0456	0.102

One model

	Coef.	Std.Err.	t	P>|t|	[0.025	0.975]
β_0	2.602	0.332	7.820	3.176e-13	1.945	3.258
β_{TV}	0.046	0.0015	29.887	6.314e-75	0.043	0.049
β_{RADIO}	0.175	0.0094	18.576	4.297e-45	0.156	0.194
β_{NEWS}	0.013	0.028	2.338	0.0203	0.008	0.035

Finding Significant Predictors: Hypothesis Testing

For checking the significance of linear regression coefficients:

1.we set up our hypotheses H_0:

$$H_0 : \beta_0 = \beta_1 = \ldots = \beta_J = 0 \qquad \textbf{(Null)}$$

$$H_1 : \beta_j \neq 0, \text{ for at least one } j \qquad \textbf{(Alternative)}$$

2. we choose the *F*-stat to evaluate the null hypothesis,

$$F = \frac{\text{explained variance}}{\text{unexplained variance}}$$

Finding Significant Predictors: Hypothesis Testing

3. we can compute the *F*-stat for linear regression models by

$$F = \frac{(\mathrm{TSS} - \mathrm{RSS})/J}{\mathrm{RSS}/(n - J - 1)}, \quad \mathrm{TSS} = \sum_i (y_i - \overline{y})^2, \mathrm{RSS} = \sum_i (y_i - \widehat{y}_i)^2$$

4. If $F = 1$ we consider this evidence for H_0; if $F > 1$, we consider this evidence against H_0.

A-T test will tell you if a *single* variable is statistically significant and an F test will tell you if a *group* of variables are jointly significant.

Qualitative Predictors

So far, we have assumed that all variables are quantitative. But in practice, often some predictors are **qualitative**.

Example: The Credit data set contains information about balance, age, cards, education, income, limit , and rating for a number of potential customers.

Income	Limit	Rating	Cards	Age	Education	Gender	Student	Married	Ethnicity	Balance
14.890	3606	283	2	34	11	Male	No	Yes	Caucasian	333
106.02	6645	483	3	82	15	Female	Yes	Yes	Asian	903
104.59	7075	514	4	71	11	Male	No	No	Asian	580
148.92	9504	681	3	36	11	Female	No	No	Asian	964
55.882	4897	357	2	68	16	Male	No	Yes	Caucasian	331

Qualitative Predictors

If the predictor takes only two values, then we create an **indicator** or **dummy variable** that takes on two possible numerical values.

For example for the gender, we create a new variable:

$$x_i = \begin{cases} 1 & \text{if } i\,\text{th person is female} \\ 0 & \text{if } i\,\text{th person is male} \end{cases}$$

We then use this variable as a predictor in the regression equation.

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i = \begin{cases} \beta_0 + \beta_1 + \epsilon_i & \text{if } i\,\text{th person is female} \\ \beta_0 + \epsilon_i & \text{if } i\,\text{th person is male} \end{cases}$$

Qualitative Predictors

Question: What is interpretation of β_0 and β_1?

Qualitative Predictors

Question: What is interpretation of β_0 and β_1?

- β_0 is the average credit card balance among males,
- $\beta_0 + \beta_1$ is the average credit card balance among females,
- and β_1 the average difference in credit card balance between females and males.

Example: Calculate β_0 and β_1 for the Credit data.

You should find $\beta_0 \sim \$509, \beta_1 \sim \$19$

More than two levels: One hot encoding

Often, the qualitative predictor takes more than two values (e.g. ethnicity in the credit data).

In this situation, a single dummy variable cannot represent all possible values.

We create additional dummy variable as:

$$x_{i,1} = \begin{cases} 1 & \text{if } i\,\text{th person is Asian} \\ 0 & \text{if } i\,\text{th person is not Asian} \end{cases}$$

$$x_{i,2} = \begin{cases} 1 & \text{if } i\,\text{th person is Caucasian} \\ 0 & \text{if } i\,\text{th person is not Caucasian} \end{cases}$$

More than two levels: One hot encoding

We then use these variables as predictors, the regression equation becomes:

$$y_i = \beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} + \epsilon_i = \begin{cases} \beta_0 + \beta_1 + \epsilon_i & \text{if } i\,\text{th person is Asian} \\ \beta_0 + \beta_2 + \epsilon_i & \text{if } i\,\text{th person is Caucasian} \\ \beta_0 + \epsilon_i & \text{if } i\,\text{th person is AfricanAmerican} \end{cases}$$

Question: What is the interpretation of β_0, β_1, β_2?

