

# Lecture 13

## Model Selection and Hyperparameter Tuning

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Stanford University  
DATASCI 112



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- ① Recap
- ② Model Selection and Hyperparameter Tuning
- ③ Grid Search



① Recap

② Model Selection and Hyperparameter Tuning

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Here's a machine learning model.

```
from sklearn.pipeline import make_pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.neighbors import KNeighborsRegressor

pipeline = make_pipeline(
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Annotations on the code:

- A blue arrow points from the word "scaler" to the `StandardScaler()` call in the pipeline.
- A blue arrow points from the letter "k" to the `n_neighbors=5` parameter in the `KNeighborsRegressor` call.
- A blue arrow points from the text "scaler method" to the `StandardScaler()` call.

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The code defines a machine learning pipeline. It starts with a `make_pipeline` call containing two steps: `StandardScaler` and `KNeighborsRegressor`. The `n_neighbors` parameter of the `KNeighborsRegressor` is set to 5, and its `metric` is set to "euclidean". Below the pipeline, there are two assignments: `X_train` and `y_train`, which are data frames containing specific columns.

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Annotations:

- scaler method
- k
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- variables

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How do we choose between all the options (scaler, *k*, etc.)?



1 Recap

2 Model Selection and Hyperparameter Tuning

3 Grid Search



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For  $k$ -nearest neighbors, hyperparameters include:

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- metric (e.g., Euclidean distance)

The distinction isn't important. We always use cross-validation and pick the model / hyperparameter with the smallest test error.



