Lecture 13
Model Selection and Hyperparameter Tuning

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

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Here's a machine learning model.

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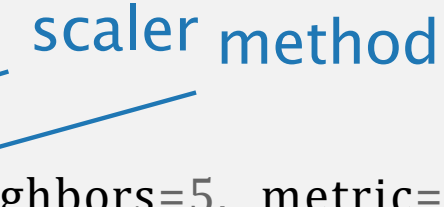

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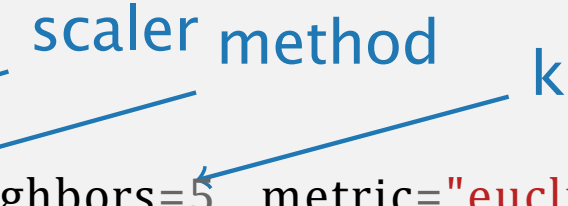

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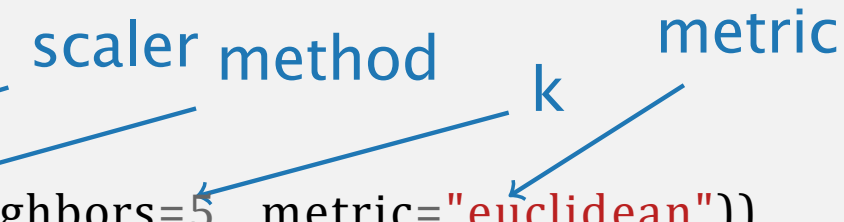

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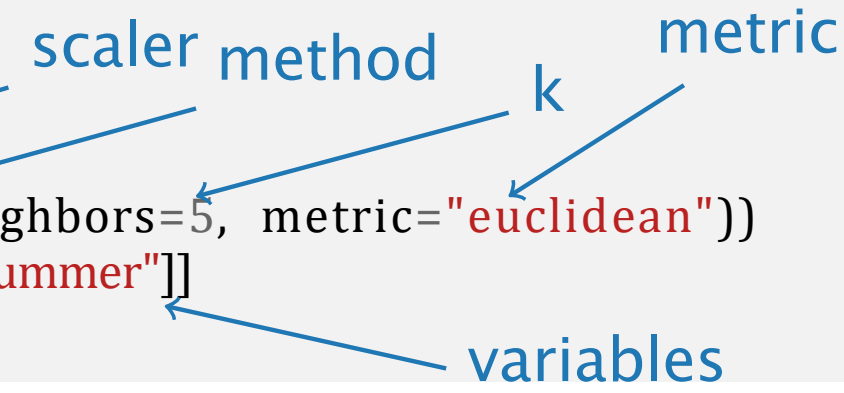

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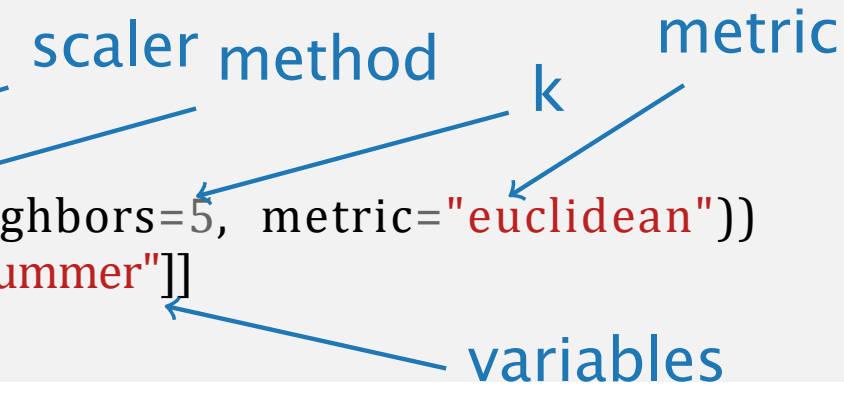

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How do we choose between all the options (scaler, k, etc.)?

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For k-nearest neighbors, hyperparameters include:

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

Example of Model Selection

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- winter rain, summer temp

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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],
      y=df_train["price"],
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      cv=4)
  print(features, -scores.mean())
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Example of Hyperparameter Tuning

What is the best value of k?

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

If k is too small, the model becomes very sensitive to noise → **overfitting.**
If k is too large, the model becomes too smooth and loses detail → **underfitting.**

Overfitting =
The model learns too much.
Very simply: The model **memorizes** the training data instead of learning general patterns.
Training performance is very good, but test performance is bad.It fits noise and irrelevant details.
Causes usually include: Model too complex,Too many features,Not enough training data,Not enough regularization.

In short: The model is like a student who memorizes the answers instead of understanding → gets perfect results on practice questions but fails the real exam.

Underfitting = The model is too simple.
Very simply: The model does not learn enough.It cannot capture patterns in the data.
Training performance is bad, and test performance is also bad.

Causes usually include: Model too simple,Not enough features,Not enough training.