Beyond linearity

In the Advertising data, we assumed that the effect on sales of increasing one advertising medium is independent of the amount spent on the other media.

If we assume linear model then the average effect on sales of a one-unit increase in TV is always β_1, regardless of the amount spent on radio.

Synergy effect or **interaction effect** states that when an increase on the radio budget affects the effectiveness of the TV spending on sales.

Beyond linearity

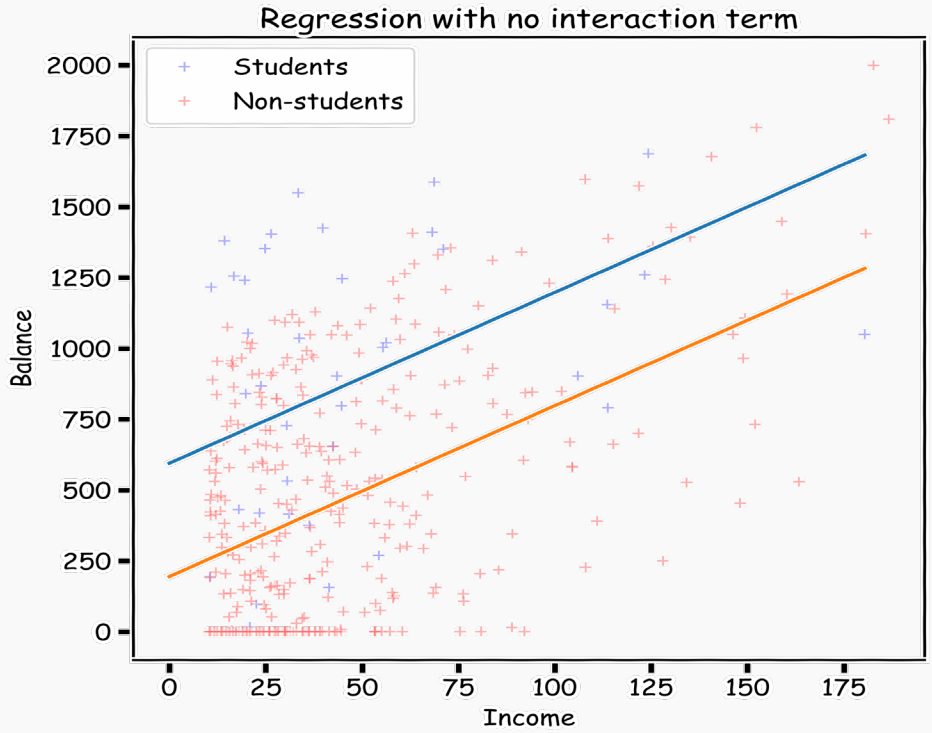
We change

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \epsilon$$

To

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \boxed{\beta_3 X_1 X_2} + \epsilon$$

What does it mean?



$$x_{Student} = \begin{cases} 0 & Balance = \beta_0 + \beta_1 \times Income. \\ 1 & Balance = (\beta_0 + \beta_2) + (\beta_1) \times Income. \end{cases}$$

$$x_{Student} = \begin{cases} 0 & Balance = \beta_0 + \beta_1 \times Income. \\ 1 & Balance = (\beta_0 + \beta_2) + (\beta_1 + \beta_3) \times Income \end{cases}$$

Predictors predictors predictors

We have a lot of predictors!

Is it a problem?

Yes: Computational Cost

Yes: Overfitting

Wait there is more …

Residuals

We started with

$$y = f(x) + \epsilon$$

We **assumed** the exact form of $f(x)$,to be,

$$f(x) = \beta_0 + \beta_1 x,$$

then estimated the $\hat{\beta}'s$.

