

# Lecture Outline

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Announcements

Data

Statistical Modeling

Regression vs. Classification

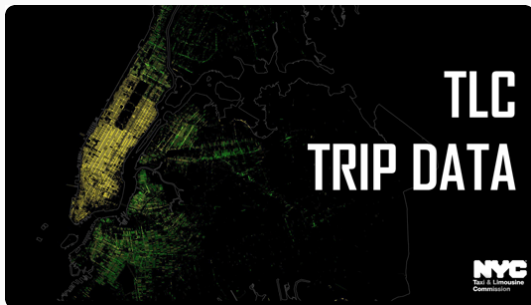
Error, Loss Functions

Model I: k-Nearest Neighbors

Model II: Linear Regression

Evaluating Model

Comparison of Two Models



The yellow and green taxi trip records include fields capturing pick-up and drop-off dates/times, pick-up and drop-off locations, trip distances, itemized fares, rate types, payment types, and driver-reported passenger counts. The data used were collected and provided to the NYC Taxi and Limousine Commission (TLC).

# NYC Car Hire Data

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More details on the data can be found here:

`http://www.nyc.gov/html/tlc/html/about/trip\_record\_data.shtml`

Notebook:

`https://github.com/cs109/a-2017/blob/master/Lectures/Lecture4-IntroRegression/Lecture4\_Notebook.ipynb`

# Statistical Modeling

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# Predicting a Variable

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Let's image a scenario where we'd like to predict one variable using another (or a set of other) variables.

## **Examples:**

- ▶ Predicting the amount of view a YouTube video will get next week based on video length, the date it was posted, previous number of views, etc.
- ▶ Predicting which movies a Netflix user will rate highly based on their previous movie ratings, demographic data etc.
- ▶ Predicting the expected cab fare in New York City based on time of year, location of pickup, weather conditions etc.

## Outcome vs. Predictor Variables

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There is an asymmetry in many of these problems: the variable we'd like to predict may be more difficult to measure, is more important than the other(s), or may be directly or indirectly influenced by the values of the other variable(s).

Thus, we'd like to define two categories of variables: variables whose value we want to predict and variables whose values we use to make our prediction.

## Definition

Suppose we are observing  $p + 1$  number variables and we are making  $n$  sets observations. We call

- ▶ the variable we'd like to predict the **outcome** or **response variable**; typically, we denote this variable by  $Y$  and the individual measurements  $y_i$ .
- ▶ the variables we use in making the predictions the **features** or **predictor variables**; typically, we denote these variables by  $X = (X_1, \dots, X_p)$  and the individual measurements  $x_{i,j}$ .

**Note:**  $i$  indexes the observation ( $i = 1, 2, \dots, n$ ) and  $j$  indexes the value of the  $j$ -th predictor variable ( $j = 1, 2, \dots, p$ ).

## True vs. Statistical Model

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We will assume that the response variable,  $Y$ , relates to the predictors,  $X$ , through some unknown function expressed generally as:

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

Here,

- ▶  $f$  is the unknown function expressing an underlying rule for relating  $Y$  to  $X$ ,
- ▶  $\epsilon$  is random amount (unrelated to  $X$ ) that  $Y$  differs from the rule  $f(X)$

A **statistical model** is any algorithm that estimates  $f$ . We denote the estimated function as  $\hat{f}$ .



## Prediction vs. Estimation

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For some problems, what's important is obtaining  $\hat{f}$ , our estimate of  $f$ . These are called **inference** problems.

When we use a set of measurements of predictors,  $(x_{i,1}, \dots, x_{i,p})$ , in an observation to predict a value for the response variable, we denote the **predicted value** by  $\hat{y}_i$ ,

$$\hat{y}_i = \hat{f}(x_{i,1}, \dots, x_{i,p}).$$

For some problems, we don't care about the specific form  $\hat{f}$ , we just want to make our prediction  $\hat{y}_i$  as close to the observed value  $y_i$  as possible. These are called **prediction problems**.

We'll see that some algorithms are better suited for inference and others for prediction.

## Regression vs. Classification

# Outcome Variables

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There are two main types of prediction problems we will see this semester:

- ▶ **Regression problems** are ones with a quantitative response variable.  
**Example:** Predicting the number of taxicab pick-ups in New York.
- ▶ **Classification problems** are ones with a categorical response variable.  
**Example:** Predicting whether or not a Netflix user will like a particular movie.

