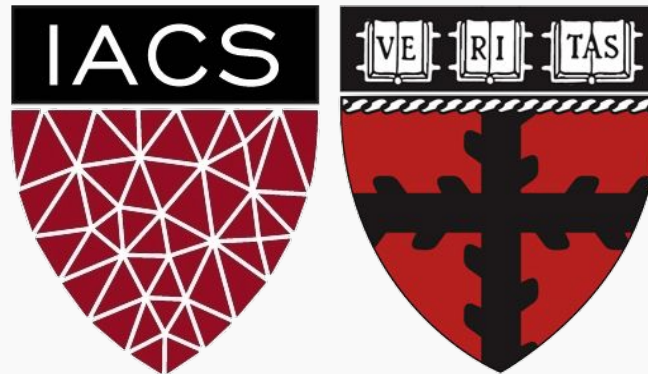


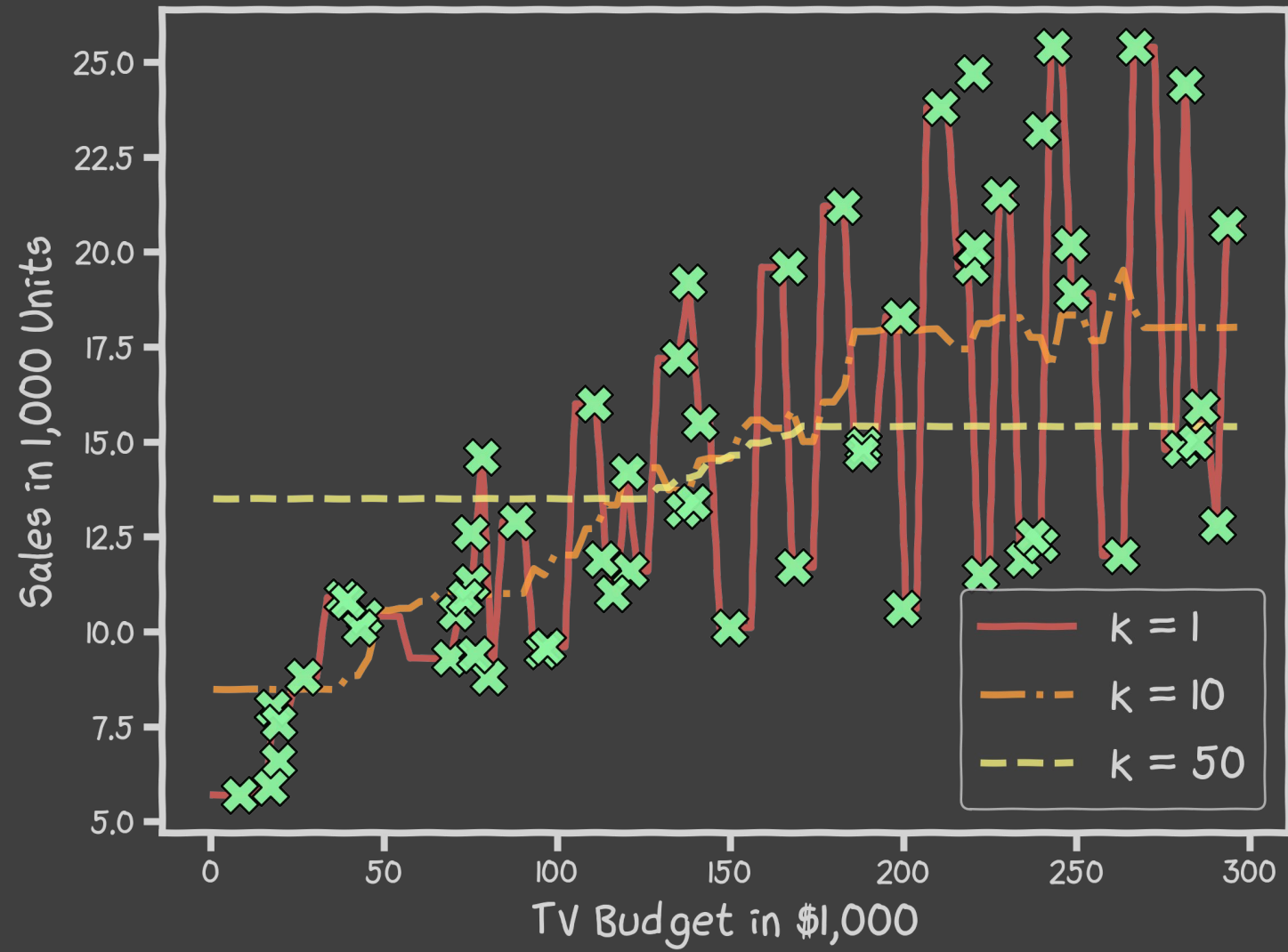
Introduction to Regression