What if that is not correct? Instead:

$$f(x) = \beta_0 + \beta_1 x + \phi(x),$$

But we model it as

$$\hat{y} = \hat{f}(x) = \hat{\beta}_0 + \hat{\beta}_1 x$$

Then the residual

$$r = (y - \widehat{y}) = \hat{f}(x) = \epsilon + \phi(x)$$

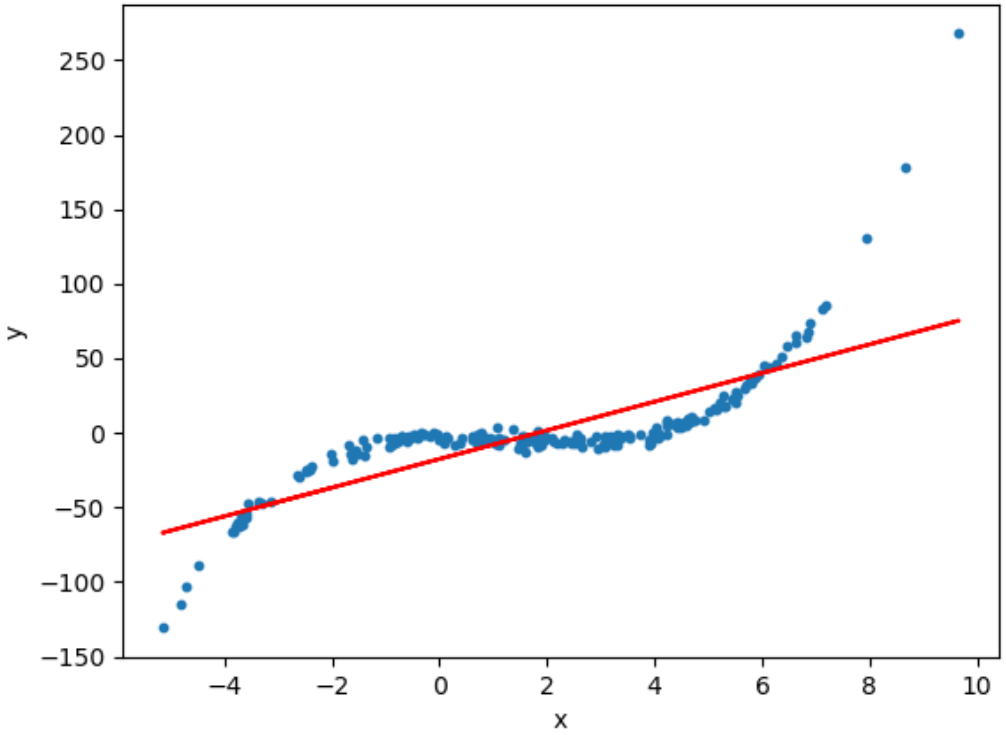
Residual Analysis

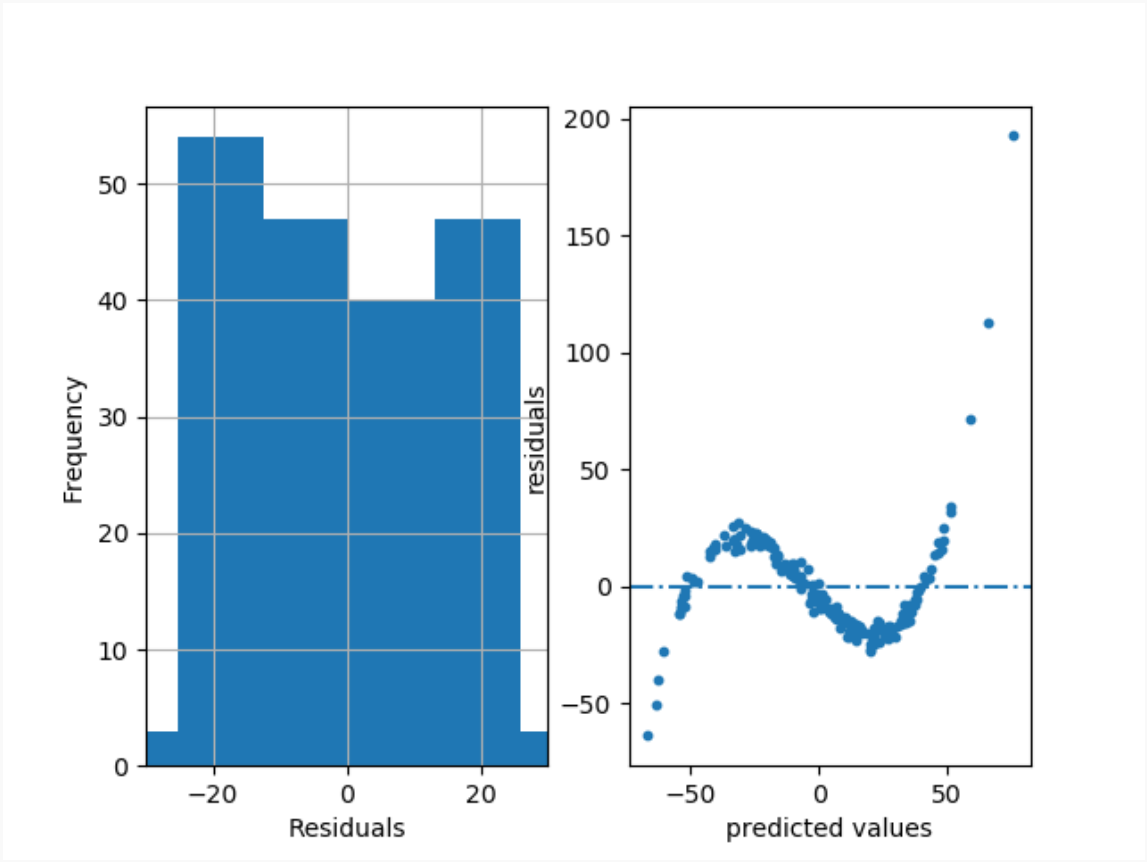
When we estimated the variance of ϵ, we assumed that the residuals $r_i = y_i - \hat{y}_i$ were uncorrelated and normally distributed with mean 0 and fixed variance.