In short: The model is like a student who didn't understand the lesson → performs poorly both in class (train) and on the exam (test).

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What is the best value of k?

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X_train = df_train[["win", "summer", "har"]]
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ks, test_mses = range(1, 7), []
for k in ks:
  pipeline = make_pipeline(
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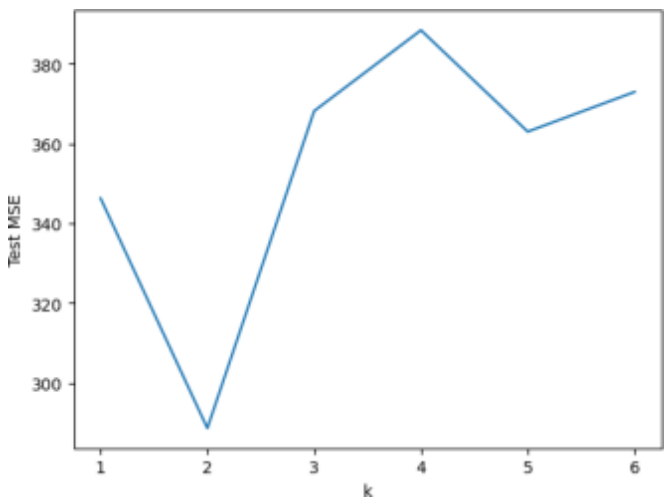

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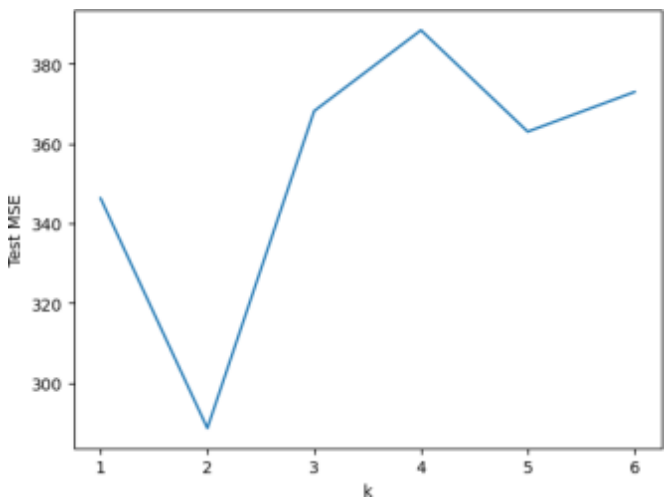
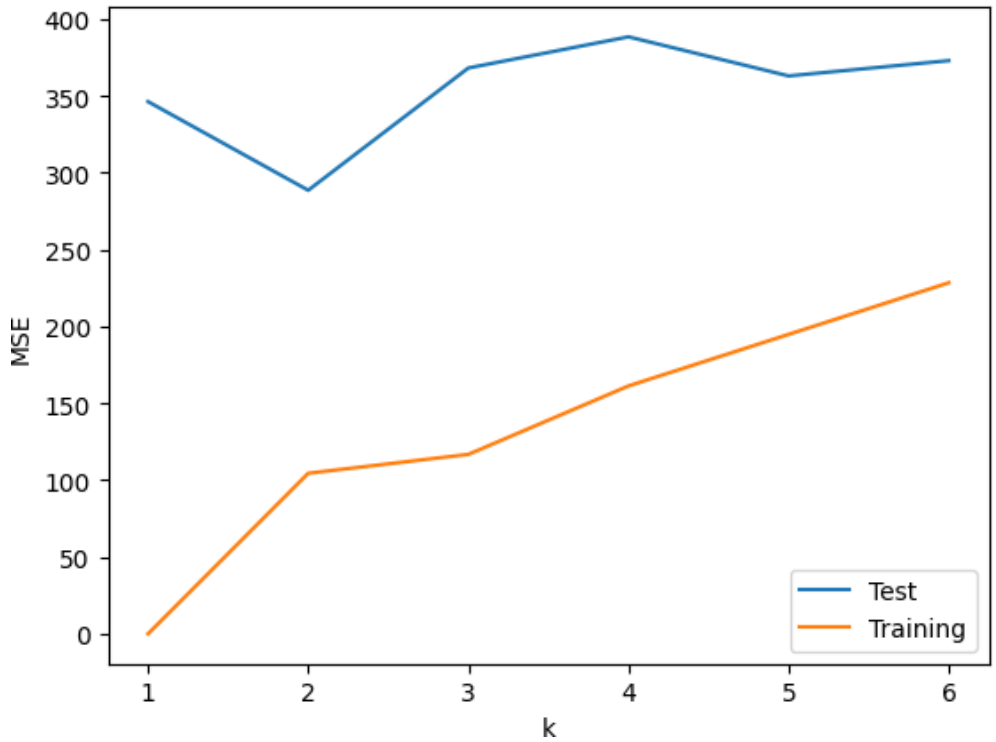


The best value of k is 2.