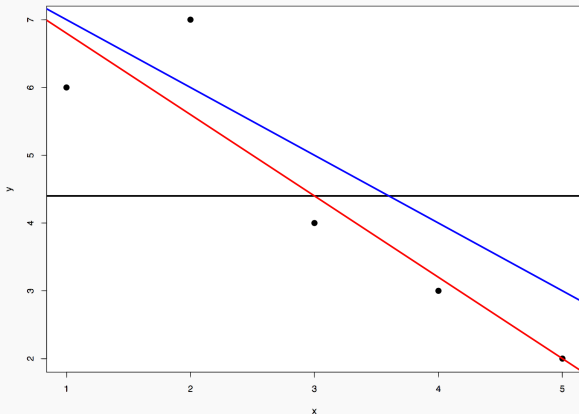
This distinction is important, as each type of problem may require it's own specialized algorithms along with metrics measuring effectiveness.

## Error, Loss Functions

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# Line of Best Fit

Which of the following linear models is the best? How do you know?



# Using Loss Functions

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Loss functions are used to choose a suitable estimate  $\hat{f}$  of  $f$ .

A statistical modeling approach is often an algorithm that:

- ▶ assumes some mathematical form for  $f$ , and hence for  $\hat{f}$ ,
- ▶ then chooses values for the unknown parameters of  $\hat{f}$  so that the loss function is minimized on the set of observations

# Error & Loss Functions

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In order to quantify how well a model performs, we define a **loss** or **error function**.

A common loss function for quantitative outcomes is the **Mean Squared Error (MSE)**:

$$MSE = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

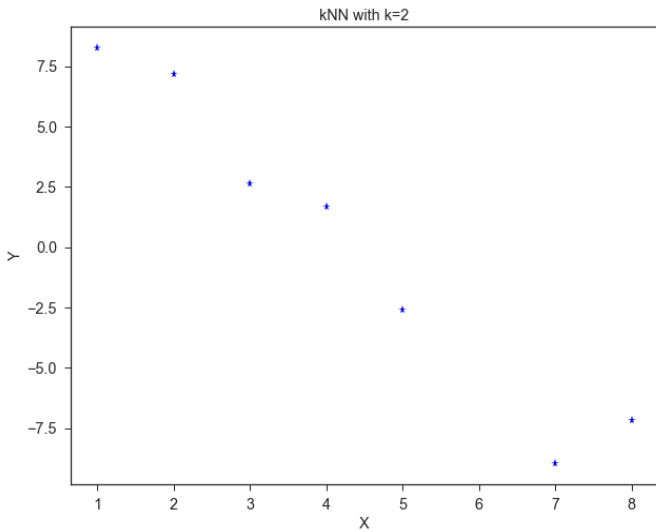
The quantity  $|y_i - \hat{y}_i|$  is called a **residual** and measures the error at the  $i$ -th prediction.

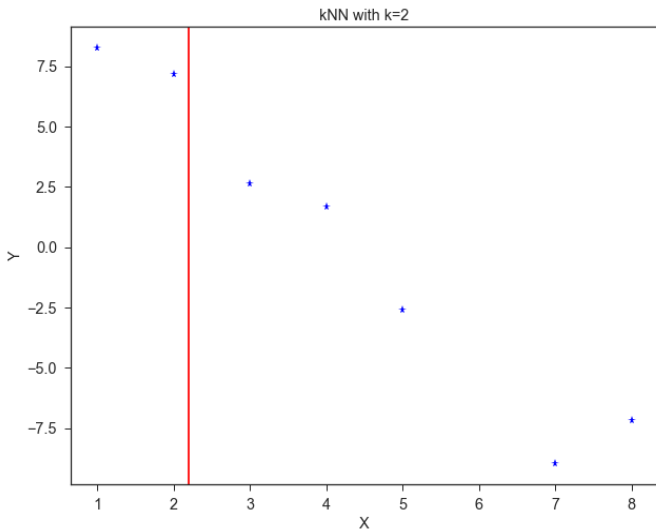
**Caution:** The MSE is by no means the only valid (or the best) loss function!

