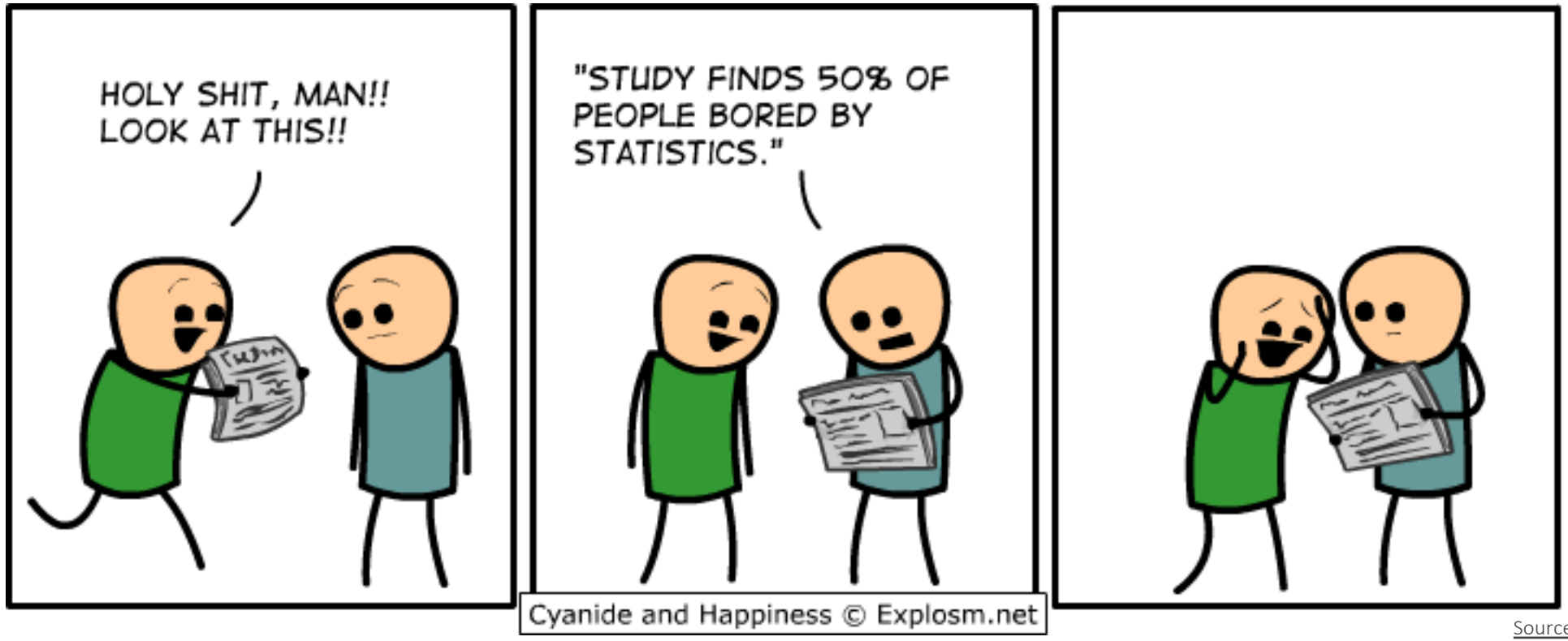
Introduction to *Urban* Data Science

Anatomy of ML

(EPA1316A)

Lecture 10

Trivik Verma



Source: Cyanide and Happiness

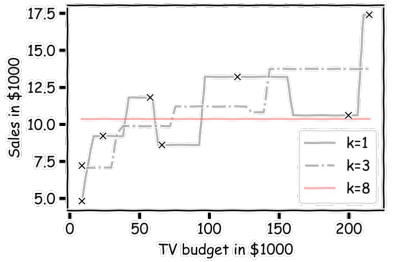
Last Time

- Machine Learning
- Predicting a Variable
- Error evaluation
- Model comparison
- Fitness of models

Today

- Linear models
- Estimate of the regression coefficients
- Model evaluation
- Interpretation

Linear Models



Note that in building our kNN model for prediction, we did not compute a closed form for $\hat{f}$.

What if we ask the question:

"how much more sales do we expect if we double the TV advertising budget?"

Alternatively, we can build a model by first assuming a simple form of f:

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

Linear Regression

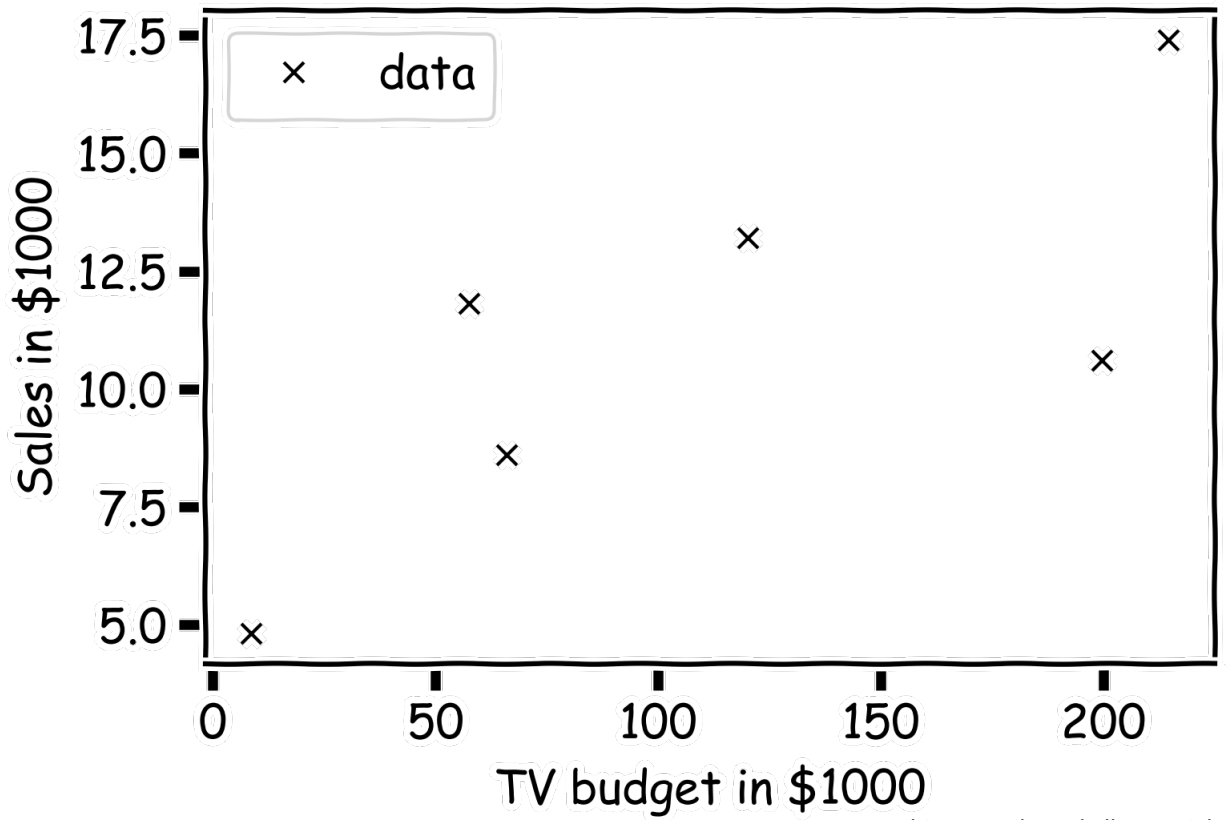
… then it follows that our estimate is:

$$\widehat{Y} = \widehat{f}(X) = \widehat{\beta_1} X + \widehat{\beta_0}$$

where $\hat{\beta}_1$ and $\hat{\beta}_0$ are **estimates** of β_1 and β_0 respectively, that we compute using observations.

Estimate of the regression coefficients

For a given data set



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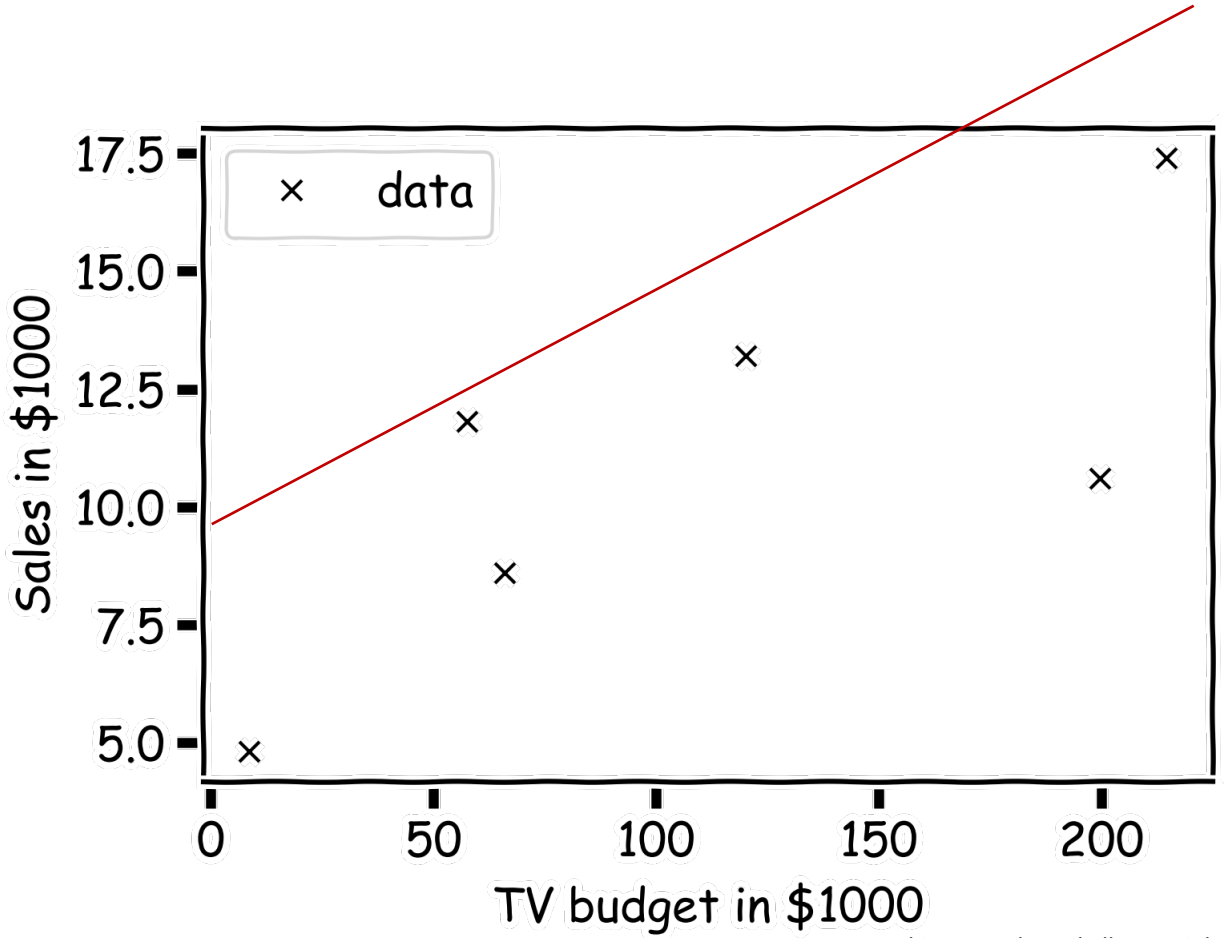
Estimate of the regression coefficients (cont)

Is this line good?



