Introduction to Regression

Part B: Error Evaluation and Model Comparison

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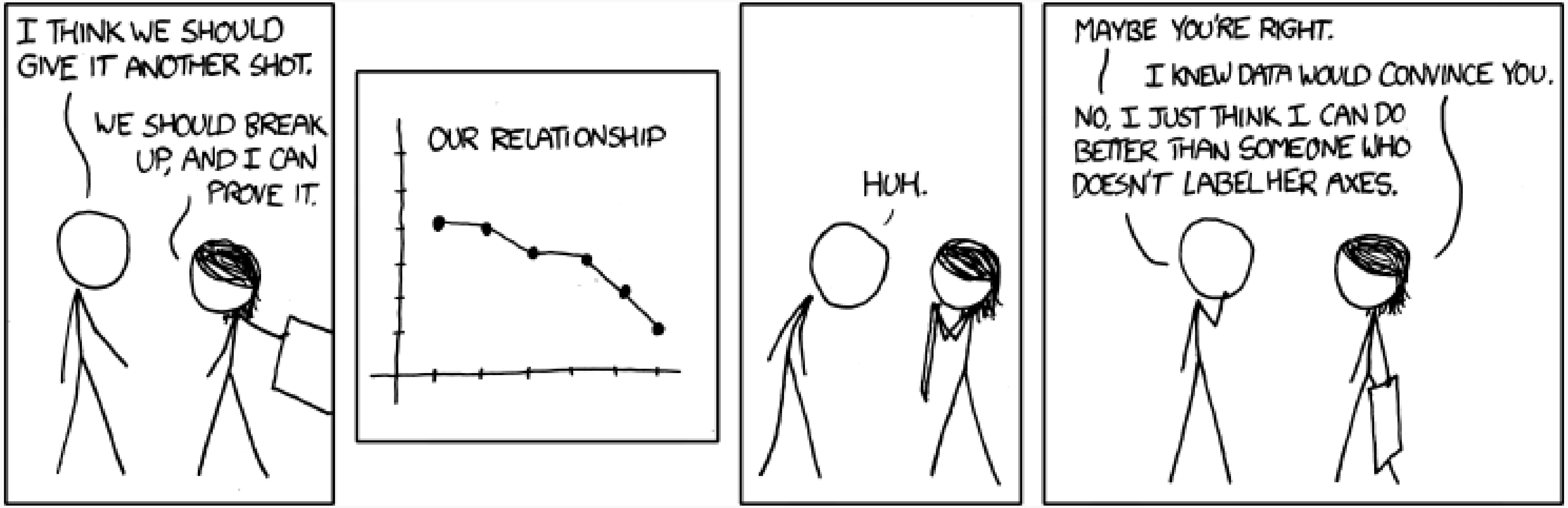
Lecture Outline

Part A: Statistical Modeling

- k-Nearest Neighbors (kNN)

Part B: Error Evaluation and Model Comparison

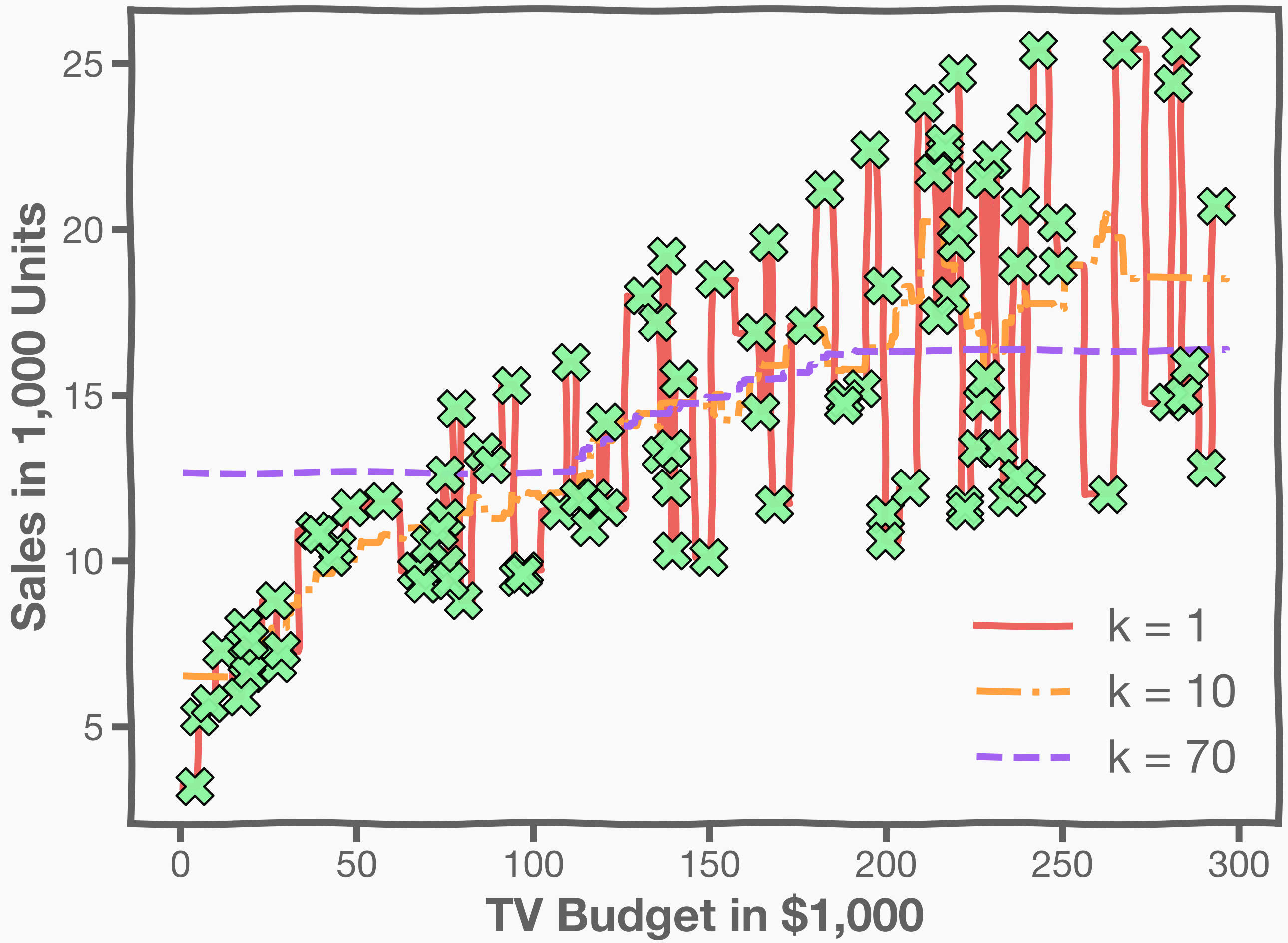
- How do we evaluate our model?
- How do we choose from two different models?