These assumptions need to be verified using the data. In residual analysis, we typically create two types of plots:

1. a plot of r_i with respect to x_i or $\hat{y}_i$. This allows us to compare the distribution of the noise at different values of x_i.
2. a histogram of r_i. This allows us to explore the distribution of the noise independent of x_i or $\hat{y}_i$.

Residual Analysis





Lecture Outline

How well do we know $\hat{f}$

The confidence intervals of our $\hat{f}$

- **Multi-linear Regression**
  - Brute Force
  - Exact method
  - Gradient Descent
- Polynomial Regression

Polynomial Regression

The simplest non-linear model we can consider, for a response *Y* and a predictor *X*, is a polynomial model of degree *M*,

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \ldots + \beta_M x^M + \epsilon.$$

Just as in the case of linear regression with cross terms, polynomial regression is a special case of linear regression - we treat each x^m as a separate predictor. Thus, we can write

$$\mathbf{Y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}, \qquad \mathbf{X} = \begin{pmatrix} 1 & x_1^1 & \ldots & x_1^M \\ 1 & x_2^1 & \ldots & x_2^M \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & \ldots & x_n^M \end{pmatrix}, \qquad \boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_M \end{pmatrix}.$$

Polynomial Regression

Again, minimizing the MSE using vector calculus yields,

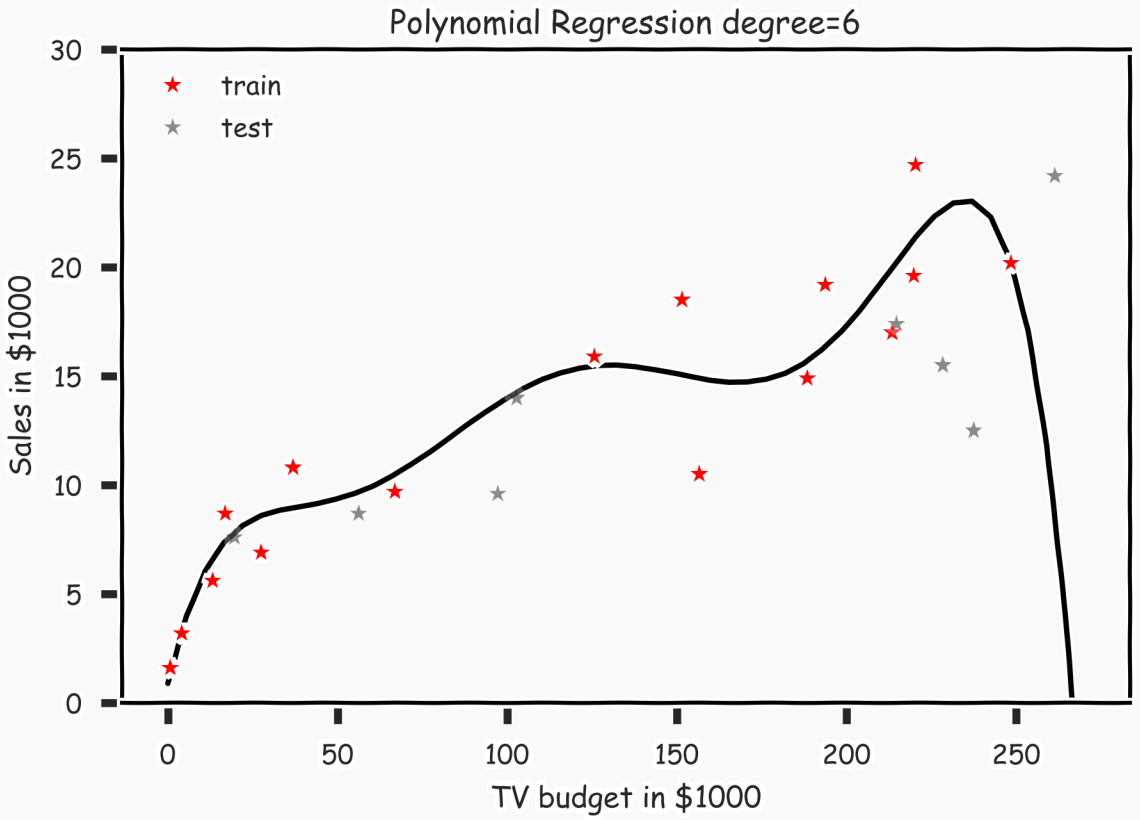
$$\widehat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \operatorname{MSE}(\boldsymbol{\beta}) = \left(\mathbf{X}^\top \mathbf{X}\right)^{-1} \mathbf{X}^\top \mathbf{Y}.$$

Polynomial Regression (cont)

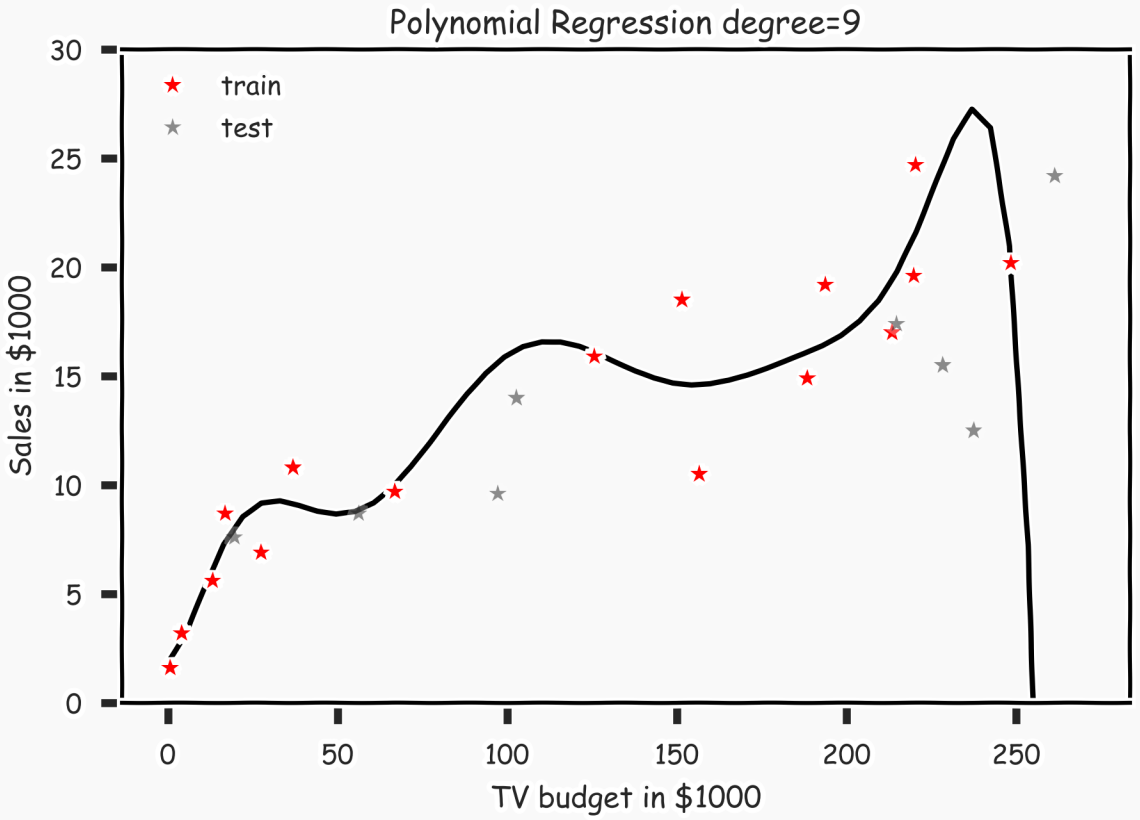
Polynomial Regression (cont)