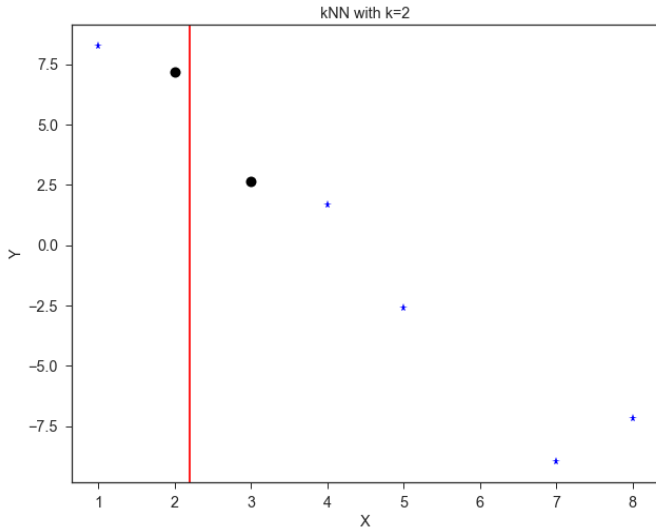
**Question:** What would be an intuitive loss function for predicting categorical outcomes?

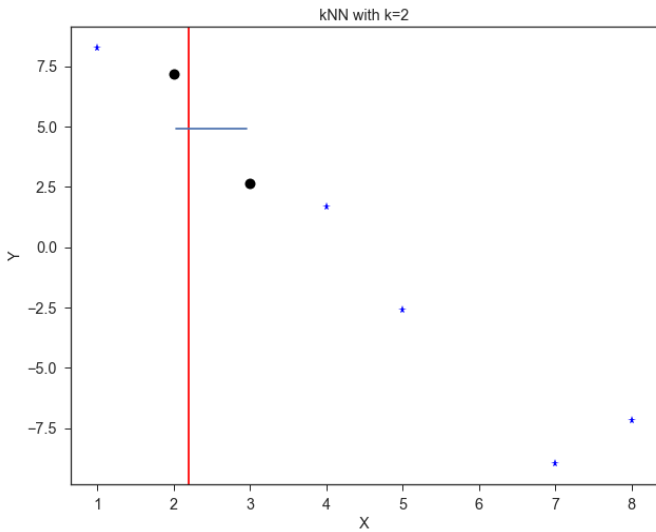
## Model I: k-Nearest Neighbors

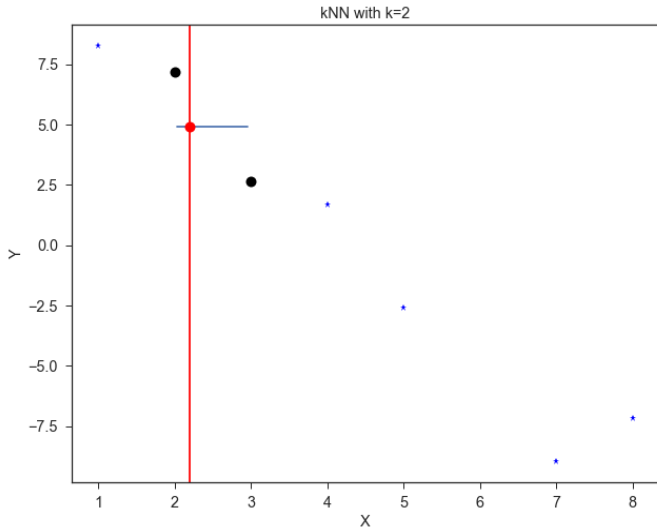












# k-Nearest Neighbors

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The *k-Nearest Neighbor (kNN) model* is an intuitive way to predict a quantitative response variable:

*to predict a response for a set of observed predictor values, we use the responses of other observations most similar to it!*

**Note:** this strategy can also be applied in classification to predict a categorical variable. We will encounter kNN again later in the semester in the context of classification.