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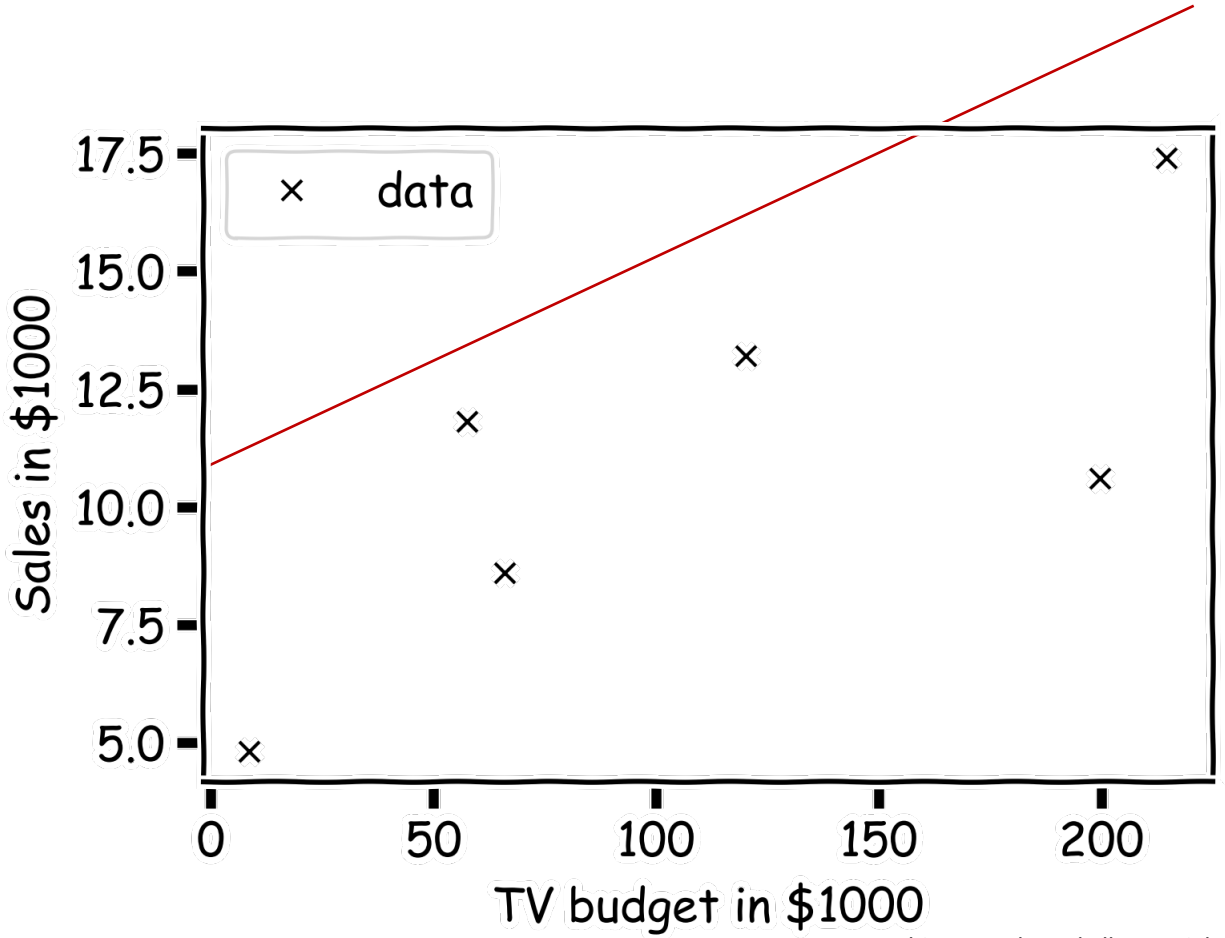
Estimate of the regression coefficients (cont)

Maybe this one?



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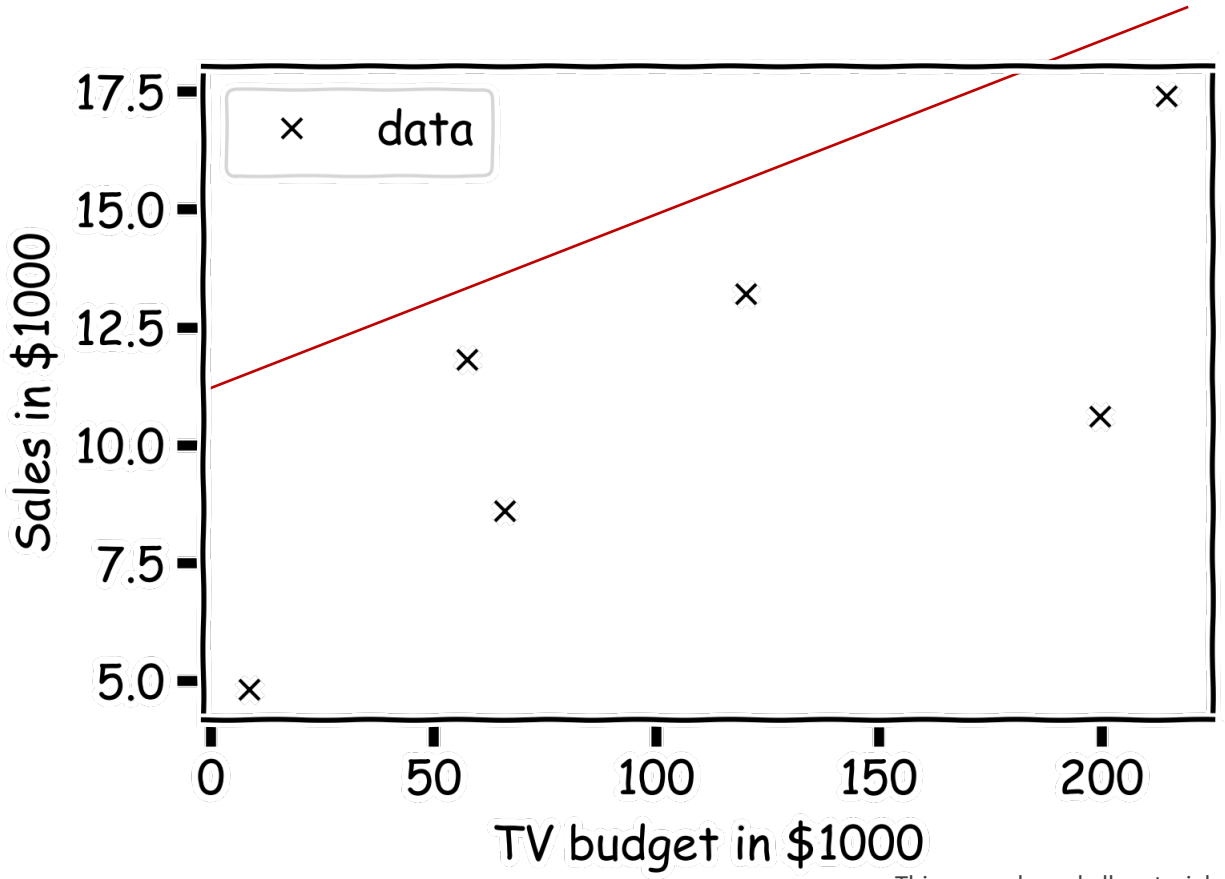
Estimate of the regression coefficients (cont)

Or this one?