Part B: Error Evaluation and Model Comparison

IACS-MACI Internship

Pavlos Protopapas

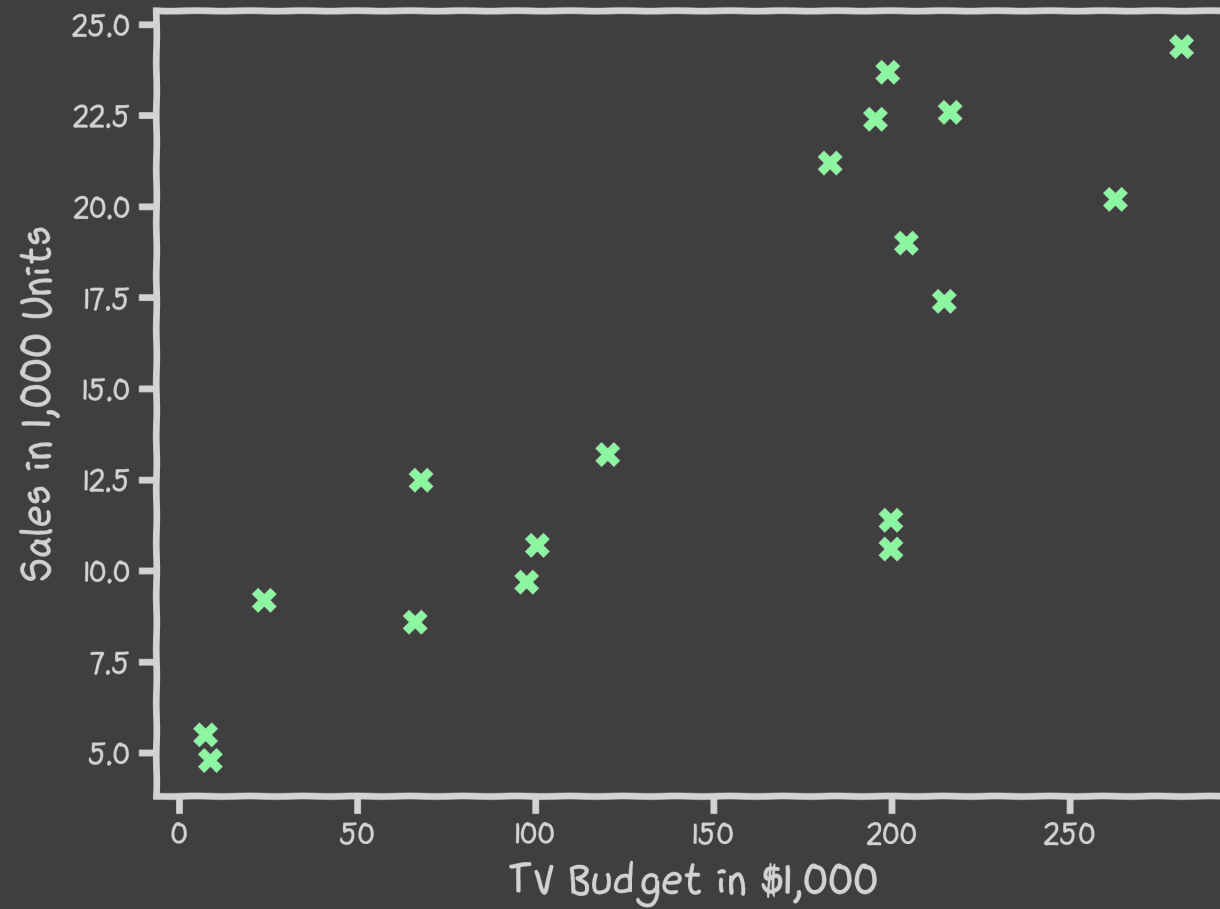