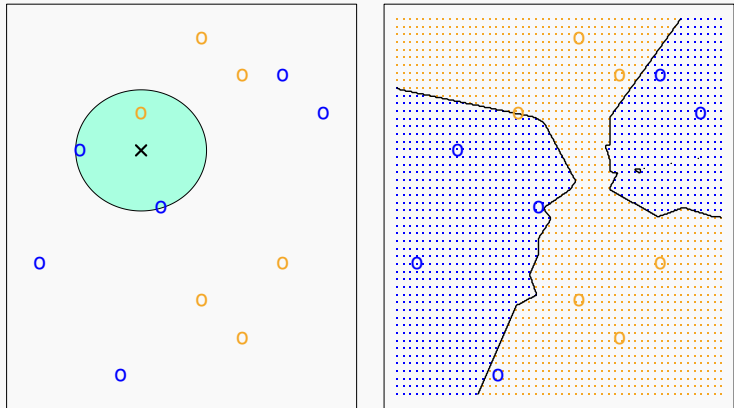
## k-Nearest Neighbors

Fixed a value of  $k$ . The predicted response for the  $i$ -th observation is the average of the observed response of the  $k$ -closest observations

$$\hat{y}_i = \frac{1}{k} \sum_{i=1}^k y_{n_i}$$

where  $\{X_{n_1}, \dots, X_{n_k}\}$  are the  $k$  observations most similar to  $X_i$  ( similar refers to a notion of distance between predictors).

# k-Nearest Neighbors for Classification





## kNN Regression: A Simple Example

Suppose you have 5 observations of taxi cab pick ups in New York City, the response is the average cab fare (in units of \$10), and the predictor is time of day (in hours after 7am):

$X$	1	2	3	4	5
$Y$	6	7	4	3	2

We calculate the predicted number of pickups using kNN for  $k = 2$ :

$$X = 1 \quad \hat{y}_1 = \frac{1}{2} (7 + 4) = 5.5$$

## kNN Regression: A Simple Example

Suppose you have 5 observations of taxi cab pick ups in New York City, the response is the average cab fare (in units of \$10), and the predictor is time of day (in hours after 7am):

$X$	1	2	3	4	5
$Y$	6	7	4	3	2

We calculate the predicted number of pickups using kNN for  $k = 2$ :

$$X = 2 \quad \hat{y}_2 = \frac{1}{2} (6 + 4) = 5.0$$

## kNN Regression: A Simple Example

Suppose you have 5 observations of taxi cab pick ups in New York City, the response is the average cab fare (in units of \$10), and the predictor is time of day (in hours after 7am):

$X$	1	2	3	4	5
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We calculate the predicted number of pickups using kNN for  $k = 2$ :

$$\hat{Y} = (5.5, 5.0, 5.0, 3.0, 3.5)$$

## kNN Regression: A Simple Example

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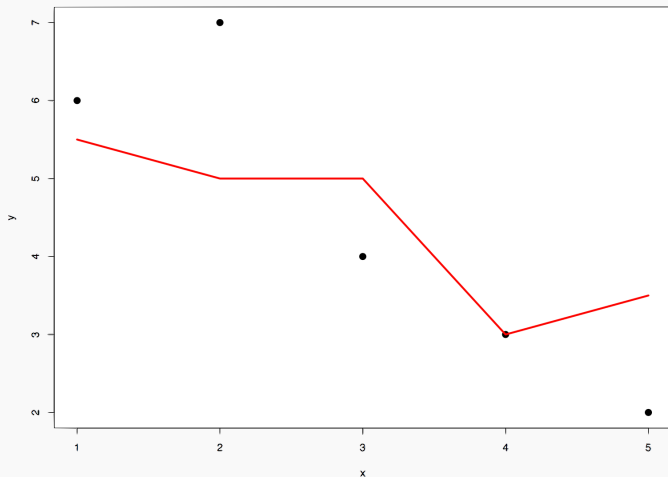
The MSE given our predictions is

$$MSE = \frac{1}{5} [(6 - 5.5)^2 + (7 - 5.0)^2 + \dots + (3.5 - 2)^2] = 1.5$$

On average, our predictions are off by \$15.