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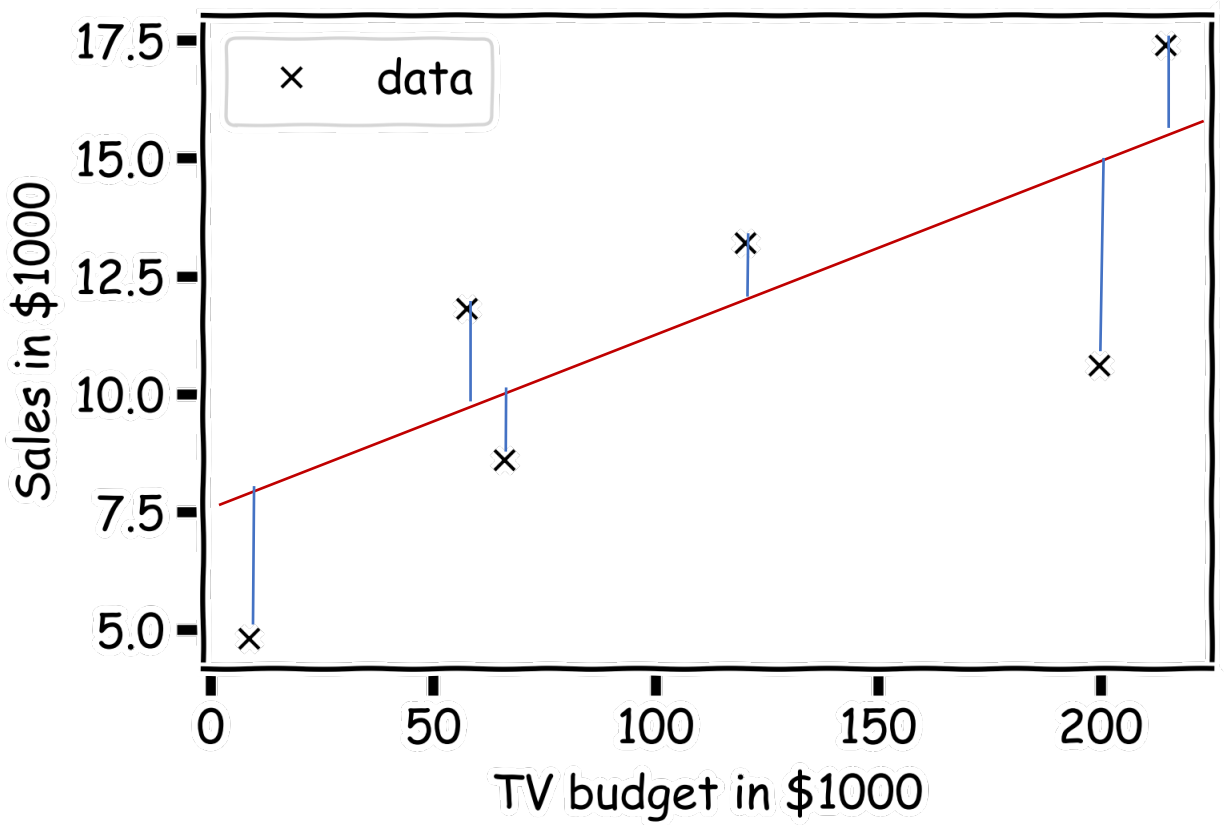
Estimate of the regression coefficients (cont)

Question: Which line is the best?

For each observation (x_n, y_n), the absolute residual is calculating the residuals $r_i = |y_i - \hat{y}_i|$.



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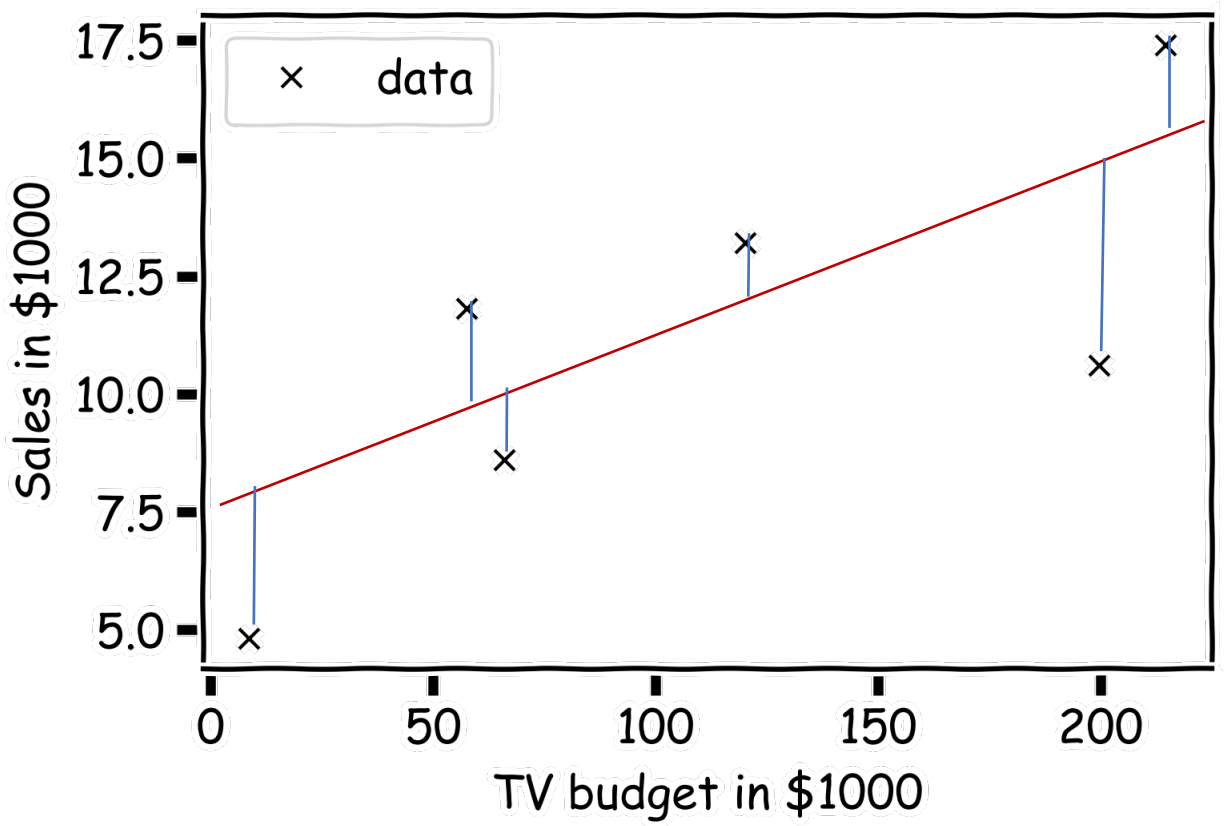
Loss Function: Aggregate Residuals

How do we aggregate residuals across the entire dataset?



1. Max Absolute Error
2. Mean Absolute Error
3. Mean Squared Error

Estimate of the regression coefficients (cont)

- Again we use MSE as our **loss function**,

$$L(\beta_0, \beta_1) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \widehat{y}_i)^2 = \frac{1}{n}\sum_{i=1}^{n}[y_i - (\beta_1 X + \beta_0)]^2 .$$

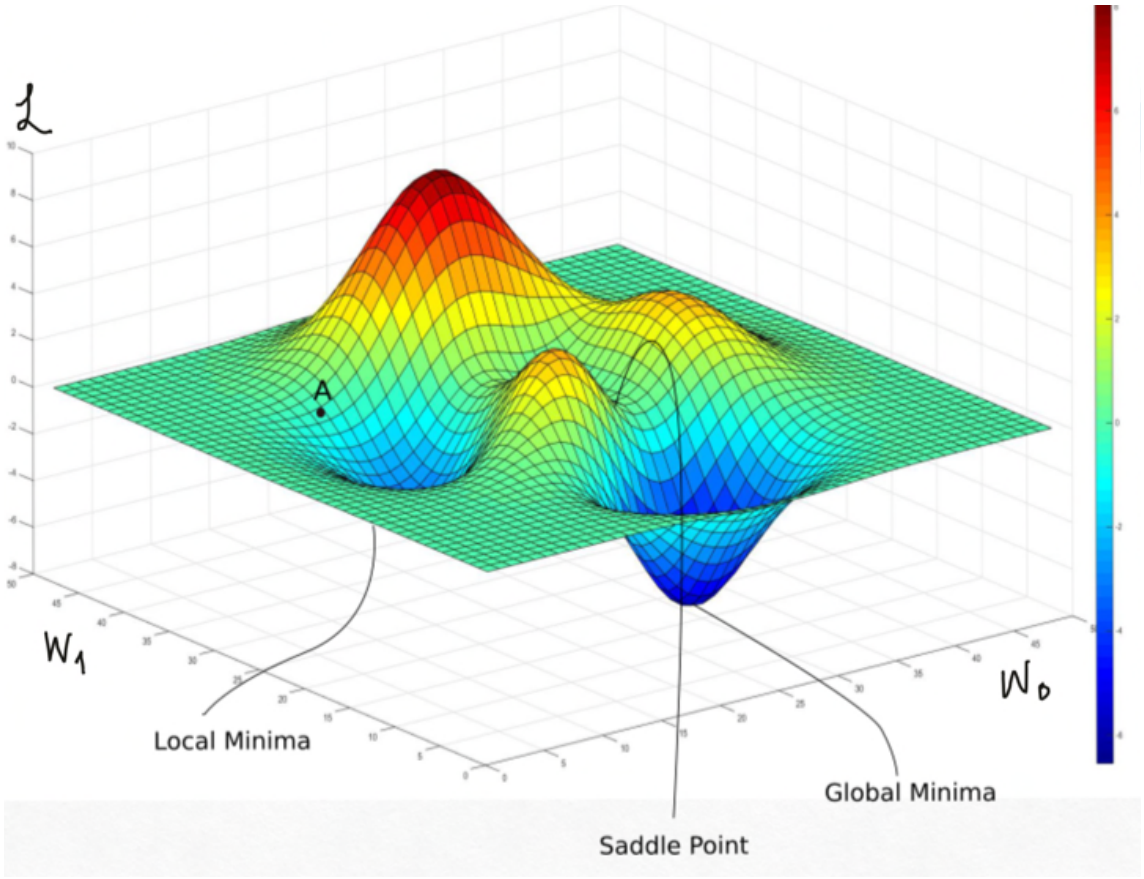
- We choose $\hat{\beta}_1$ and $\hat{\beta}_0$ in order to minimize the predictive errors made by our model, i.e. minimize our loss function.
- Then the optimal values for $\hat{\beta}_0$ and $\hat{\beta}_1$ should be:

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

WE CALL THIS **FITTING** OR **TRAINING** THE MODEL

Optimization

How does one minimize a loss function?