Error Evaluation

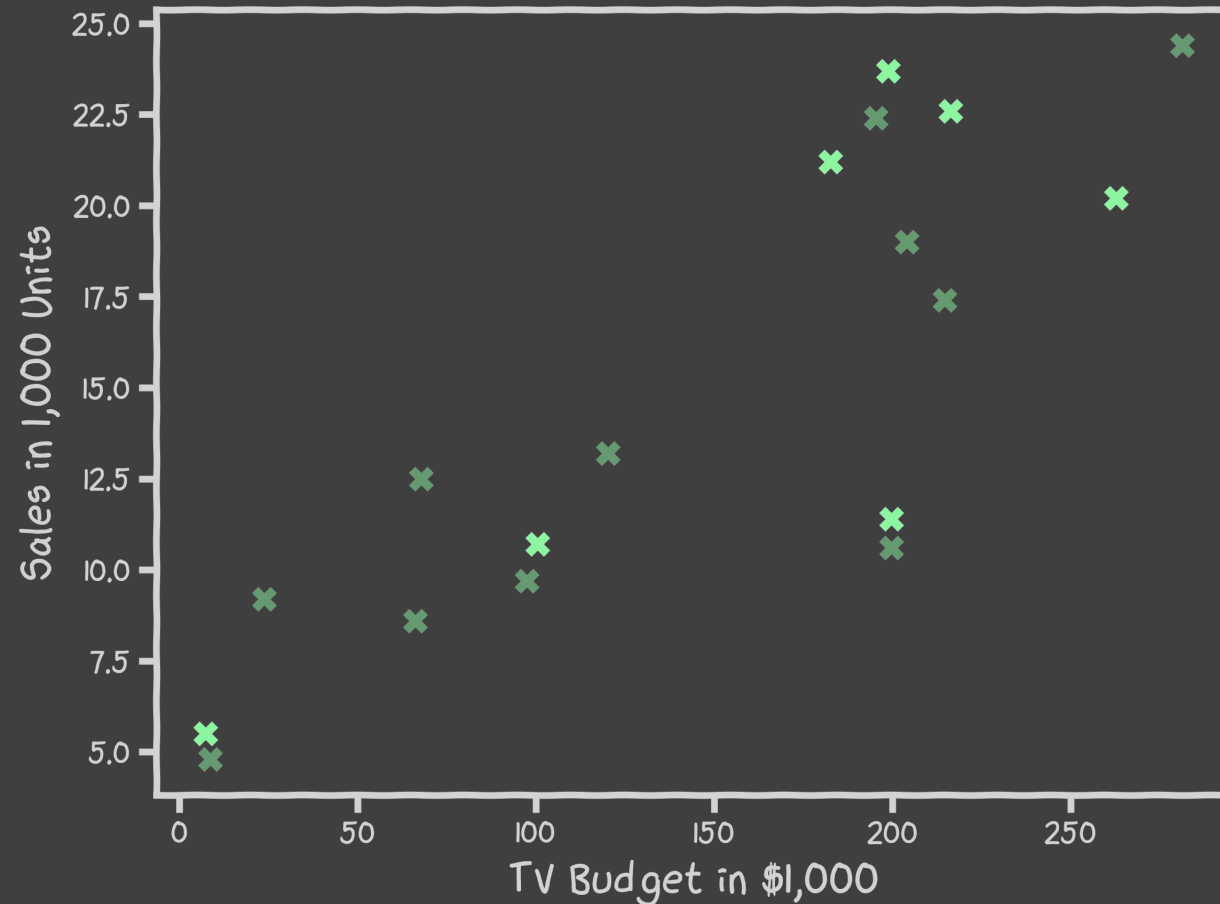
Error Evaluation

Start with some data.