# Example of Model Selection

Which input features should we include?



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- winter rain, summer temp



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- winter rain, summer temp
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- winter rain, summer temp, harvest rain
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- winter rain, summer temp, harvest rain
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```
for features in [["win", "summer"],  
                  ["win", "summer", "har"],  
                  ["win", "summer", "har", "sep"]]:  
    scores = cross_val_score(  
        pipeline,  
        X=df_train[features],  
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    print(features, -scores.mean())
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['win', 'summer'] 375.2716666666665
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['win', 'summer', 'har'] 363.04047619047617
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['win', 'summer', 'har', 'sep'] 402.4507142857142
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# Example of Hyperparameter Tuning

What is the best value of  $k$ ?

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# Example of Hyperparameter Tuning

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X_train = df_train[["win", "summer", "har"]]

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pd.Series(test_mses, index=ks).plot.line()
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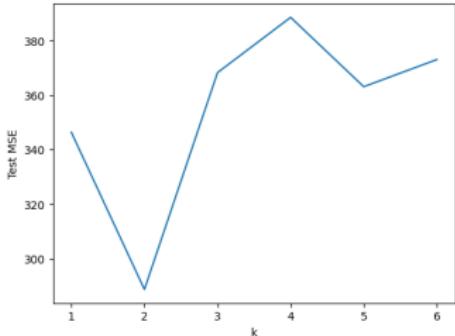
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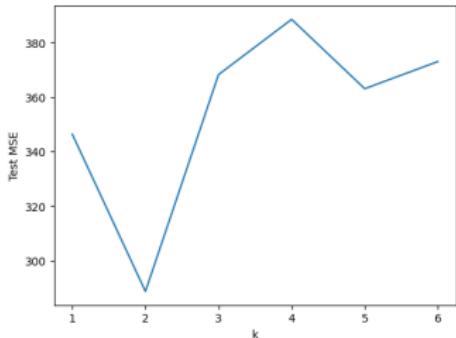
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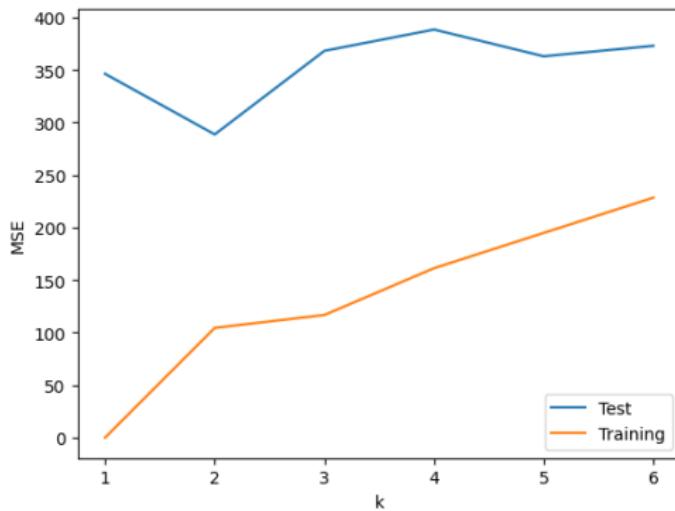


The Best value of  $k$  is 2



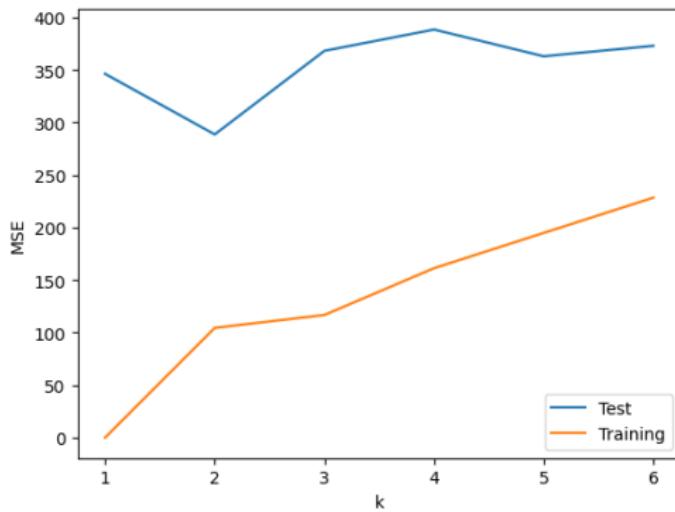
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Here are the training and test MSEs on the same graph.



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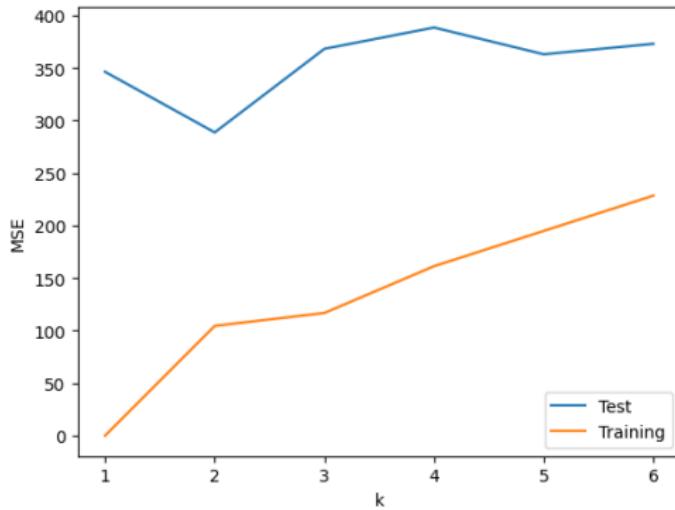
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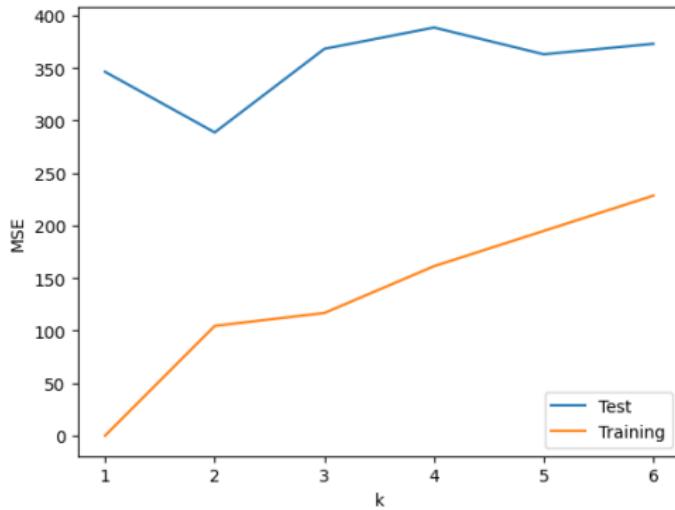