The global minima or maxima of $L(\beta_0, \beta_1)$ must occur at a point where the gradient (slope)

$$\nabla L = \left[\frac{\partial L}{\partial \beta_0}, \frac{\partial L}{\partial \beta_1}\right] = 0$$

- Brute Force: Try every combination
- Exact: Solve the above equation
- Greedy Algorithm: Gradient Descent

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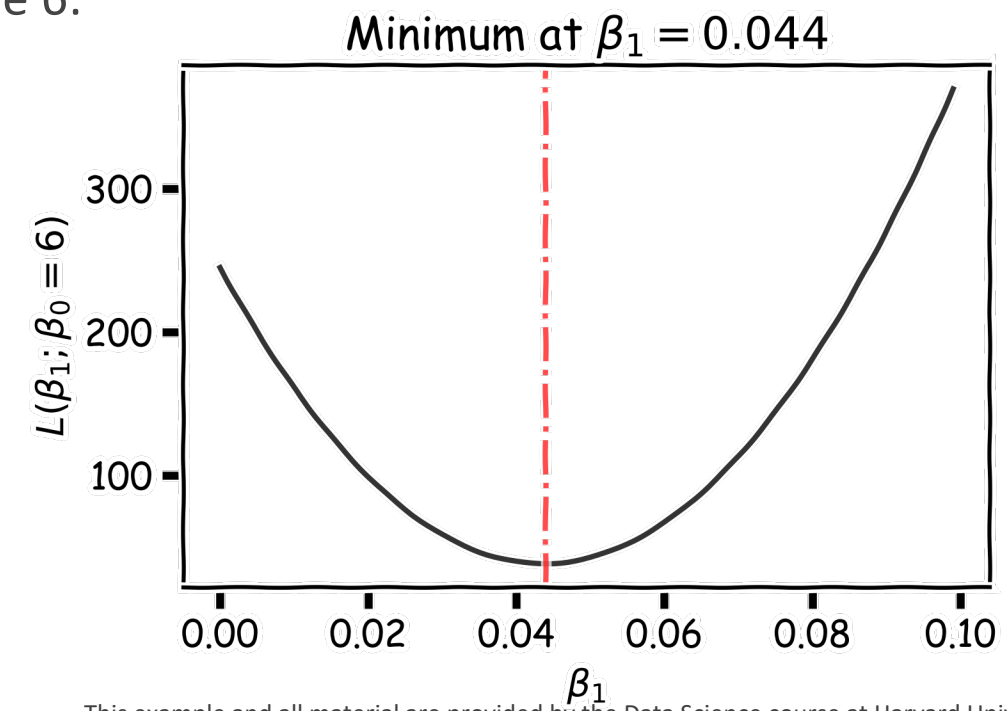
Optimization: Estimate of the regression coefficients

Brute force

- A way to estimate $\text{argmin}_{\beta_0,\beta_1} L$ is to calculate the loss function for every possible β_0 and β_1. Then select the β_0 and β_1 where the loss function is minimum.
- E.g. the loss function for different β_1 when β_0 is fixed to be 6:

Very **computationally expensive** with many coefficients



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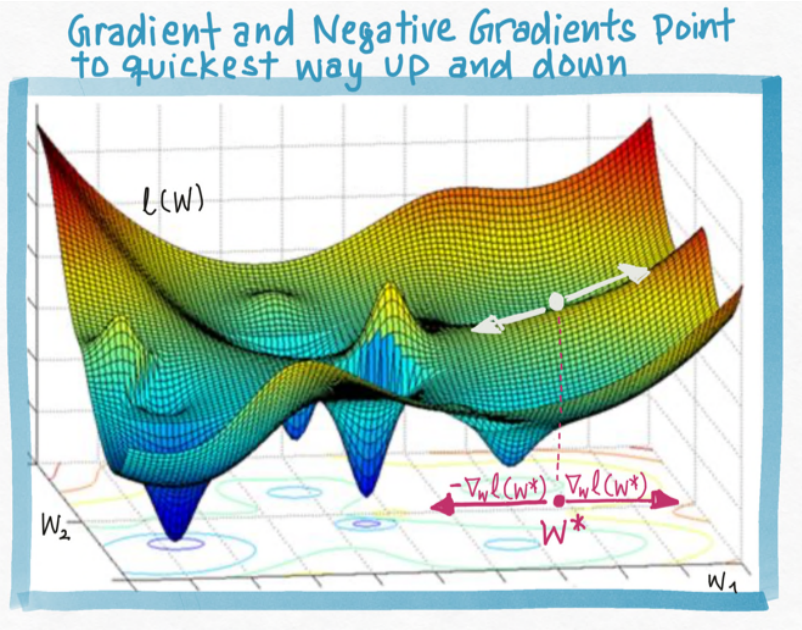
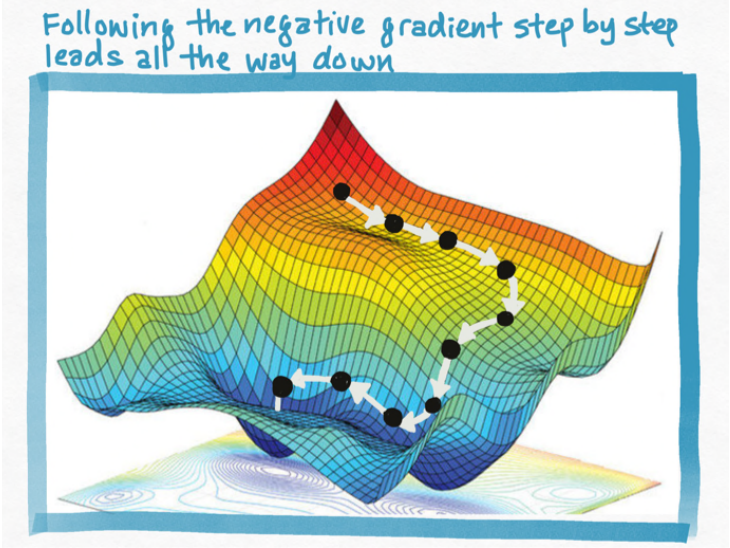
Gradient Descent

- When we can't analytically solve for the stationary points of the gradient, we can still exploit the information in the gradient.
- The gradient ∇L at any point is the direction of the steepest increase. The negative gradient is the direction of steepest decrease.
- By following the –ve gradient, we can eventually find the lowest point.
- This method is called Gradient Descent.





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Estimate of the regression coefficients: analytical solution

Take the gradient of the loss function and find the values of $\hat{\beta}_0$ and $\hat{\beta}_1$ where the gradient is zero: $\nabla L = \left[\frac{\partial L}{\partial \beta_0}, \frac{\partial L}{\partial \beta_1}\right]$=0

This does not usually yield to a close form solution. However, for linear regression this procedure gives us
explicit formulae for $\hat{\beta}_0$ and $\hat{\beta}_1$:

$$\hat{\beta}_1 = \frac{\sum_i (x_i - \overline{x})(y_i - \overline{y})}{\sum_i (x_i - \overline{x})^2}$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

where $\bar{y}$ and $\bar{x}$ are sample means.

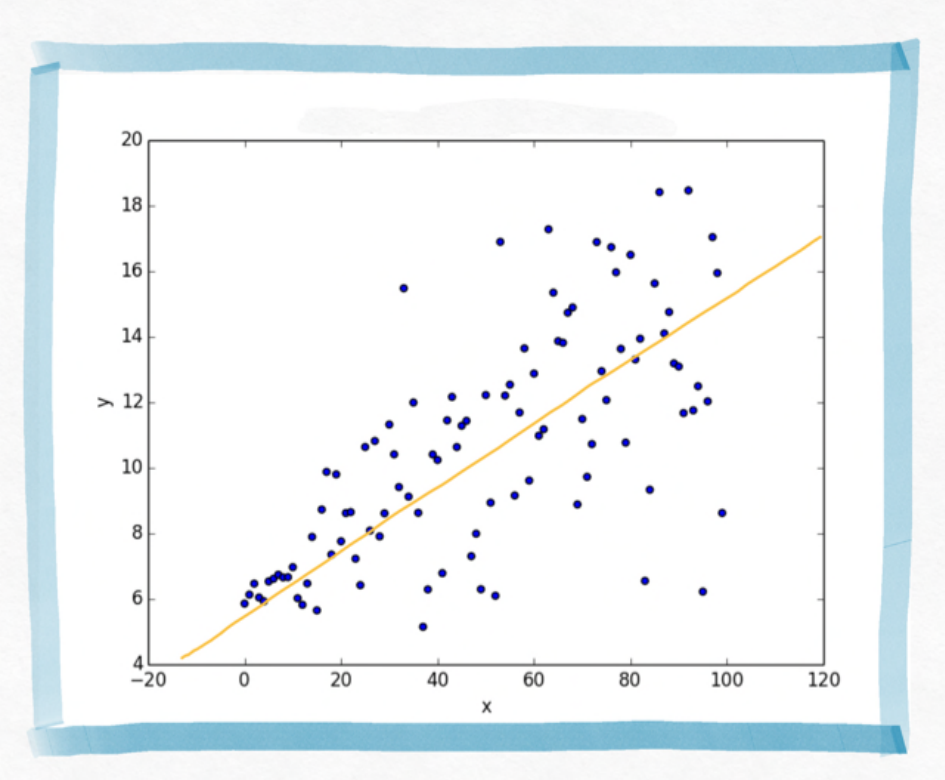
The line:

$$\widehat{Y} = \widehat{\beta}_1 X + \widehat{\beta}_0$$

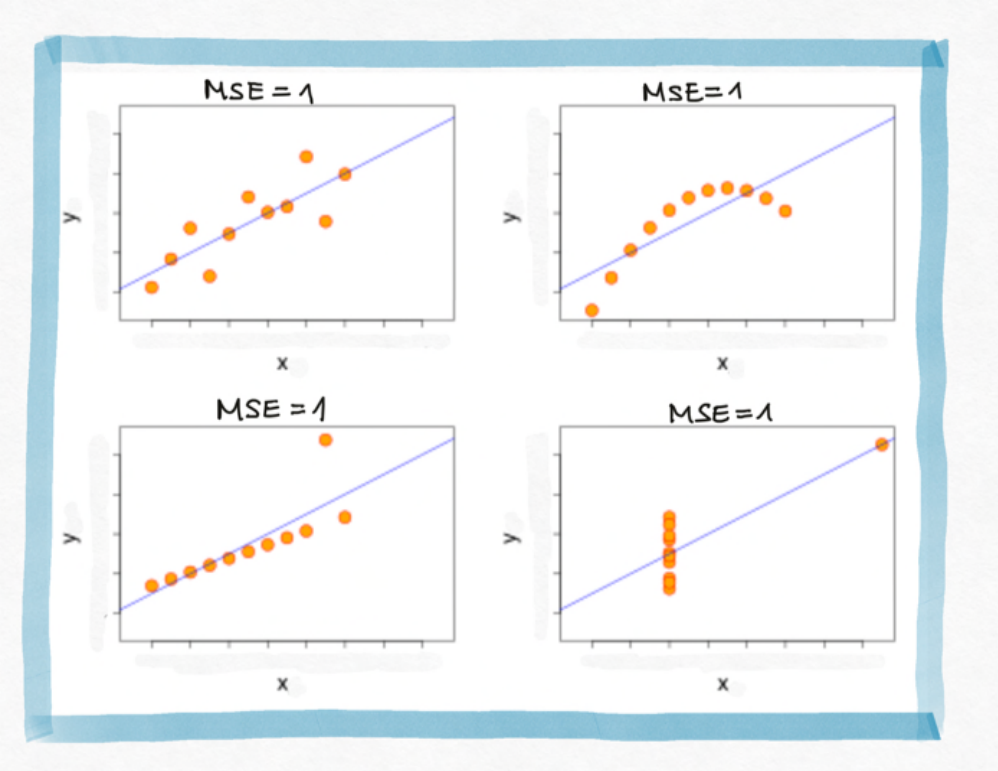
is called the **regression line**.