https://xkcd.com/833/

k-Nearest Neighbors – kNN

We have tested various models using different k-values on the data.



Choices for model

Which model do you think is the best?

Options:

$A.\quad k = 1$

$B.\quad k = 10$

$C.\quad k = 70$

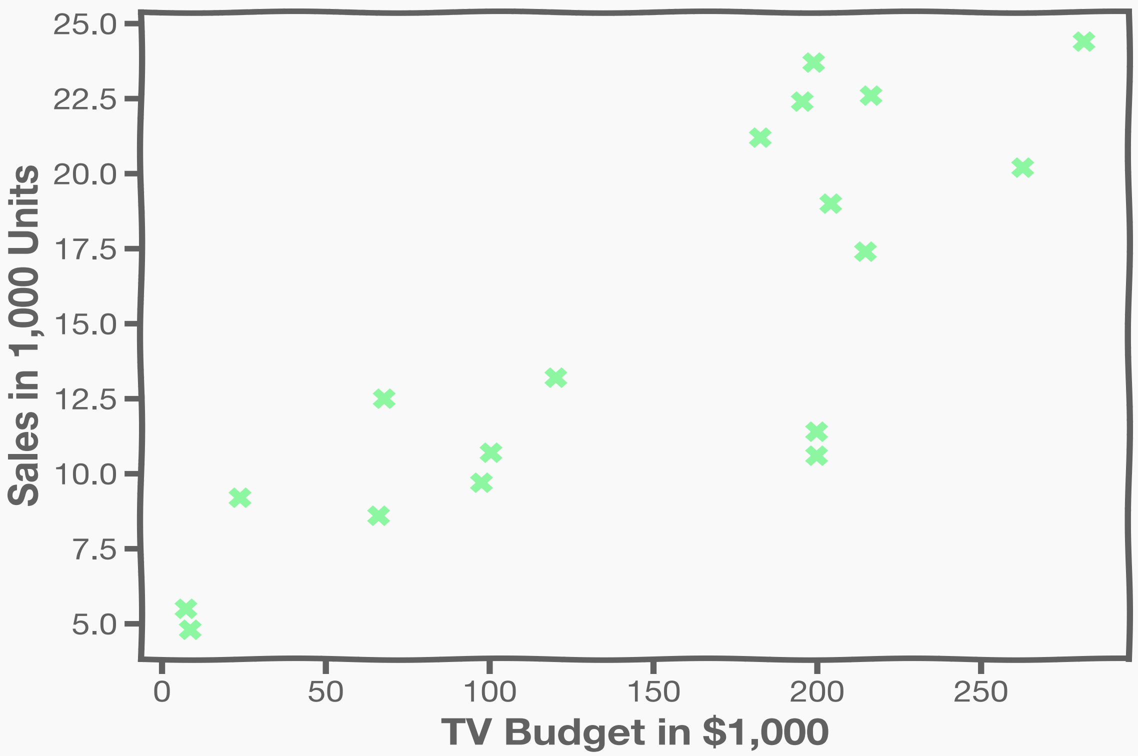
$D.\quad k = 15$

E. 🤷‍♂️

Error Evaluation

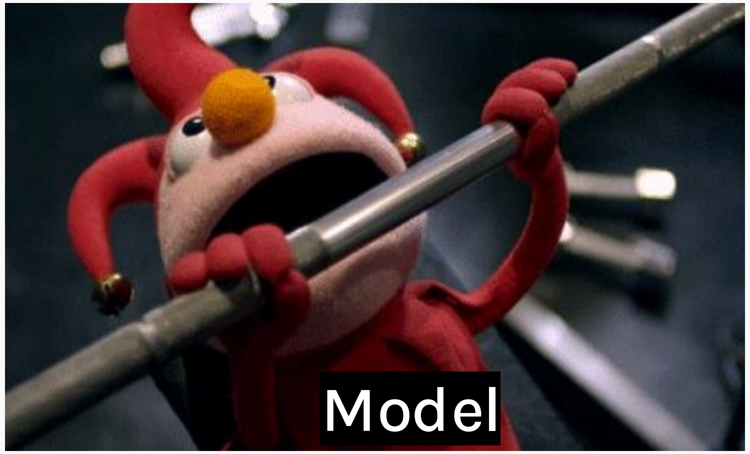
Error Evaluation

We need to define what we mean by ***best***. To do so, we start with our data.



Error Evaluation

We first **withhold** a portion of the data from the model; this process is called **train-test** split.



Train Set

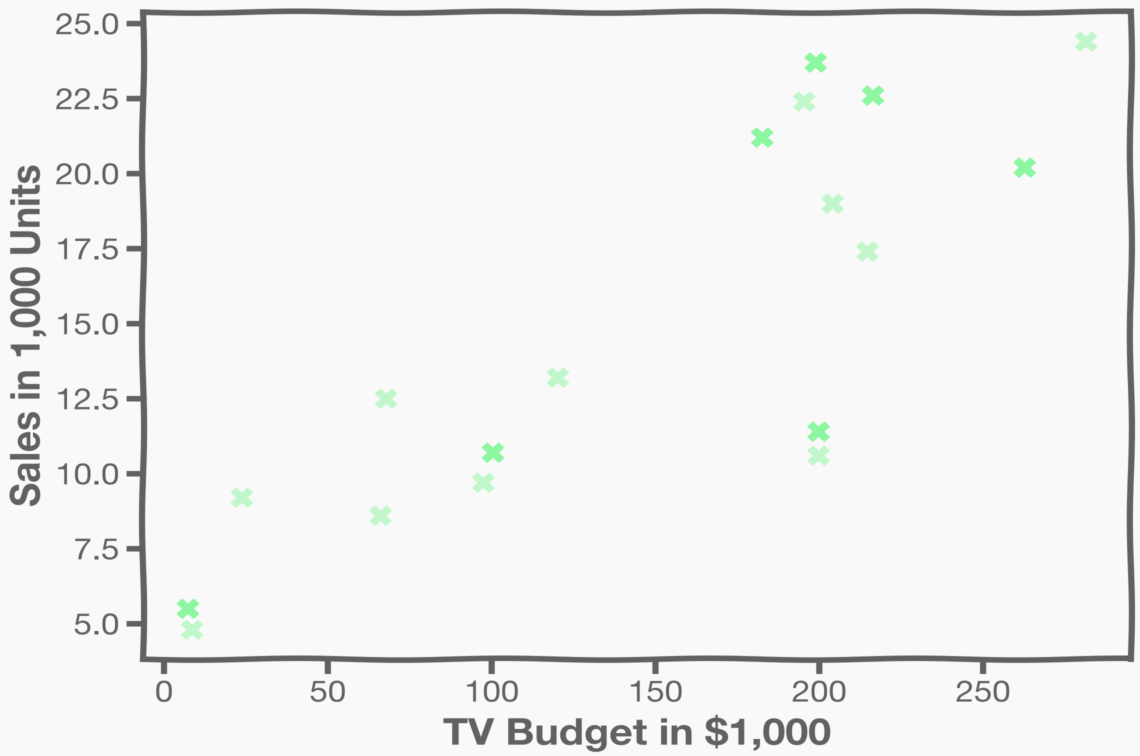
The data that we use to train our model to estimate, $\hat{y}$.

Test Set

The data that we use to evaluate our model's performance.