Error Evaluation

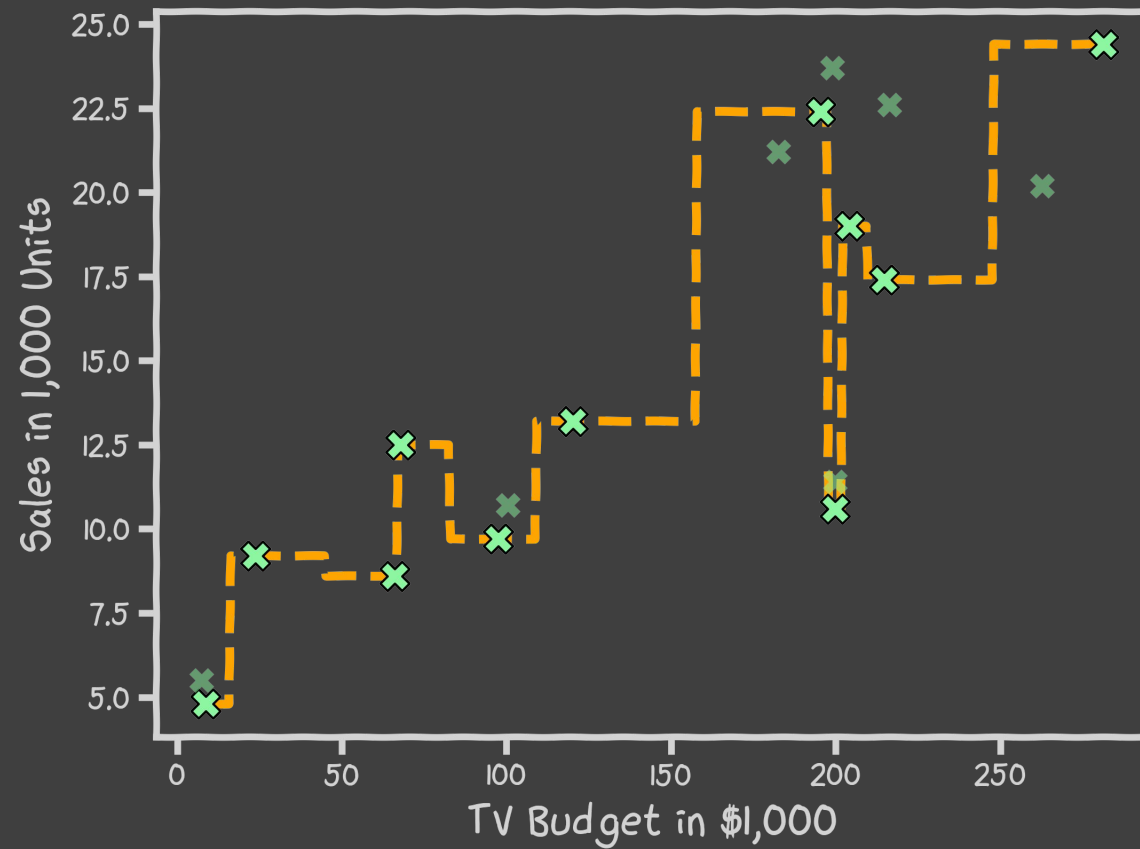
Randomly hide some of the data from the model. This is called **train-validation** split.



We use the train set to estimate \hat{y} , and the validation set to evaluate the model.