Evaluation: Training Error

Just because we found the model that minimizes the squared error it doesn't mean that it's a good model. We investigate the R2 but also:



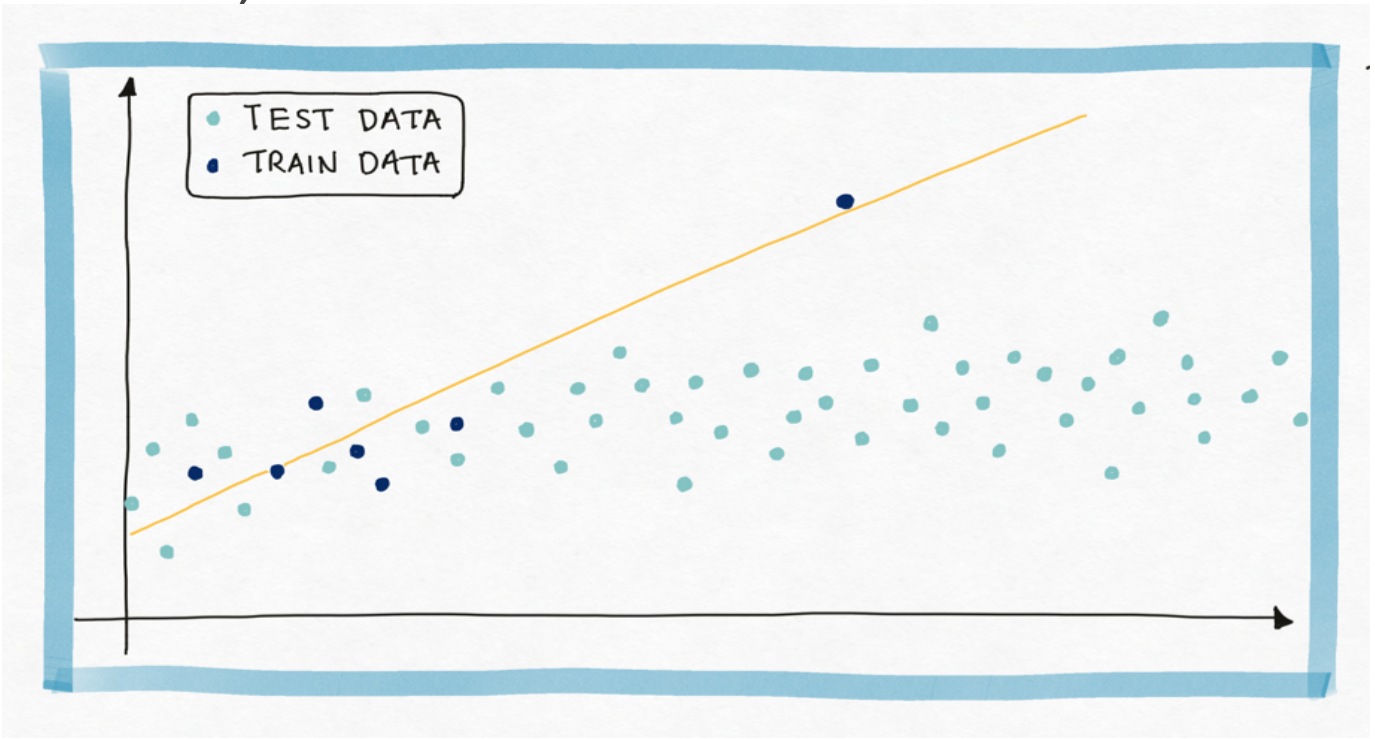
The MSE is high due to noise in the data.



The MSE is high in all four models but the models are not equal.

Evaluation: Test Error

We need to evaluate the fitted model on new data, data that the model did not train on, the test data.



The training MSE here is 2.0 where the test MSE is 12.3.

The training data contains a strange point – **an outlier** – which confuses the model.

Fitting to meaningless patterns in the training is called **overfitting.**

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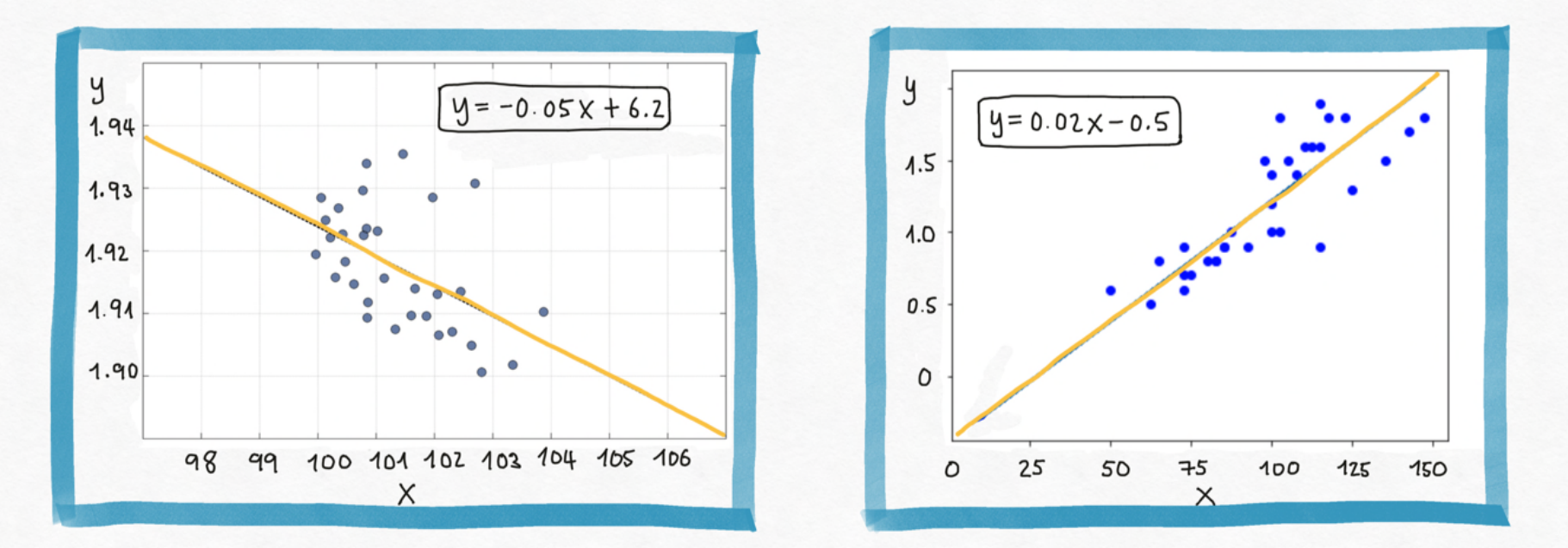
Evaluation: Model Interpretation

For linear models it's important to interpret the parameters



The MSE of this model is very small. But the slope is -0.05. That means the larger the budget the less the sales.

The MSE is very small but the intercept is -0.5 which means that for very small budget we will have negative sales.

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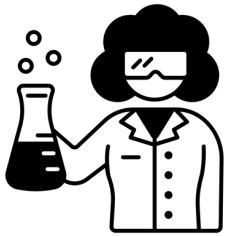
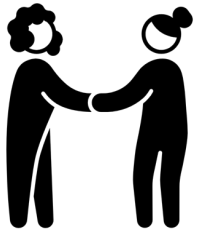
Break

CHILL

WALK



COFFEE OR TEA



MAKE FRIENDS

Icons by Iconathon on The Noun Project

Multiple Linear Regression

If you must 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

X
predictors
features
covariates

Y
outcome
response variable
dependent variable

TV	radio	newspaper	sales
230.1	37.8	69.2	22.1
44.5	39.3	45.1	10.4
17.2	45.9	69.3	9.3
151.5	41.3	58.5	18.5
180.8	10.8	58.4	12.9

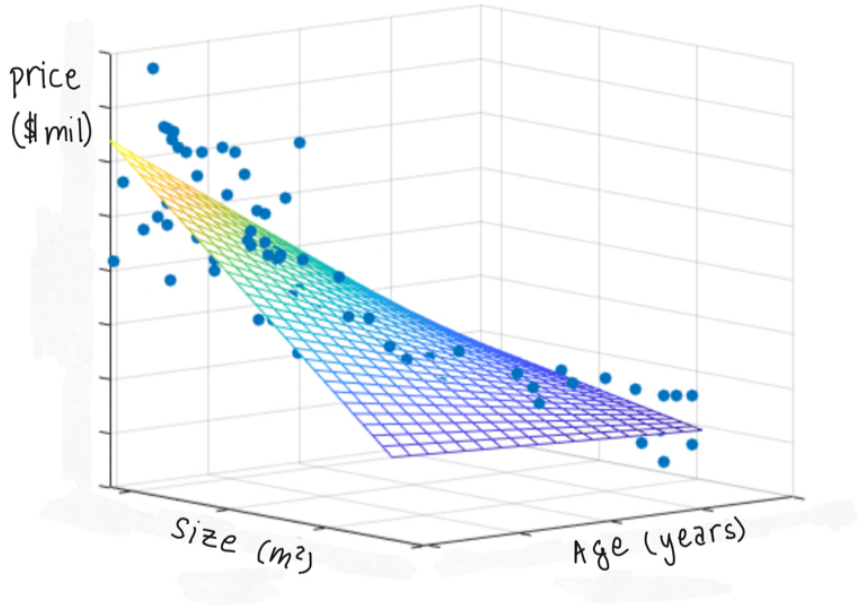
n observations

p predictors

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 last lecture,

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



we can still assume a simple form for f -a multilinear form:

$$f(X_1, \dots, X_J) = \beta_0 + \beta_1 X_1 + \cdots + \beta_J X_J$$

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

$$\hat{f}(X_1, \dots, X_J) = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \cdots + \hat{\beta}_J X_J$$