Error Evaluation

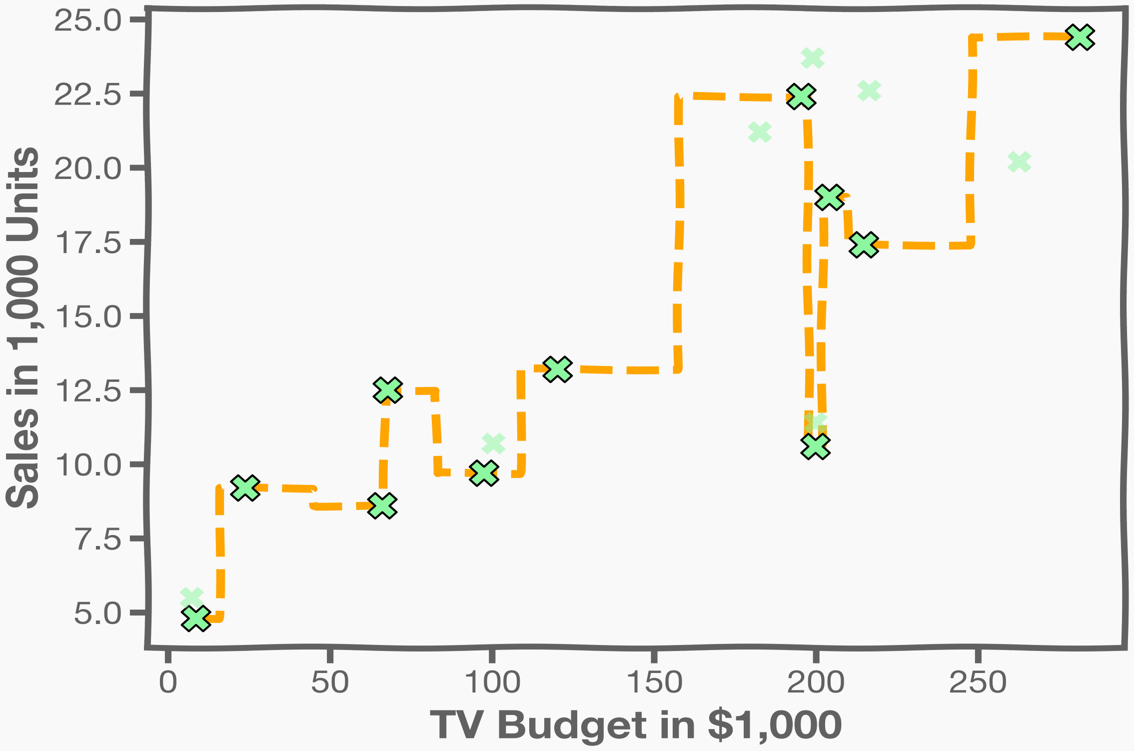
We first **withhold** a portion of the data from the model; this process is called **train-test** split.



We use the training set to estimate $\hat{y}$, and the test set to evaluate the model's performance.

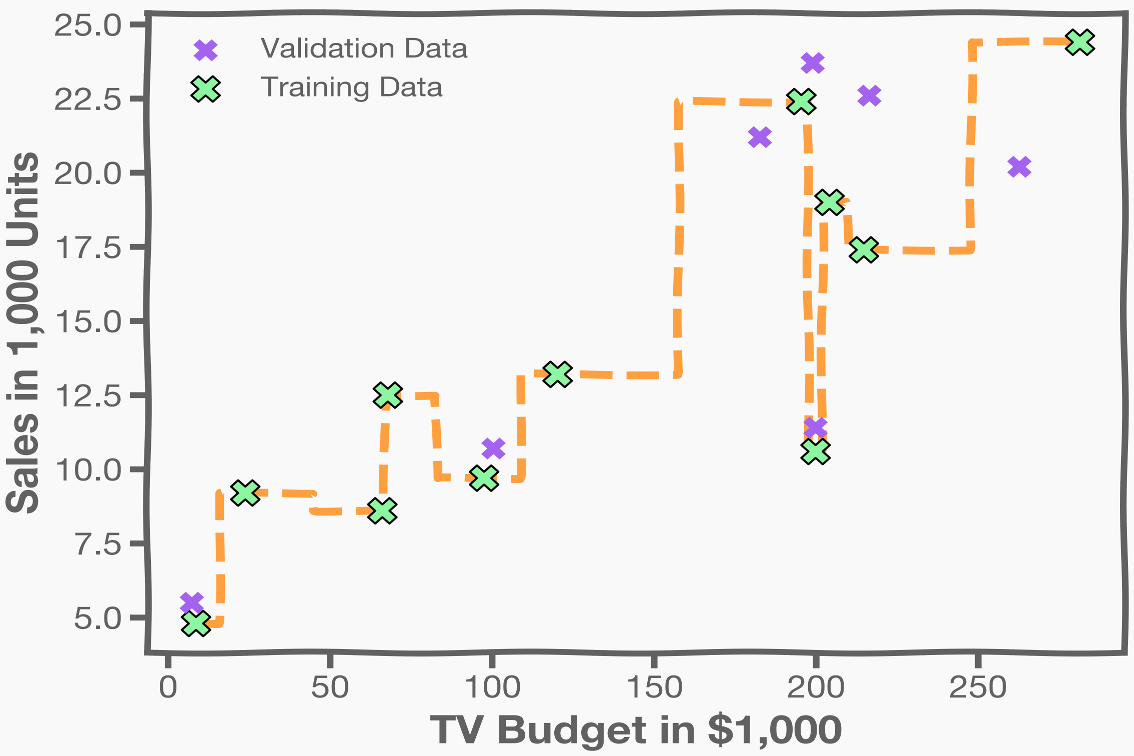
Error Evaluation

Estimate $\hat{y}'s$ values for all the data points in the training set when ***k=1*.**