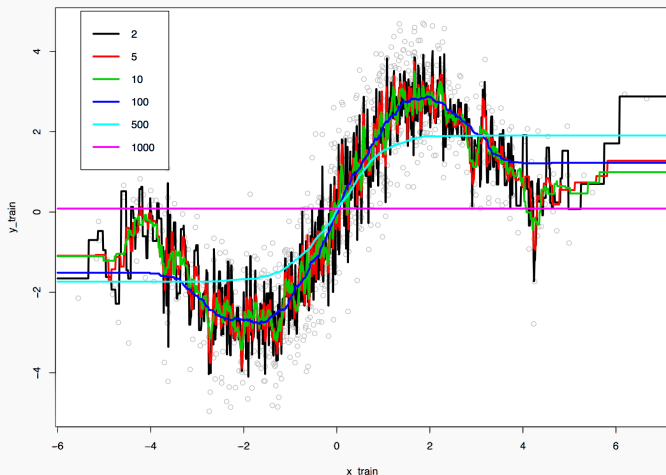
# kNN Regression: A Simple Example

We plot the observed responses along with predicted responses for comparison:



# Choice of $k$ Matters

But what value of  $k$  should we choose? What would our predicted responses look like if  $k$  is very small? What if  $k$  is large (e.g.  $k = n$ )?



## kNN with Multiple Predictors

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In our simple example, we used absolute value to measure the distance between the predictors in two different observations,  $|x_i - x_j|$ .

When we have multiple predictors in each observation, we need a notion of distance between two **sets** of predictor values. Typically, we use Euclidean distance:

$$d(x_i - x_j) = \sqrt{(x_{i,1} - x_{j,1})^2 + \dots + (x_{i,p} - x_{j,p})^2}$$

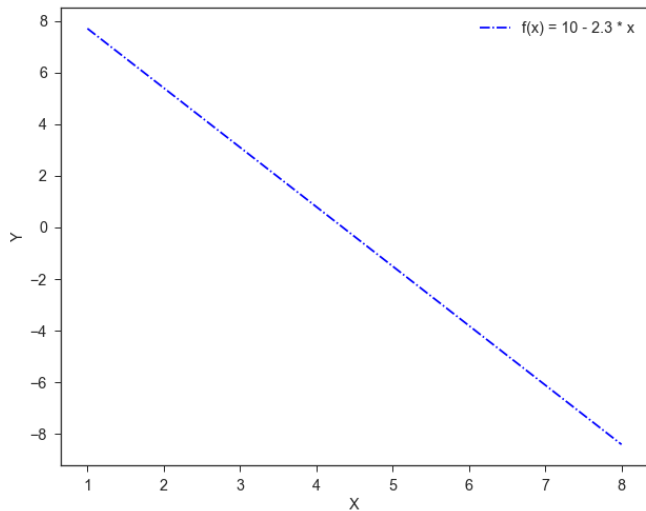
**Caution:** when using Euclidean distance, the scale (or units) of measurement for the predictors matter! Predictors with large values, comparatively, will dominate the distance measurement.

## Model II: Linear Regression

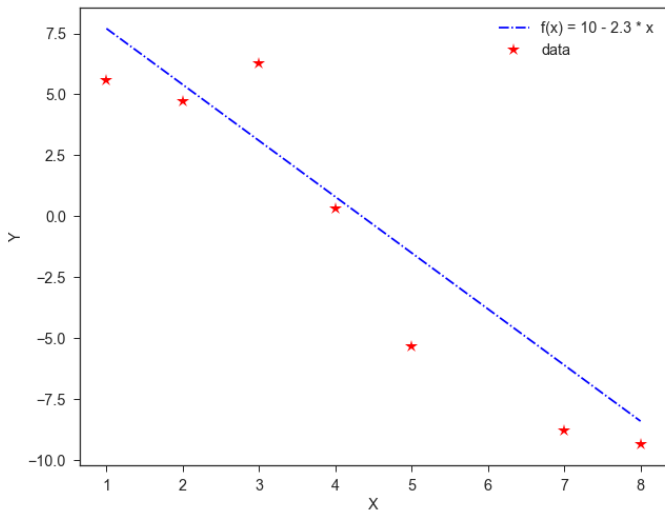
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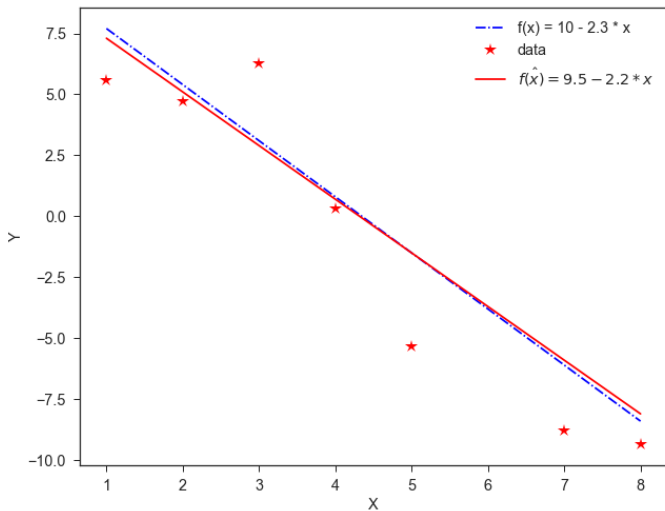
# Linear Models in One Variable