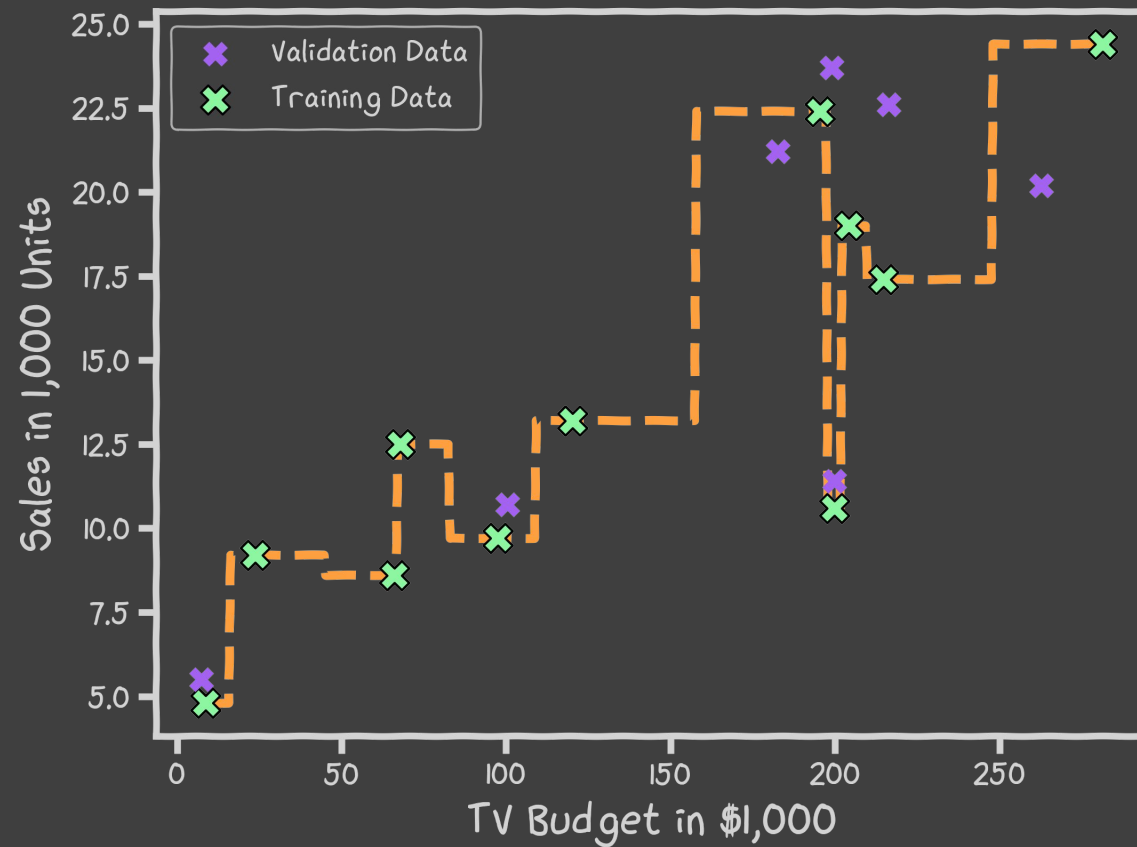
Error Evaluation

Estimate \hat{y} for $k=1$.



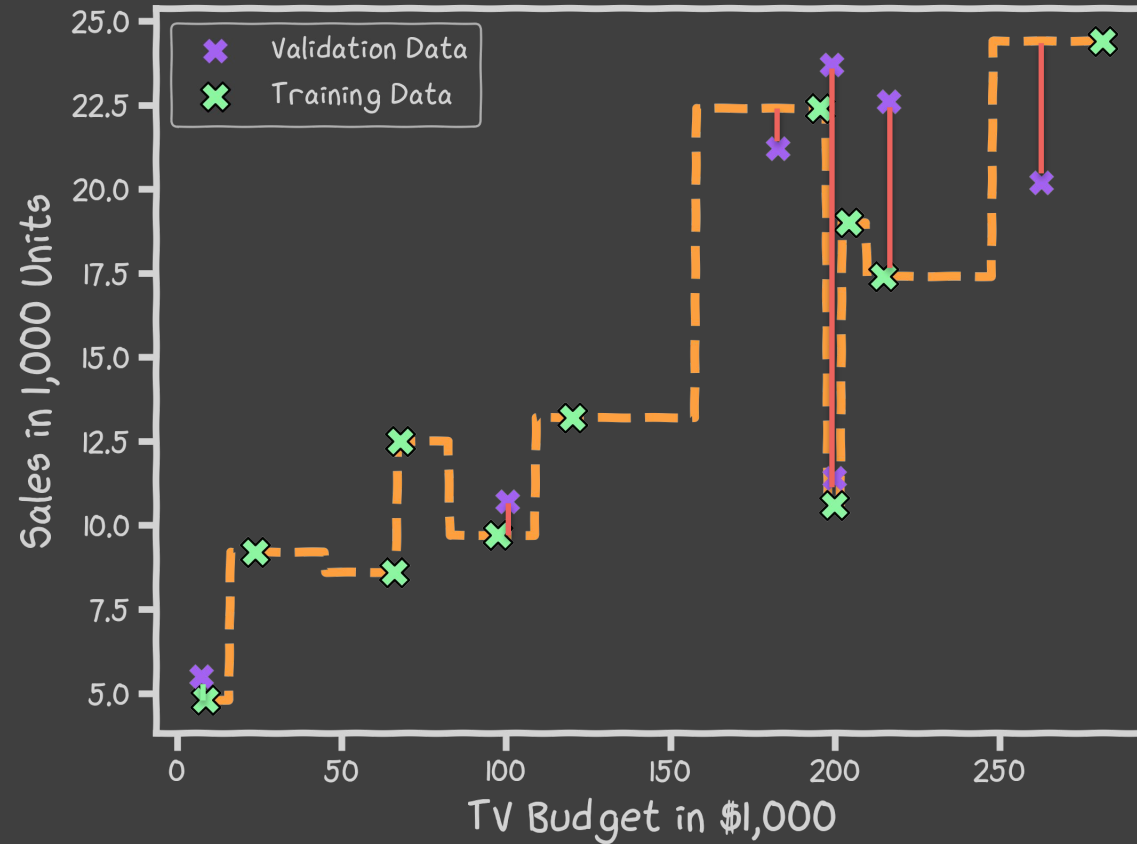
Error Evaluation

Now, we look at the data we have not used, the **validation data** (red crosses).



Error Evaluation

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.

In order to quantify how well a model performs, we aggregate the errors, and we call that the *loss* or *error* or *cost function*.

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

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

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

Other choices for loss function:

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

Note: The square Root of the Mean of the Squared Errors (RMSE) is also commonly used.

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

Error Evaluation

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

Other choices for loss function:

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

We will motivate MSE when we introduce probabilistic modeling.