Polynomial Regression (cont)

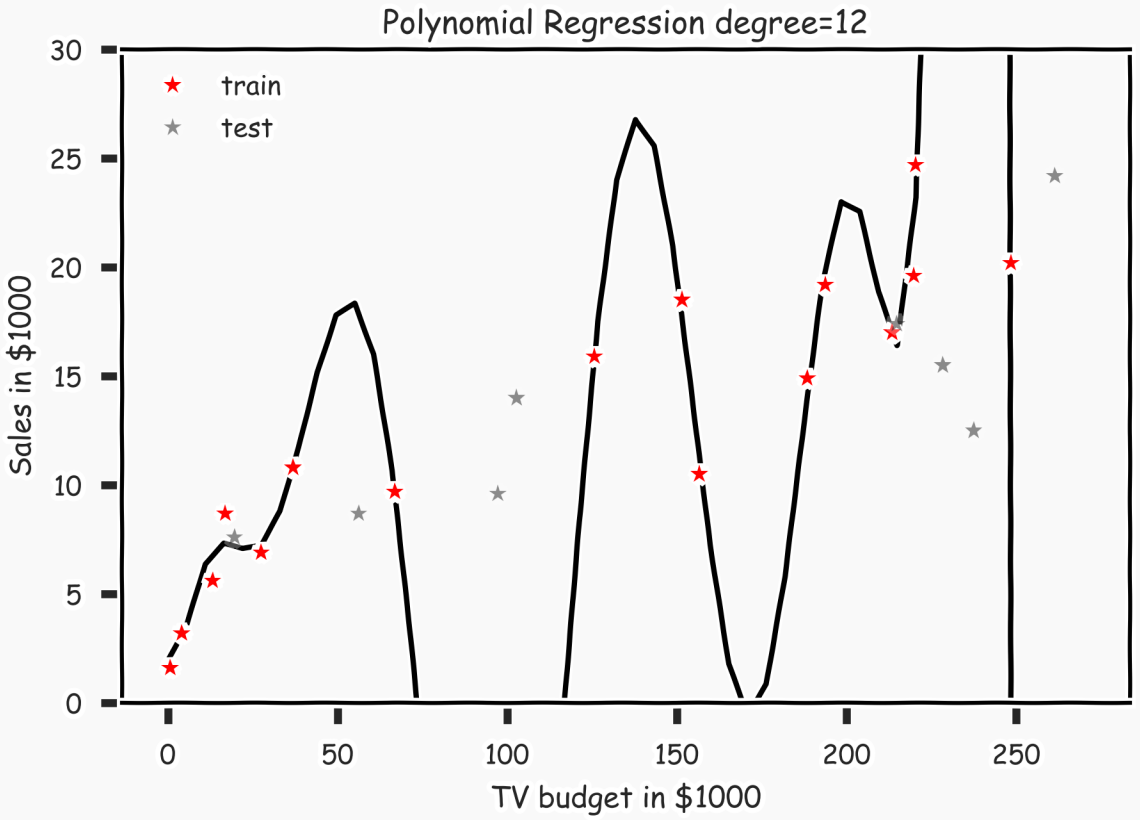
Polynomial Regression (cont)



Polynomial Regression (cont)



Polynomial Regression (cont)



Overfitting

In statistics, **overfitting** is "the production of an analysis that corresponds too closely or exactly to a particular set of data, and may therefore fail to fit additional data or predict future observations reliably”

More on this next week

Summary

How well do we know $\hat{f}$

The confidence intervals of our $\hat{f}$

- Multi-linear Regression
  - Formulate it in Linear Algebra
  - Categorical Variables
- Interaction terms
- Polynomial Regression
  - Linear Algebra Formulation