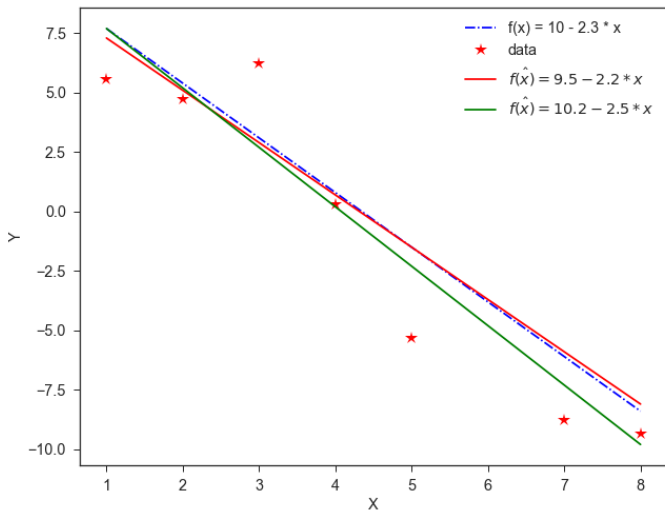
# Linear Models in One Variable



# Linear Models in One Variable



# Linear Models in One Variable



# Linear Models in One Variable

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Note that in building our kNN model for prediction, we did not compute a closed form for  $\hat{f}$ , our estimate of the function,  $f$ , relating predictor to response.

Alternatively, if each observation has only one predictor, we can build a model by first assuming a simple form for  $f$  (and hence  $\hat{f}$ ), say a **linear form**,

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

Again,  $\epsilon$  is the random quantity or **noise** by which observed values of  $Y$  differ from the rule  $f(X)$ .

# Inference for Linear Regression

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If our statistical model is

$$Y = f(X) + \epsilon = \beta_1^{\text{true}} X + \beta_0^{\text{true}} + \epsilon,$$

then it follows that our estimate is

$$\hat{Y} = \hat{f}(X) = \hat{\beta}_1 X + \hat{\beta}_0$$

where  $\hat{\beta}_1$  and  $\hat{\beta}_0$  are estimates of  $\beta_1$  and  $\beta_0$ , respectively, that we compute using observations.

Recall that our intuition says to 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.

# Inference for Linear Regression

Again we use MSE as our loss function,

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

Then the optimal values for  $\hat{\beta}_1$  and  $\hat{\beta}_0$  should be

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

Now, taking the partial derivatives of  $L$  and finding the global minimum will give us explicit formulae for  $\hat{\beta}_0, \hat{\beta}_1$ ,

$$\hat{\beta}_1 = \frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\sum_i (x_i - \bar{x})^2}, \quad \hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

where  $\bar{y}$  and  $\bar{x}$  are sample means. The line  $\hat{Y} = \hat{\beta}_1 X + \hat{\beta}_0$  is called the **regression line**.

# Linear Regression: A Simple Example

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Recall our simple example from before, where we observe the average cab fare in NYC using the time of day,

$X$	1	2	3	4	5
$Y$	6	7	4	3	2

By our formula, we compute the regression line to be

$$\hat{Y} = -1.2X + 8$$

Using this model, we can generate predicted responses:

$$\hat{Y} = (6.8, 5.6, 4.4, 3.2, 2.0)$$

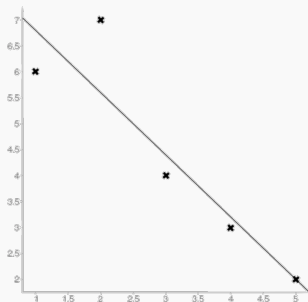
Let's graph our linear model against the observations.