Note: The square Root of the Mean of the Squared Errors (RMSE) is also commonly used.

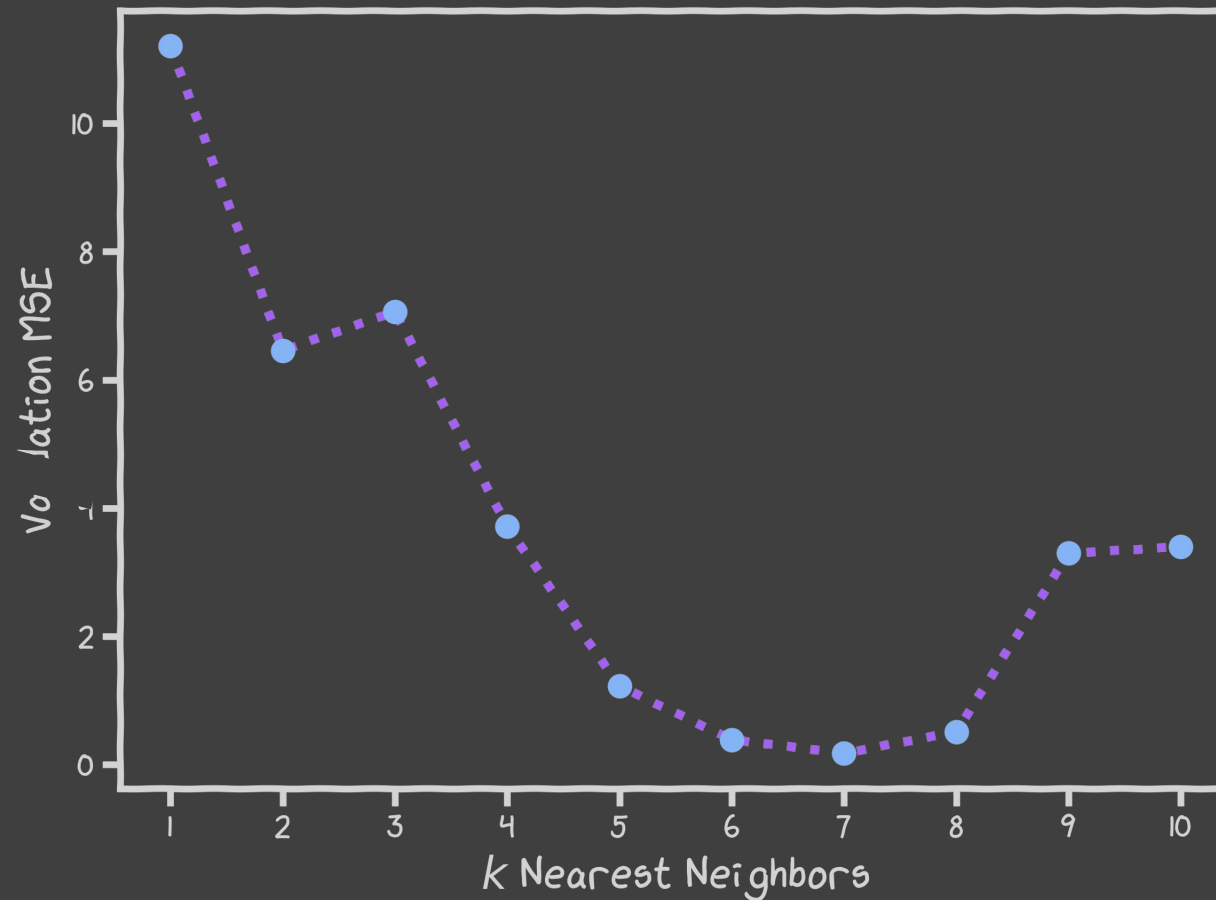
$$RMSE = \sqrt{MSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2}$$

Model Comparison

Model Comparison



Do the same for all k 's and compare the MSEs.



Which model is the best?