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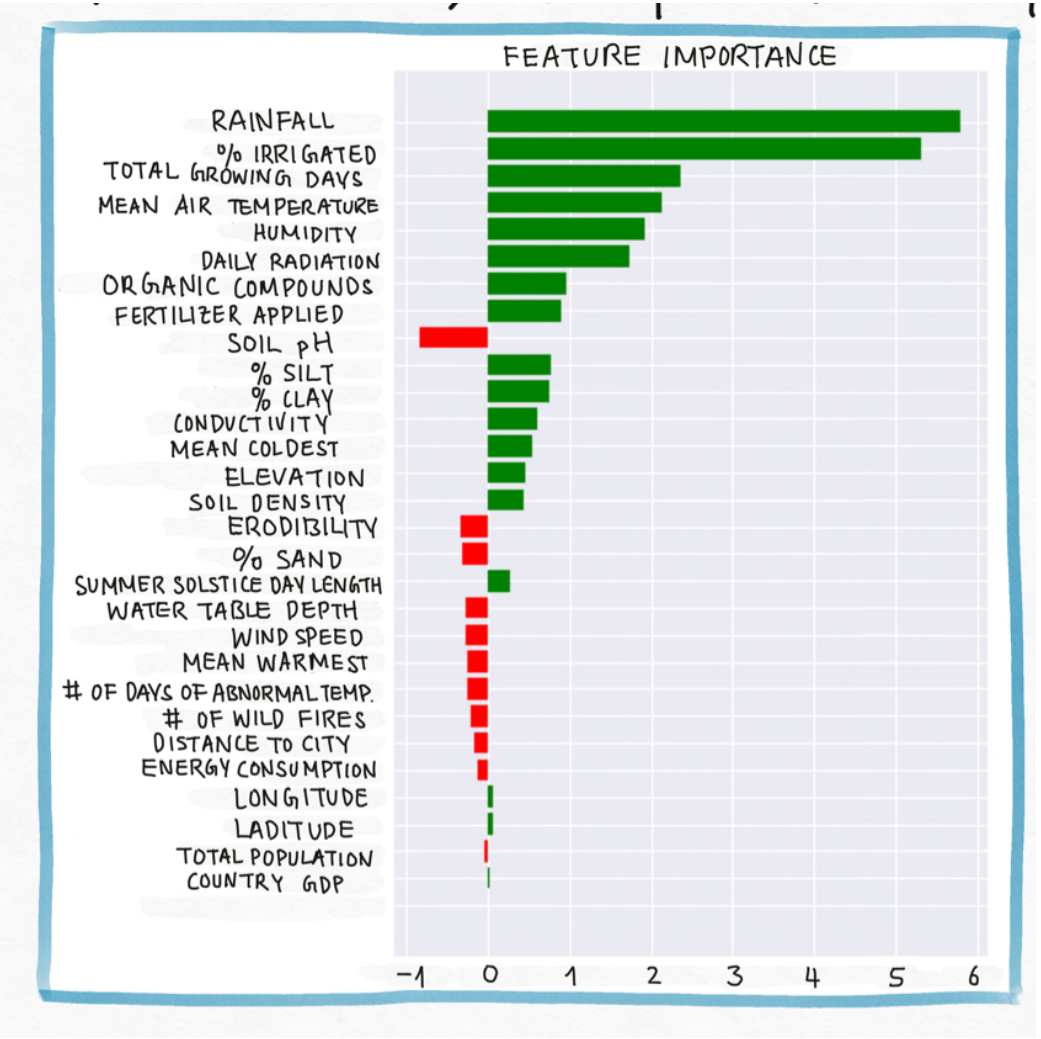
Multilinear Model, example

For our data

$$Sales = \beta_0 + \beta_1 \times TV + \beta_2 \times Radio + \beta_3 \times Newspaper$$

Interpreting multi-linear regression

For linear models, it is easy to interpret the model parameters.



When we have many predictors: $X_1, \ldots, X_J$, there will be many model parameters, $\beta_1, \beta_2, \ldots, \beta_J$.

Looking at the values of β's is impractical, so we visualize these values in a feature importance graph.

The feature importance graph shows which predictors has the most impact on the model's prediction.

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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 several 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

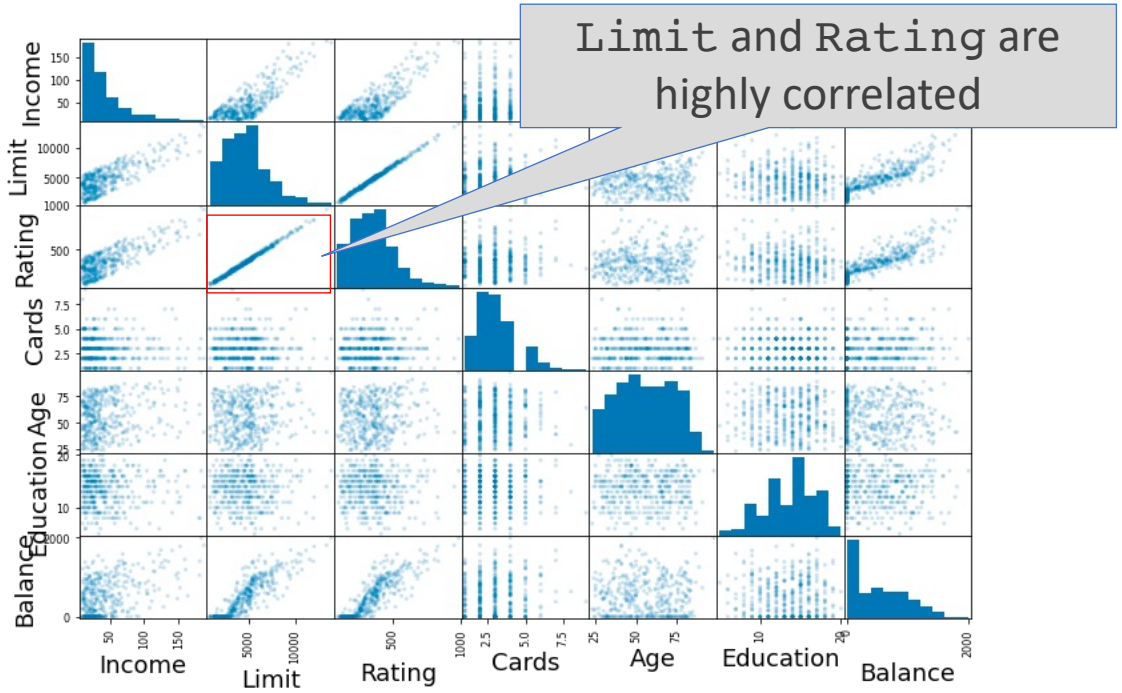
We then use these variables as predictors, the regression equation becomes:

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

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

Collinearity

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



	Columns	Coefficients
0	Income	-7.802001
1	Limit	0.193077
2	Rating	1.102269
3	Cards	17.923274
4	Age	-0.634677
5	Education	-1.115028
6	Gender	10.406651
7	Student	426.469192
8	Married	-7.019100

	Columns	Coefficients
0	Income	-7.770915
1	Rating	3.976119
2	Cards	4.031215
3	Age	-0.669308
4	Education	-0.375954
5	Gender	10.368840
6	Student	417.417484
7	Married	-13.265344

The regression coefficients are not uniquely determined. In turn it hurts the interpretability of the model as then the regression coefficients are not unique and have influences from other features.

Both limit and rating have positive coefficients, but it is hard to understand if the balance is higher because of the rating or is it because of the limit? If we remove limit then we achieve almost the same model performance but the coefficients change.

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Beyond linearity

So far we assumed:

- linear relationship between X and Y
- the residuals $r_i = y_i - \hat{y}_i$ were uncorrelated (taking the average of the square residuals to calculate the MSE implicitly assumed uncorrelated residuals).

These assumptions need to be verified using the data and **visually inspecting the residuals.**

Residual Analysis

If the correct model is not linear then,

$$y = \beta_0 + \beta_1 x + \boldsymbol{\phi}(\boldsymbol{x}) + \epsilon$$

our model assuming linear relationship is:

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

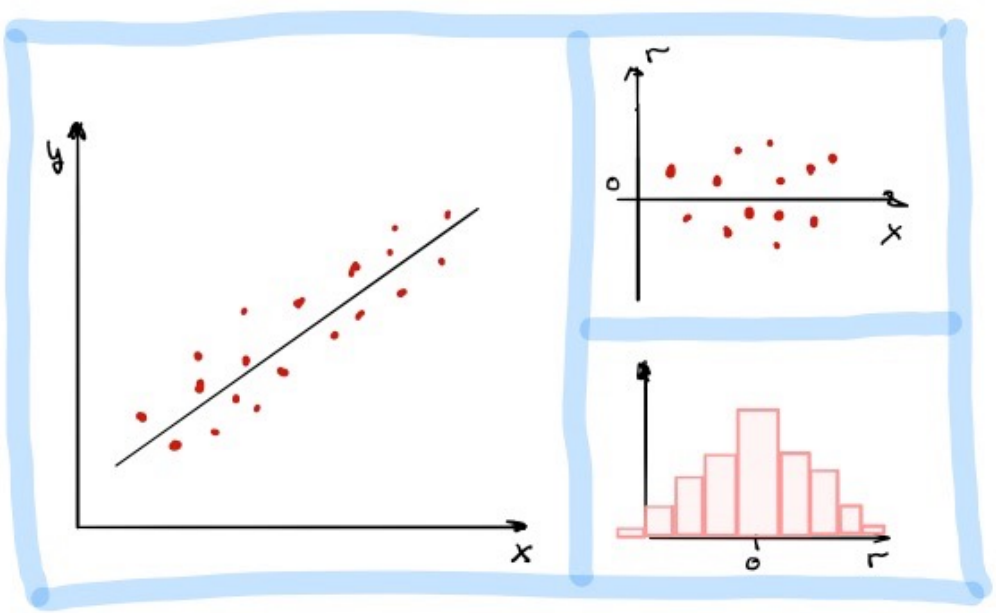
Then the residuals, $r = (y - \hat{y}) = \epsilon + \boldsymbol{\phi}(\boldsymbol{x})$, are not independent of $\boldsymbol{x}$