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Notice that training MSE only goes down as we decrease  $k$ .

If we optimize for training MSE, then we will pick  $k = 1$ , but this has worse test MSE.

In other words, the  $k = 1$  model has **overfit** to the training data.



① Recap

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③ Grid Search



# Grid Search

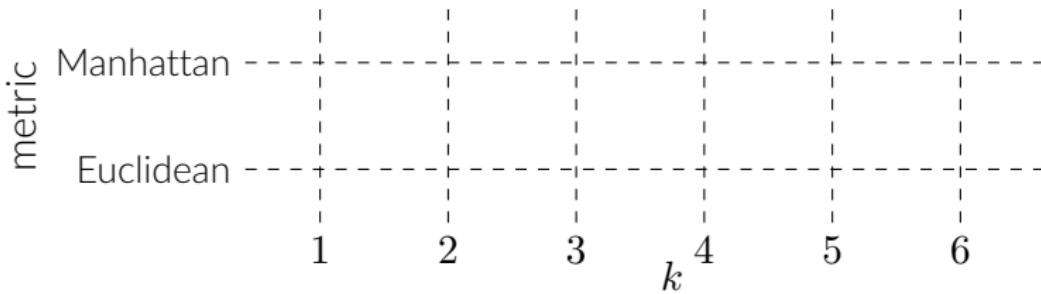
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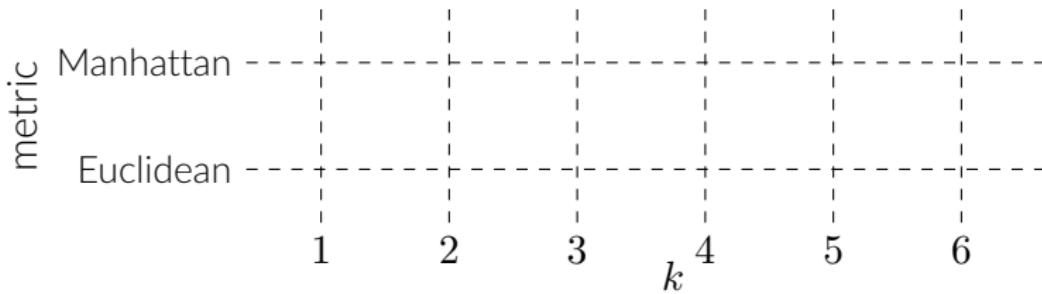
We need to try all 12 combinations on the following grid:



# Grid Search

Suppose we want to choose  $k$  and the distance metric (Euclidean or Manhattan).

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Scikit-Learn's `GridSearchCV` automates the creation of a grid with all combinations.



# Grid Search in Scikit-Learn

Let's try out `GridSearchCV` in a Colab.



# Challenges with Grid Search

Why can't all machine learning be automated by grid search?



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### Why can't all machine learning be automated by grid search?

There were 5 input features in the original data (summer temp, harvest rainfall, winter rainfall, Sept. temperature, age).



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Now, combine this with the choice of  $k$ , distance metric, and scaler.



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That's already  $32 \times 6 \times 2 \times 2 = 768$  models.



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And that's not even considering models besides  $k$ -nearest neighbors!



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- **coordinate optimization:**
  - start with guesses for all parameters,
  - try all values for *one* parameter (holding the rest constant) and find the best value of that parameter,
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You will have the chance to practice this on Lab 4, which is a **kaggle** competition to build the best machine learning model. There will be prizes for the winners!