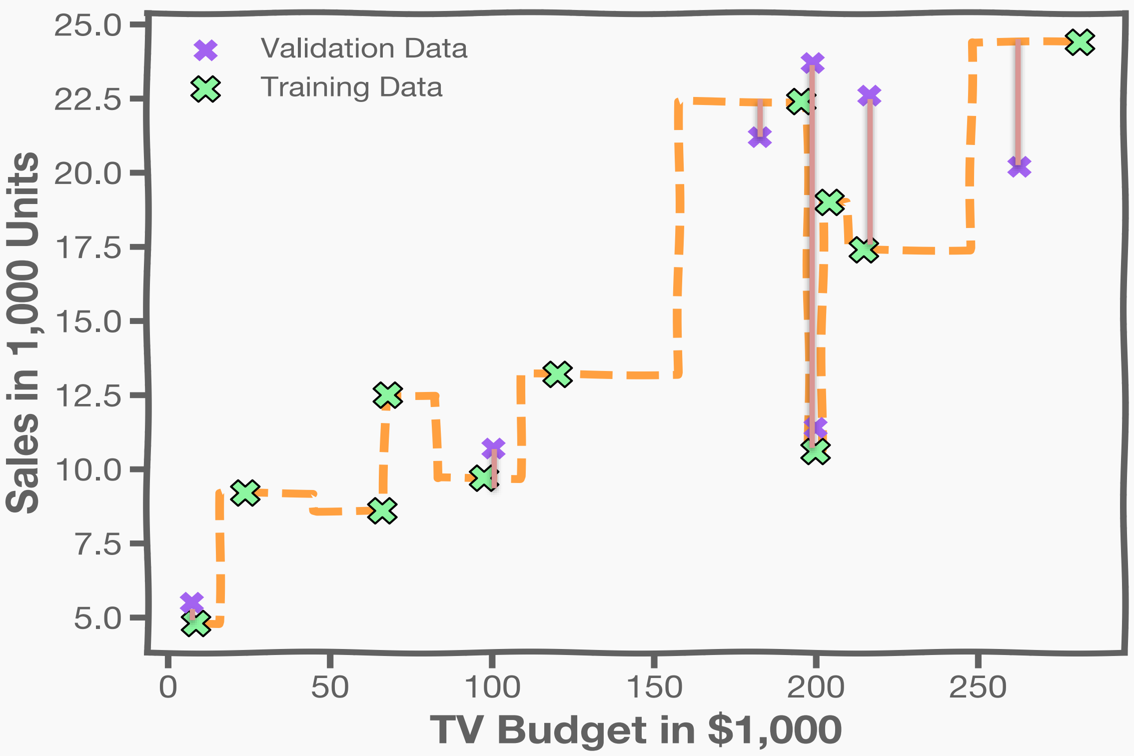
Error Evaluation

Now, we examine the data that was not used for estimating $\hat{y}$, the **test data** represented by purple crosses.



Error Evaluation

And we calculate the **residuals** $(y_i - \hat{y}_i)$.



For each observation (x_n, y_n), the absolute residuals, $r_i = |y_i - \hat{y}_i|$ quantify the error at each observation point.

Error Evaluation

To quantify the performance of a model, we aggregate the errors. This aggregated value is commonly referred to as the ***loss***, ***error***, or ***cost function***.

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

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

Note: Loss and cost function refer to the same thing. Cost usually refers to the total loss where loss refers to a single training point.

Error Evaluation

Caution: MSE is not the only valid, or necessarily the best, loss function for all scenarios.

Other choices for loss function:

1. Max Absolute Error
2. Mean Absolute Error
3. Huber Loss

We will motivate MSE when we introduce probabilistic modeling.

Note: The square **R**oot of the **M**ean of the **S**quared **E**rrors (RMSE) is also commonly used.