Residual Analysis

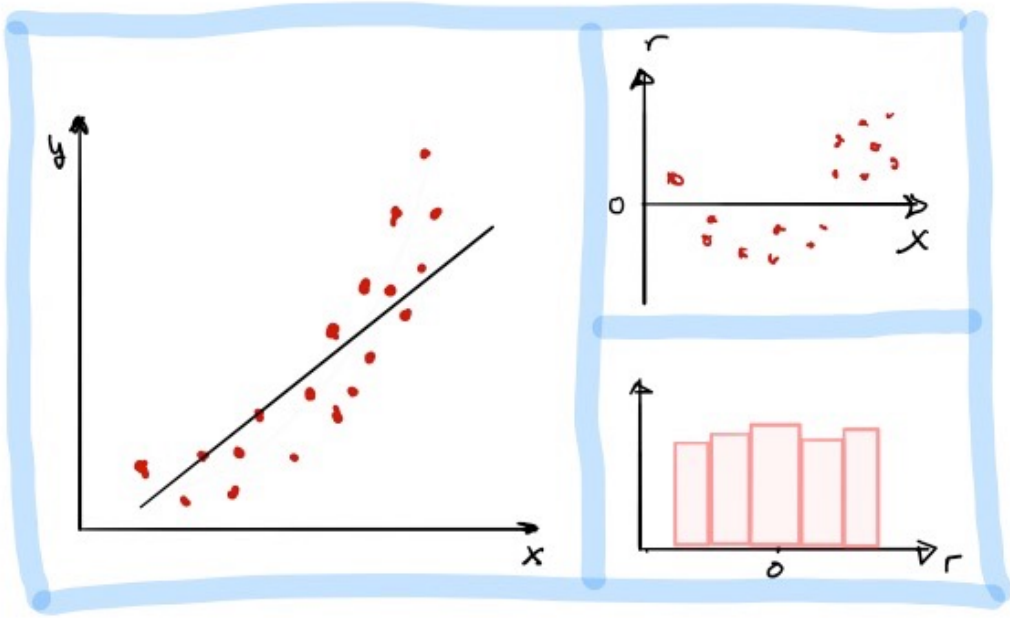
In residual analysis, we typically create two types of plots:

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 or $\hat{y}_i$.
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



Linear assumption is correct. There is no obvious relationship between residuals and *x*. Histogram of residuals is symmetric and normally distributed.



Linear assumption is incorrect. There is an obvious relationship between residuals and *x*. Histogram of residuals is symmetric but not normally distributed.

Note: For multi-regression, we plot the residuals vs predicted values, $\hat{y}$, since there are too many x's and that could wash out the relationship.

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Beyond linearity: **synergy effect** or **interaction effect**

- We also assume that 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.

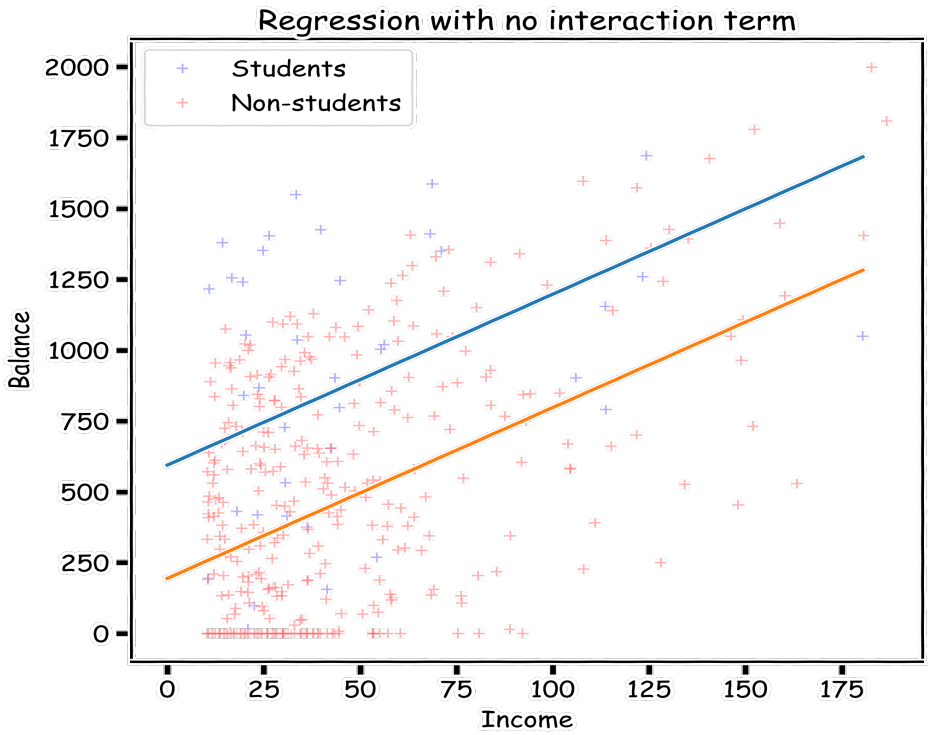
  We change

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

  to:

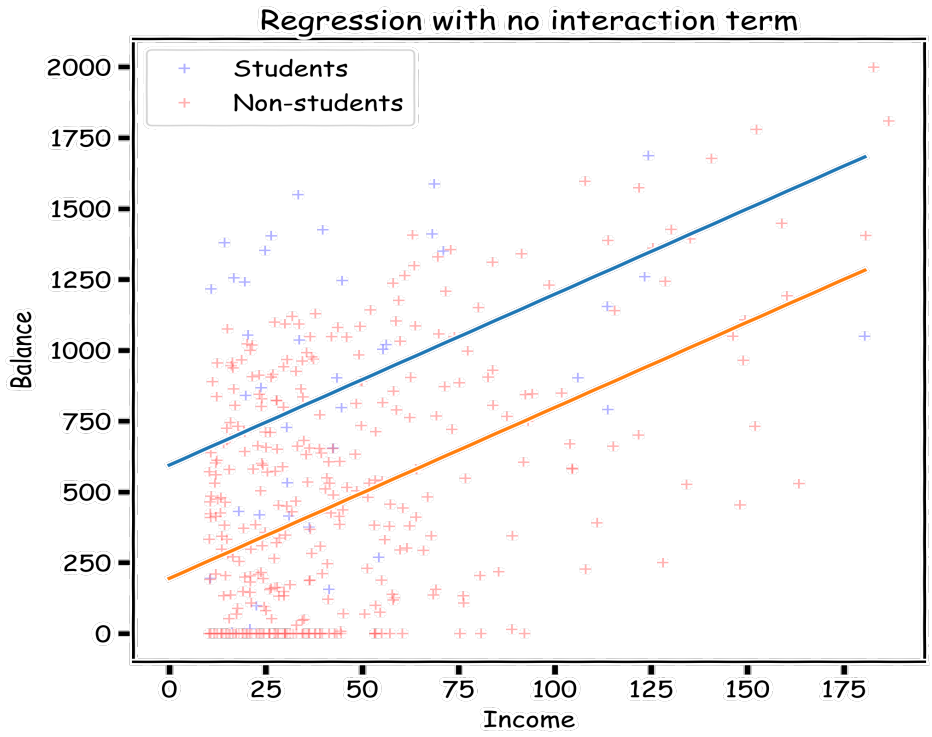
$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \boxed{\beta_3 X_1 X_2} + \epsilon$$

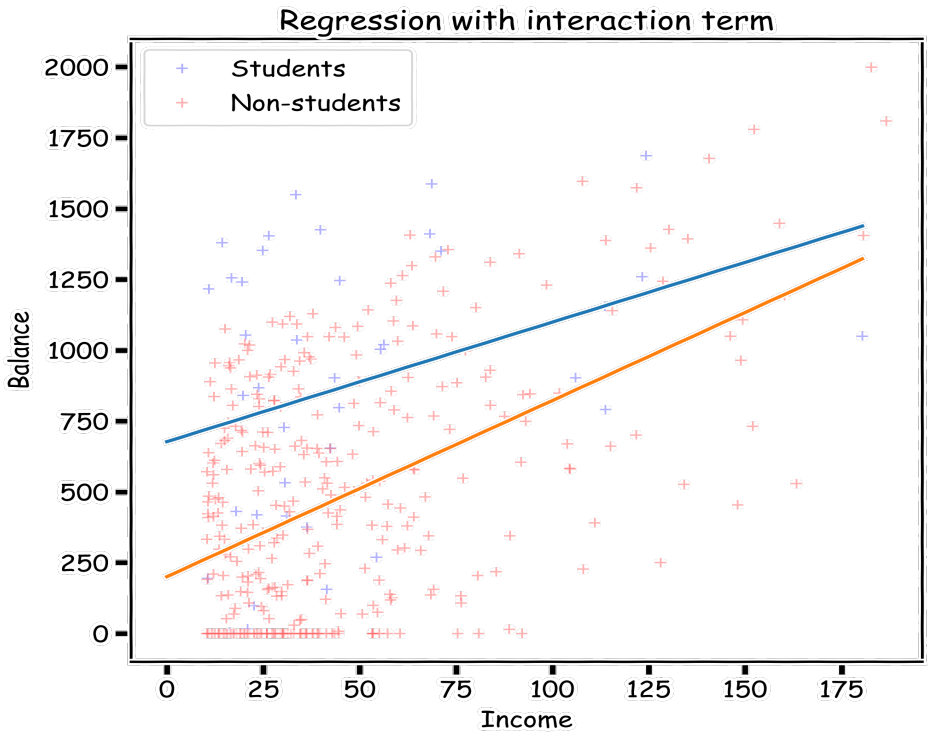
What does it mean?



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

What does it mean?