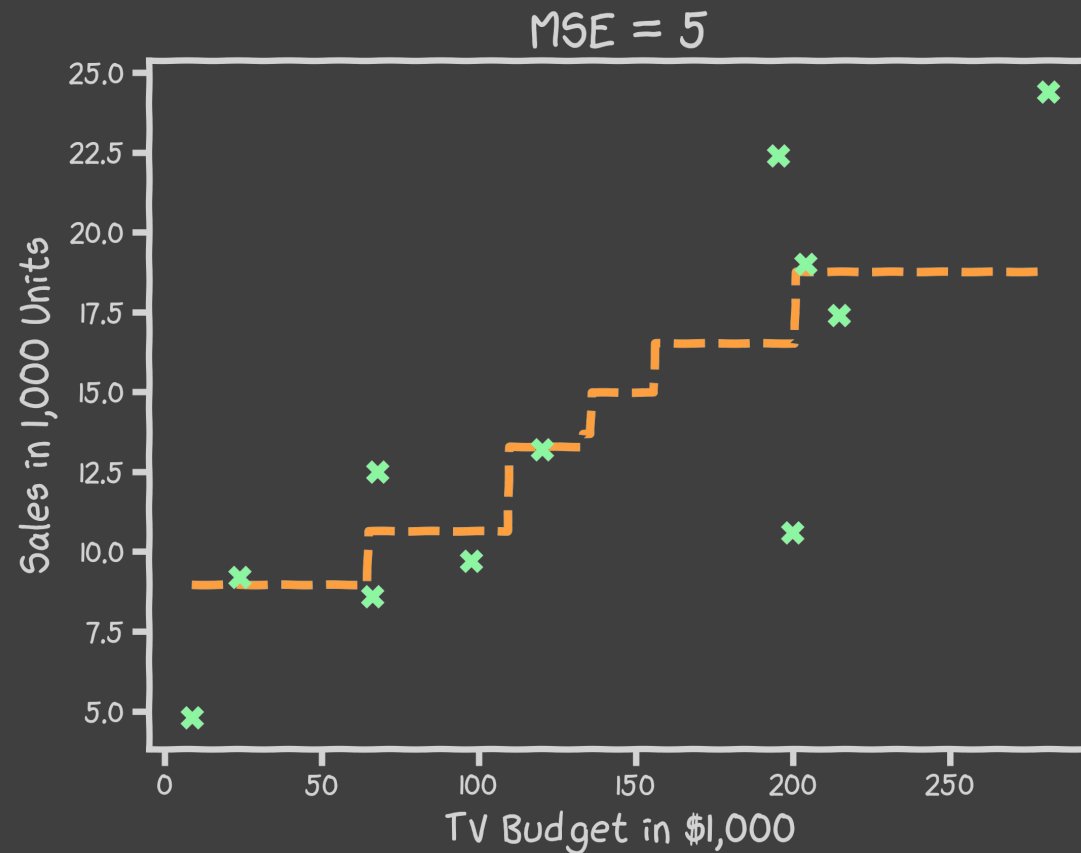
$k=7$ seems to be the **best model**.

Model Fitness

Model fitness



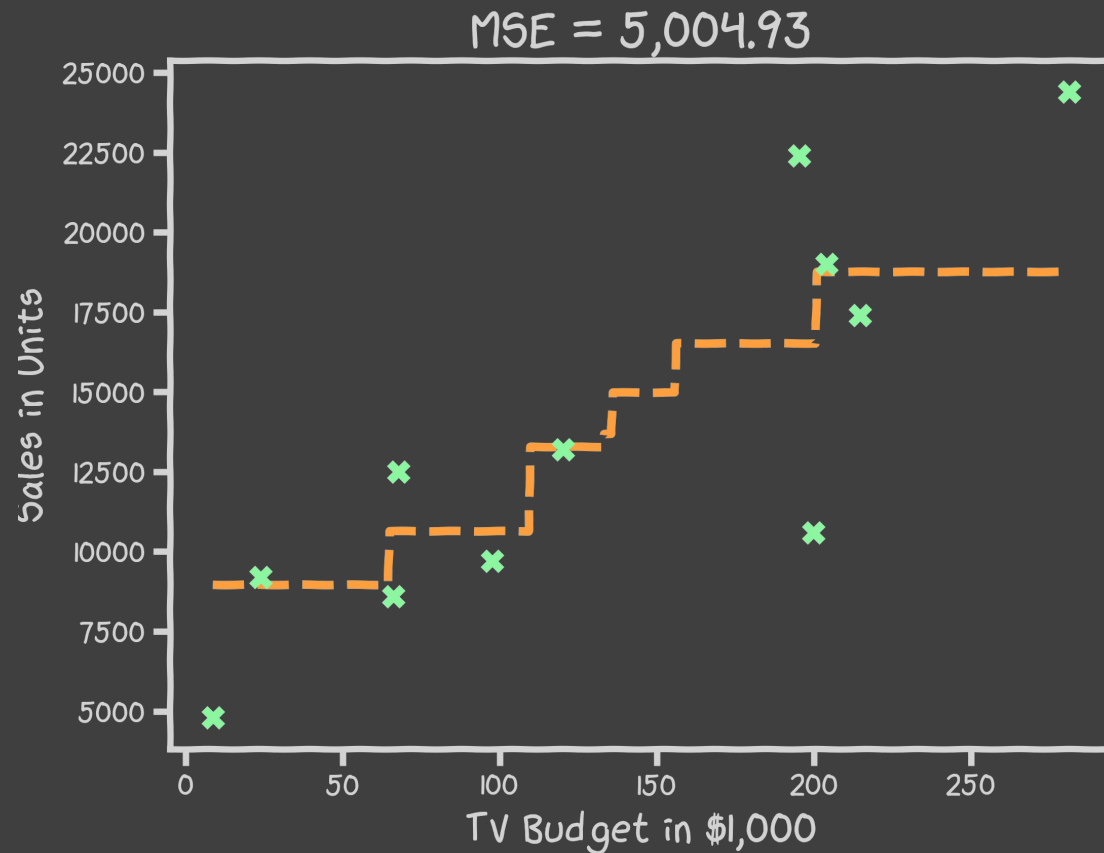
For a subset of the data, calculate the MSE for $k=3$.