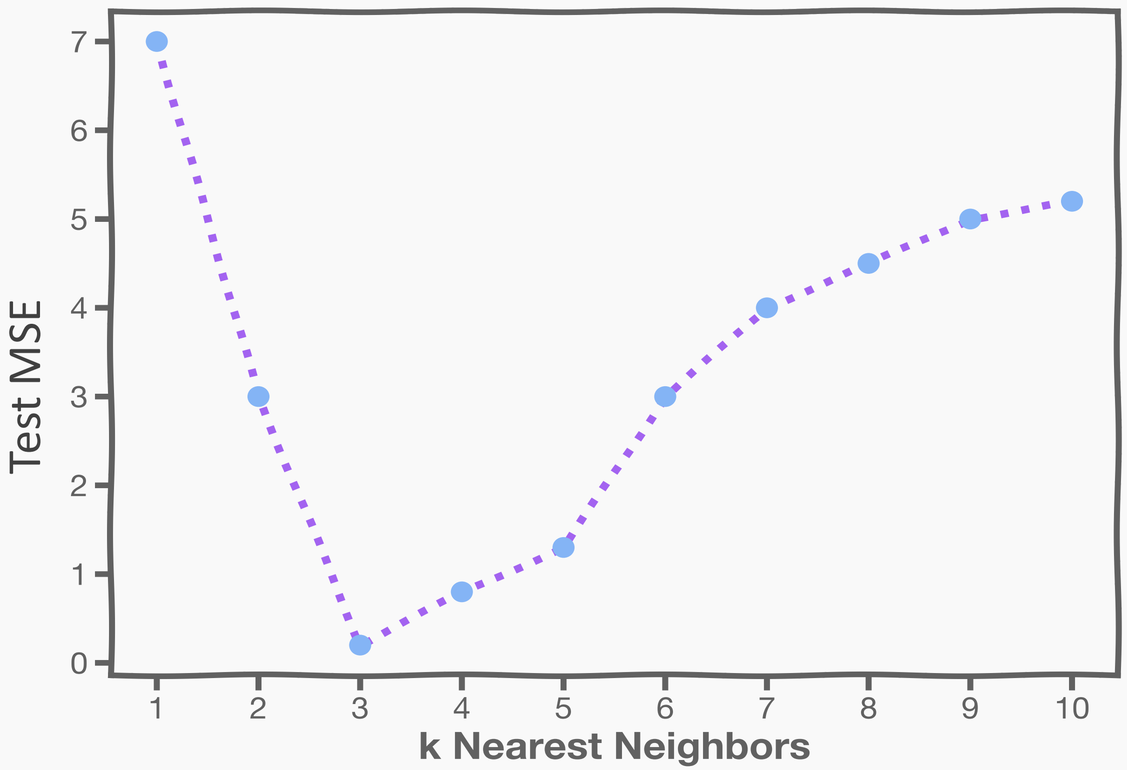
$$RMSE = \sqrt{MSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \widehat{y_i})^2}$$

Model Comparison

Model Comparison

We repeat this process for all values of ***k*** and compare the MSEs on the test set**.**

We will introduce validation set soon



Which model is the best?

Question

Which model do you think is the best now

Options:

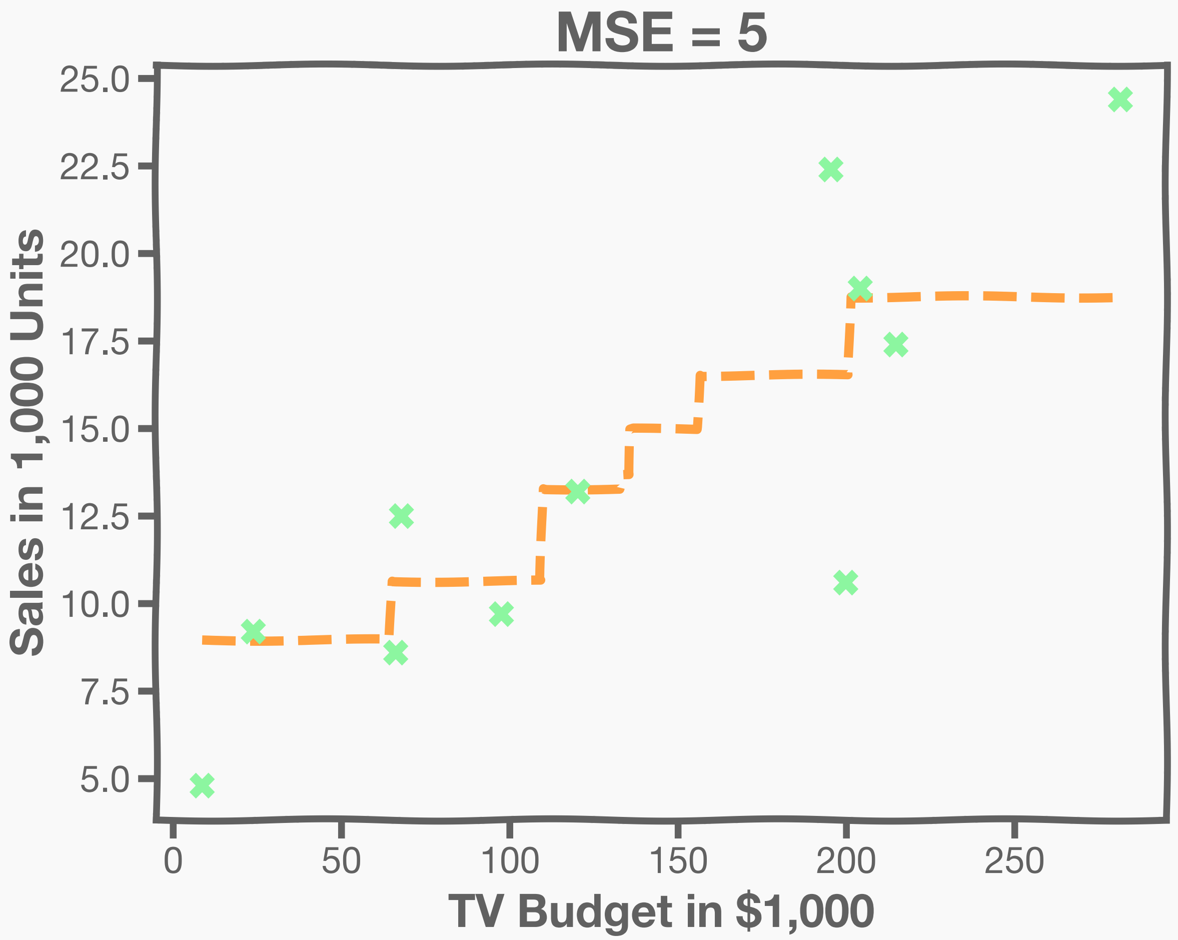
A. $k = 3$

B. $k = 3$ but why don’t we experiment with different train/test splits?

Model Fitness

Model fitness

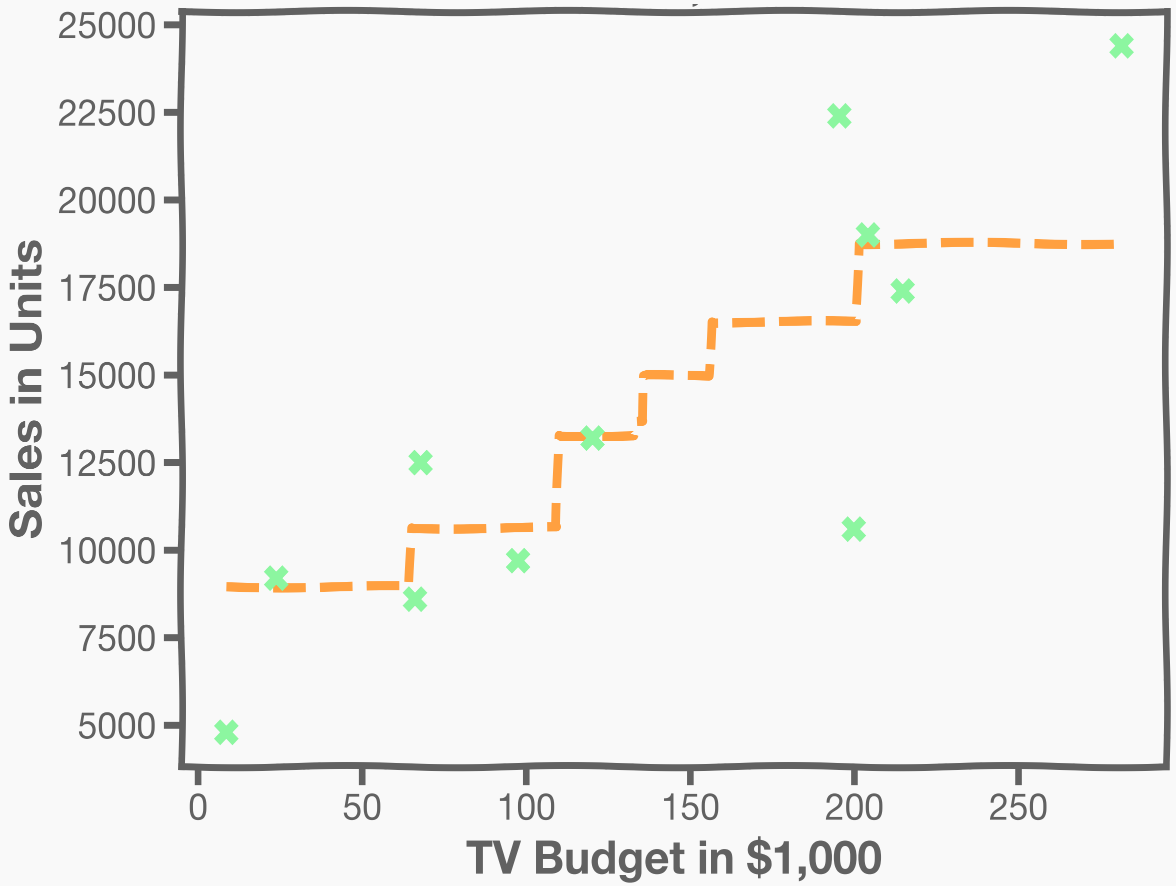
Calculate the MSE for $k = 3$ using a subset of the data.



Is MSE=5.0 good enough?

Model fitness

What would happen if we measure the ***Sales*** in single units instead of 1000 units?



MSE is now 5,004,930.

Is that good?

Model fitness

It would be more meaningful to compare it to a benchmark or a known value.