# Linear Regression: A Simple Example

Why doesn't our line fit the observations exactly? There are two possibilities:

- ▶  $f$  is not a linear function
- ▶ the difference between prediction and observation is due to the noise term in  $Y = f(X) + \epsilon$ .



Regardless of the form of  $f$ , the presence of the random term  $\epsilon$  means that the predictions made using  $\hat{f}$  will never exactly match the observations.

**Question:** Is it possible to measure how confidently  $\hat{\beta}_0$ ,  $\hat{\beta}_1$  approximate the true parameters of  $f$ ?

## Evaluating Model

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# Evaluating Model Things to Consider

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- ▶ How well do we know  $\hat{f}$  ?  
The confidence intervals of our  $\hat{\beta}_0$  and  $\hat{\beta}_1$ ?
- ▶ Evaluating Significance of Predictors  
Does the outcome depend on the predictors?
- ▶ Model Fitness  
How does the model perform predicting?
- ▶ Comparison of Two Models  
How do we choose from two different models?

# Understanding Model Uncertainty

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We interpret the  $\epsilon$  term in our observation

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

to be noise introduced by random variations in natural systems or imprecisions of our scientific instruments.

We call  $\epsilon$  the measurement error or **irreducible error**.

Since even predictions made with the actual function  $f$  will not match observed values of  $Y$ .

Due to  $\epsilon$ , every time we measure the response  $Y$  for a fix value of  $X$  we will obtain a different observation, and hence a different estimate of  $\beta_0$  and  $\beta_1$ .

## Uncertainty In $\hat{\beta}_0$ and $\hat{\beta}_1$

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Again due to  $\epsilon$ , if we make only a few observations, the noise in the observed values of  $Y$  will have a large impact on our estimate of  $\beta_0$  and  $\beta_1$ .

If we make many observations, the noise in the observed values of  $Y$  will 'cancel out'; noise that biases some observations towards higher values will be canceled by the noise that biases other observations towards lower values.

This feels intuitively true but requires some assumptions on  $\epsilon$  and a formal justification - or at least an example.

## Uncertainty In $\hat{\beta}_0$ and $\hat{\beta}_1$

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In summary, the variations in  $\hat{\beta}_0, \hat{\beta}_1$  (estimates of  $\beta_0$  and  $\beta_1$  respectively) are affected by

- ▶ **(Measurement)**  $\text{Var}[\epsilon]$ , the variance (the scale of the variation) in the noise,  $\epsilon$
- ▶ **(Sampling)**  $n$ , the number of observations we make

The variances of  $\hat{\beta}_0, \hat{\beta}_1$  are also called **standard errors**, which we will see later.

# A Simple Example

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# Bootstrapping for Estimating Sampling Error

With some assumption on  $\epsilon$ , we can compute the variances or standard errors of  $\hat{\beta}_0$  and  $\hat{\beta}_1$  analytically.

The standard errors can also be estimated empirically through **bootstrapping**.

## Definition

Bootstrapping is the practice of estimating properties of an estimator by measuring those properties by, for example, sampling from the observed data.

For example, we can compute  $\hat{\beta}_0$  and  $\hat{\beta}_1$  multiple times by randomly sampling from our data set. We then use the variance of our multiple estimates to approximate the true variance of  $\hat{\beta}_0$  and  $\hat{\beta}_1$ .



## Comparison of Two Models

## Parametric vs. Non-parametric Models

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Linear regression is an example of a **parametric model**, that is, it is a model with a fixed form and a fixed number of parameters that does not depend on the number of observations in the training set.

kNN is an example of a **non-parametric model**, that is, it is a model whose structure depends on the data. The set of parameters of the kNN model is the entire training set.

In particular, the number of parameters in kNN depends on the number of observations in the training set.

# kNN vs. Linear Regression

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So which model is better? Rather than answer this question, let's define 'better'.

To compare two models, we can consider any combination of the following criteria (and possibly more):

- ▶ Which model gives less predictive error, with respect to a loss function?
- ▶ Which model takes less space to store?
- ▶ Which model takes less time to train (perform inference)?
- ▶ Which model takes less time to make a prediction?