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

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

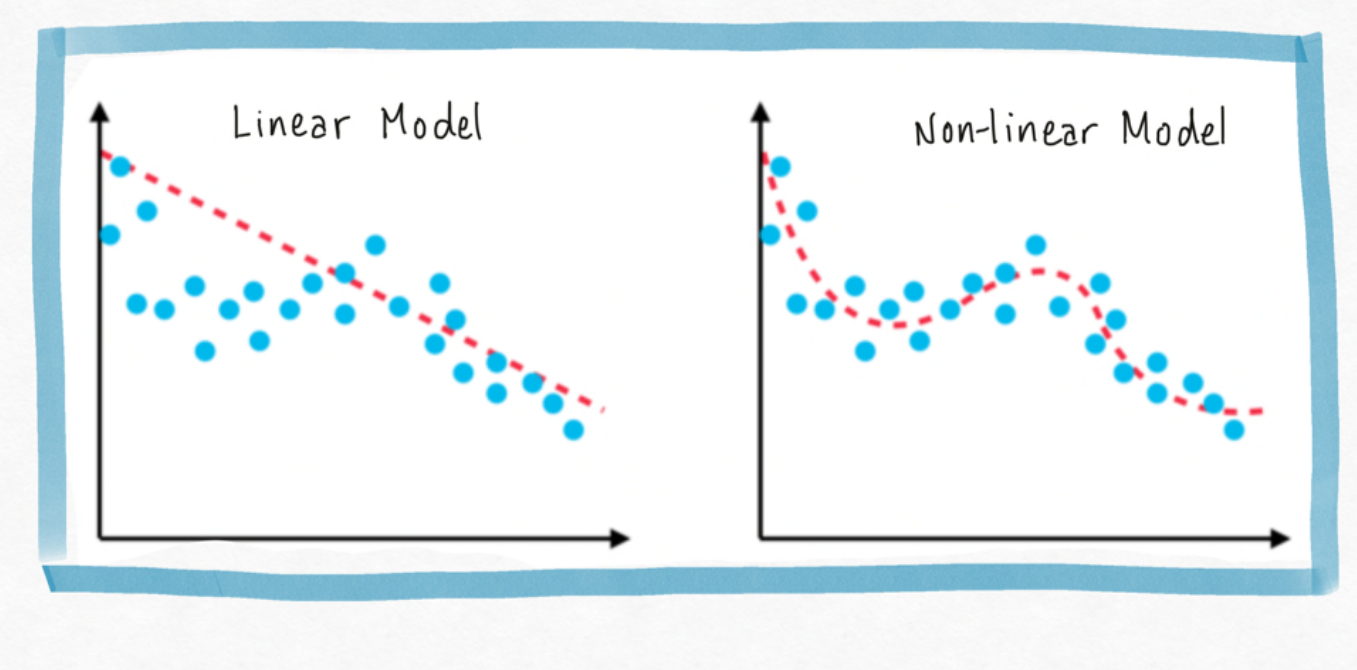
Too many predictors, collinearity and too many interaction terms leads to **OVERFITTING!**

Cartoon on data points & regression analysis involving drug trials, December 13, 2012. (http://www.landers.co.uk).

Polynomial Regression

Fitting non-linear data

Multi-linear models can fit large datasets with many predictors. But the relationship between predictor and target isn't always linear.



We want a model:

$$y = f_\beta(x)$$

Where f is a non-linear function and β is a vector of the parameters of f.

This example and all material are provided by the Data Science course at Harvard University

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*,

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_M x^M$$

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

$$y = \beta_0 + \beta_1 x1 + \beta_2 x2 \quad + \cdots + \beta_M xM$$

This looks a lot like multi-linear regression where the predictors are powers of x!

Model Training

Give a dataset $\{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$, we find the optimal polynomial model:

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_M x^M$$

We transform the data by adding new predictors:

$$\tilde{x} = [1, \tilde{x}_1, \tilde{x}_2, \dots, \tilde{x}_M]$$

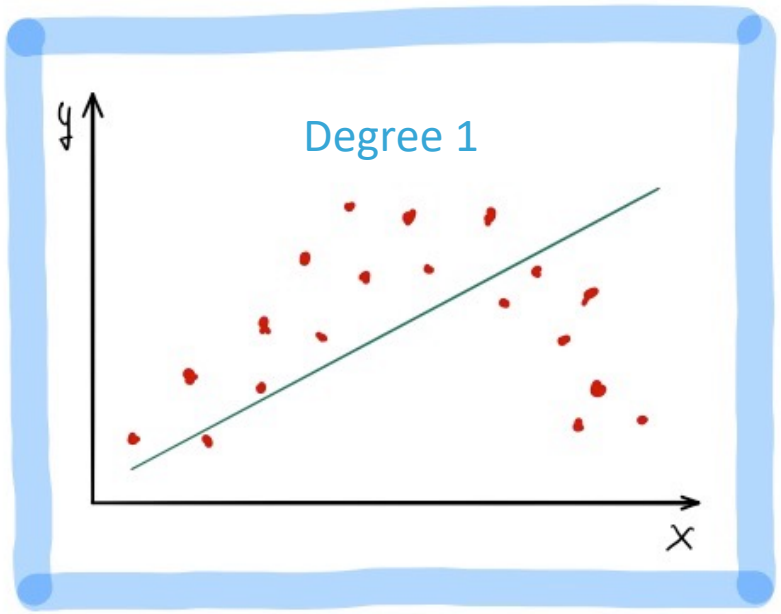
where $\tilde{x}_k = x^k$

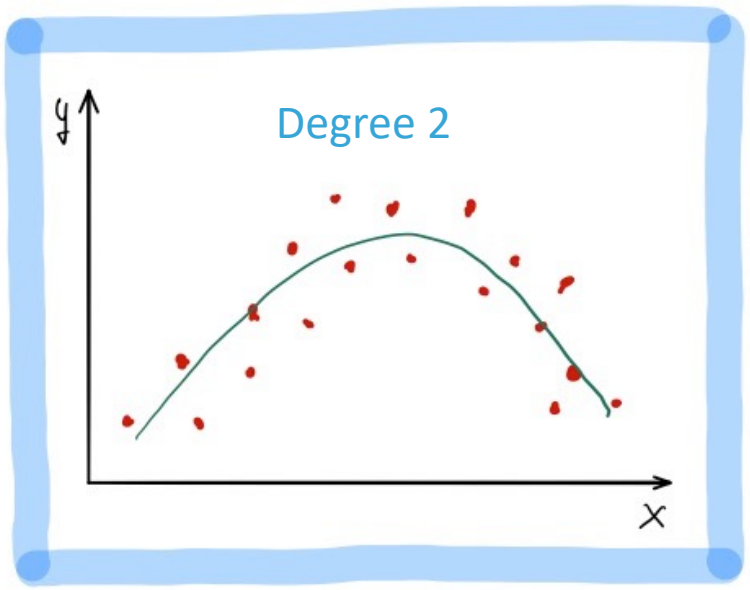
Fit the parameters by minimizing the MSE using vector calculus. As in multi-linear regression:

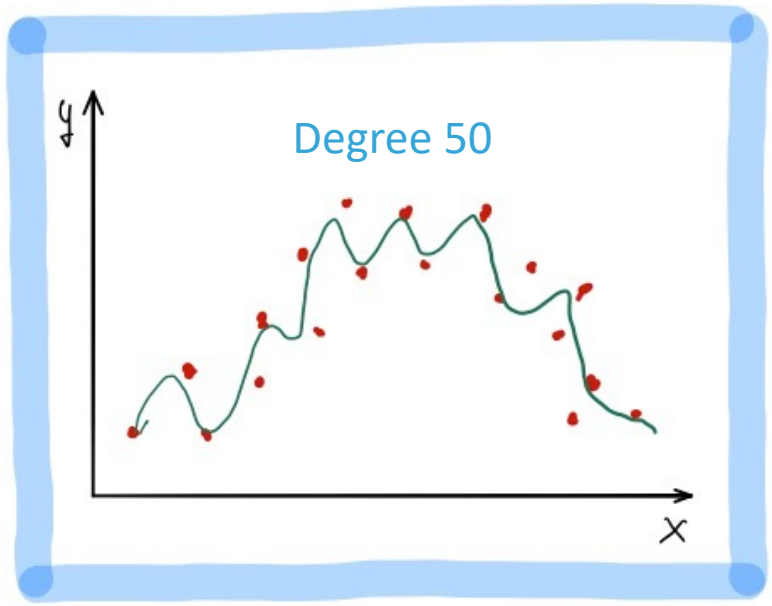
$$y = \beta_0 + \beta_1 \tilde{x}_1 + \beta_2 \tilde{x}_2 + \cdots + \beta_M \tilde{x}_M$$

Polynomial Regression (cont)

Fitting a polynomial model requires choosing a degree.







Underfitting: when the degree is too low, the model cannot fit the trend.

We want a model that fits the trend and ignores the noise.

Overfitting: when the degree is too high, the model fits all the noisy data points.

This example and all material are provided by the Data Science course at Harvard University

Feature Scaling

Do we need to scale out features for polynomial regression?

Linear regression, $Y = X\beta$, is invariant under scaling. If X is called by some number λ then β will be scaled by $\frac{1}{\lambda}$ and MSE will be identical.

However if the range of X is low or large then we run into troubles. Consider a polynomial degree of 20 and the maximum or minimum value of any predictor is large or small. Those numbers to the 20th power will be problematic.

- It is always a good idea to scale X when considering polynomial regression:

$$X^{norm} = \frac{X - \bar{X}}{\sigma_X}$$

Note: sklearn's `StandardScaler()` can do this.

High degree of polynomial leads to **OVERFITTING!**

Recapitulation

- Consider collinearity
- Consider interaction effects
- Consider residual analysis
- Too many predictors, collinearity and too many interaction terms leads to **OVERFITTING!**
- High degree of polynomial leads to **OVERFITTING!**

For next class..

Finish Labs to practice programming

Complete Homework and review your peers' work

Check Assignment contents and due date

See "To do before class" for next lecture (~ 1 hour of self study)

Read paper for **Discussion** session before next week (~ 1 hour)

Post questions on the **Discussion** forum on Brightspace