A benchmark that isn't affected by the scale of the data.

Model fitness

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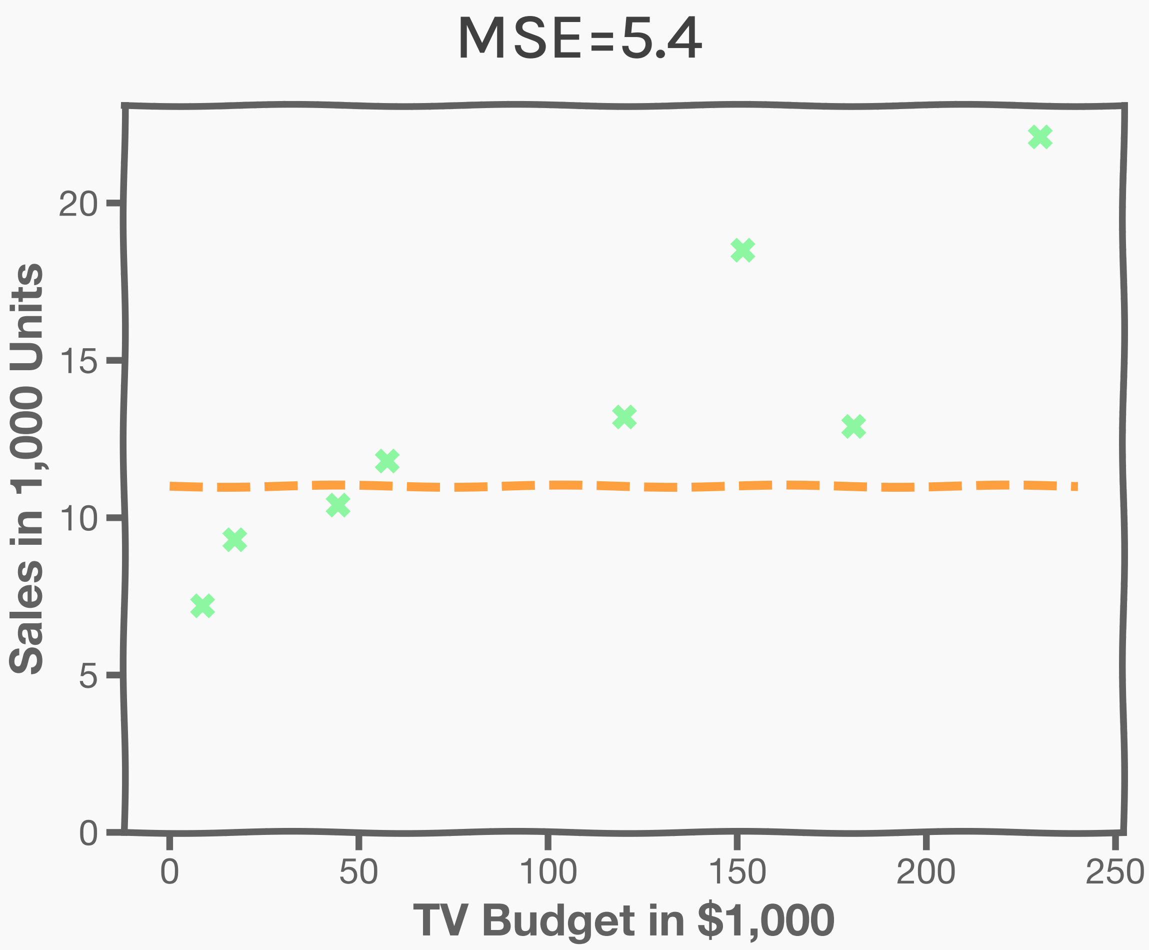

We will use the simplest model:

$$\hat{y} = \bar{y} = \frac{1}{n}\sum_i y_i$$

as the worst possible model and

$\hat{y}_i = y_i$ as the best possible model.

R-squared

Though is called R-squared, it is not the square of a quantity R as given in this formula.

We will use two reference models for comparison:

1. The simplest model, often considered the worst possible, where the predicted value $\hat{y}$ is the mean of all observations:

$$\hat{y} = \bar{y} = \frac{1}{n}\sum_i y_i$$

2. The ideal or best possible model, where the predicted value $\hat{y}$ is identical to the actual value y.

Using these two reference models, we define the R^2 (R-squared) value as:

$$\boxed{R^2 = 1 - \frac{\sum_i (\hat{y}_i - y_i)^2}{\sum_i (\bar{y} - y_i)^2}}$$

R-squared

$$R^2 = 1 - \frac{\sum_i (\hat{y}_i - y_i)^2}{\sum_i (\bar{y} - y_i)^2}$$

- If our model is as good as the mean value, $\bar{y}$, then $R^2 = 0$
- If our model is perfect, then $R^2 = 1$
- R^2 can be negative if the model is worse than the average. This can happen when we evaluate the model in the **test** set.


TRENDIZISST
THANK YOU!!