Is $MSE=5.0$ good enough?

Model fitness

What if we measure the Sales in single units instead of thousands?

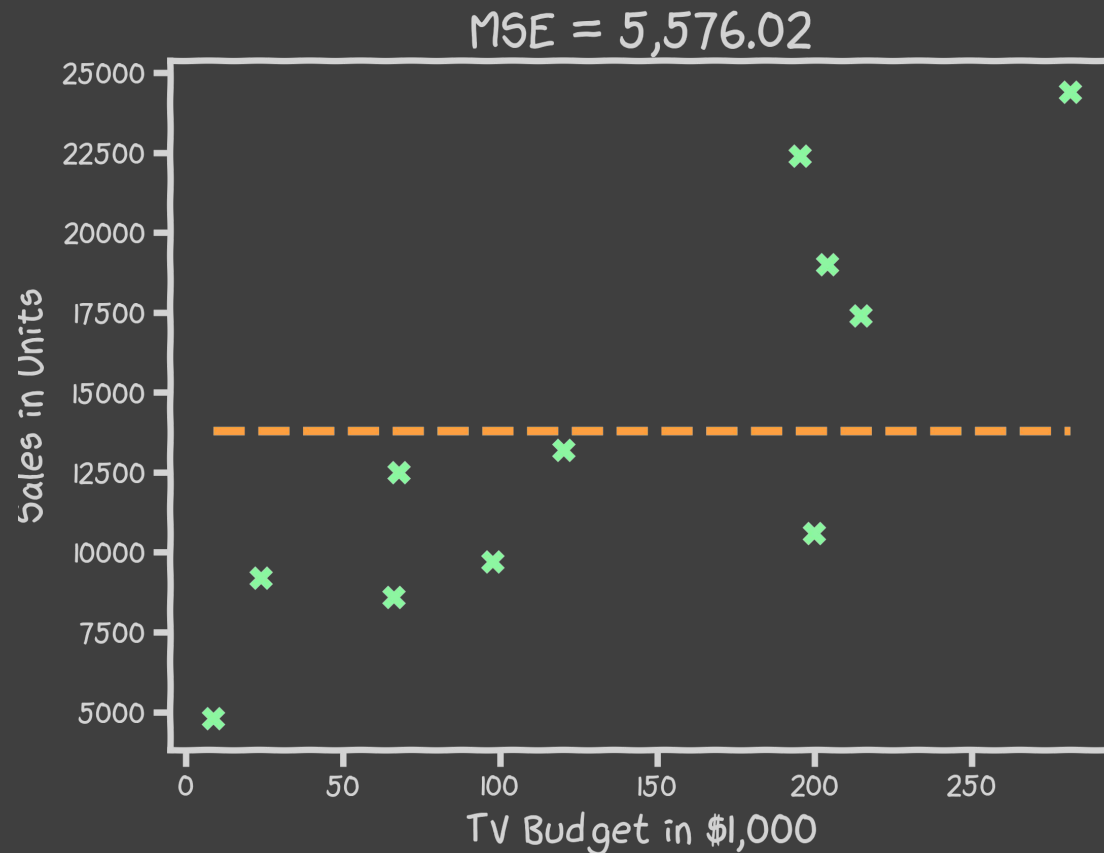


MSE is now 5004.93.

Is that good?

Model fitness

It is better if we compare it to something.



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 R

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

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