Training vs. Test Error

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



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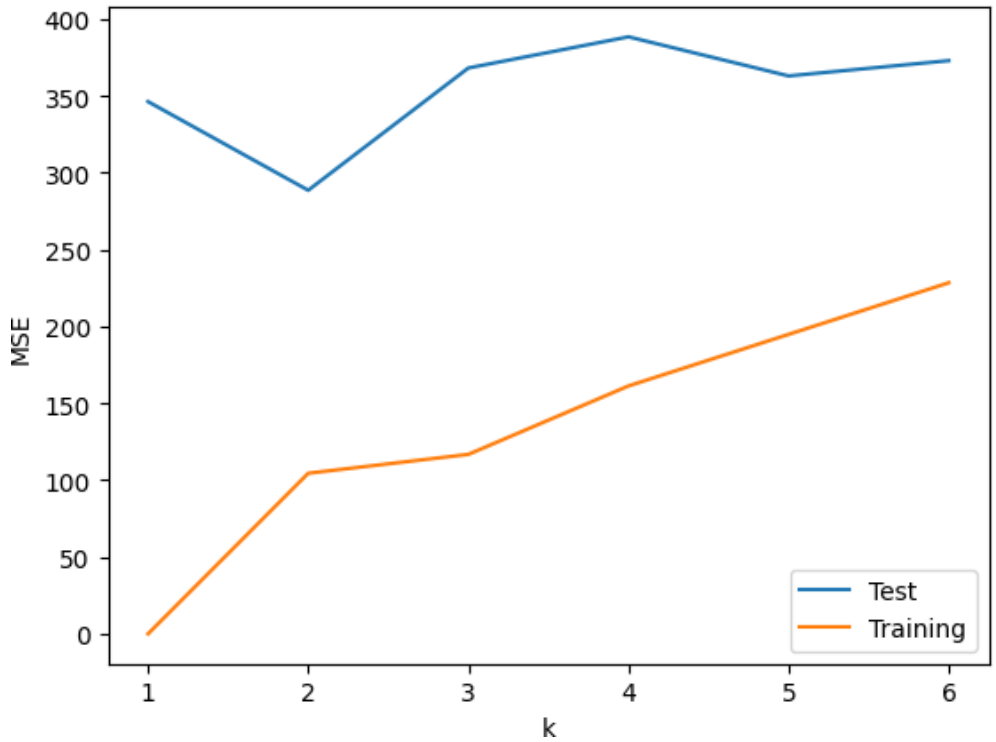

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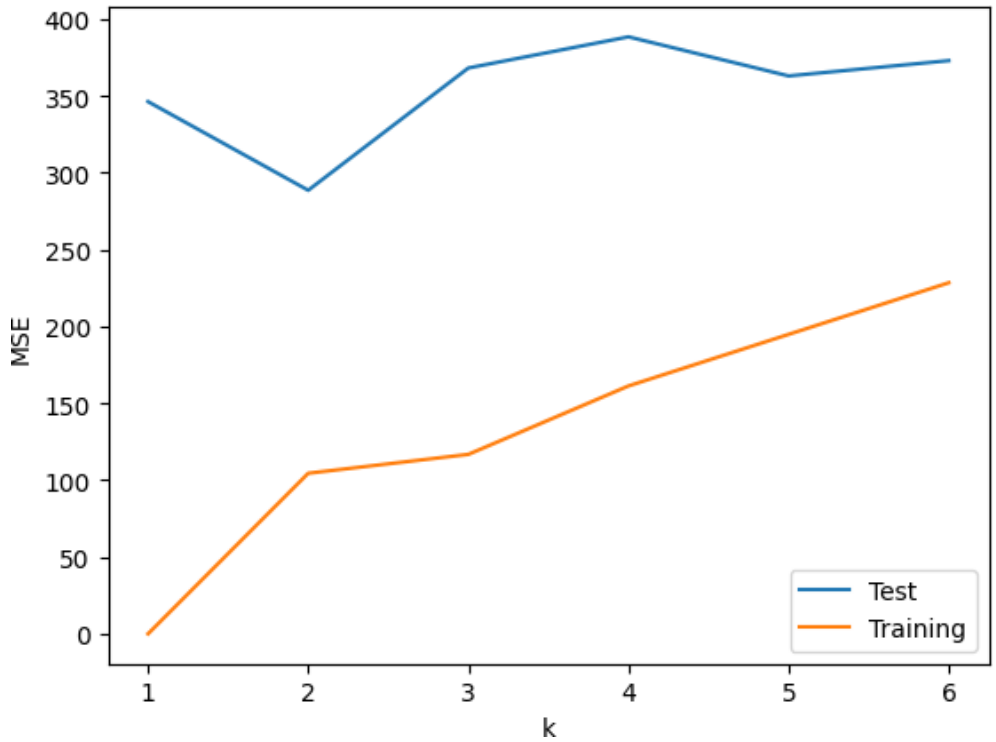

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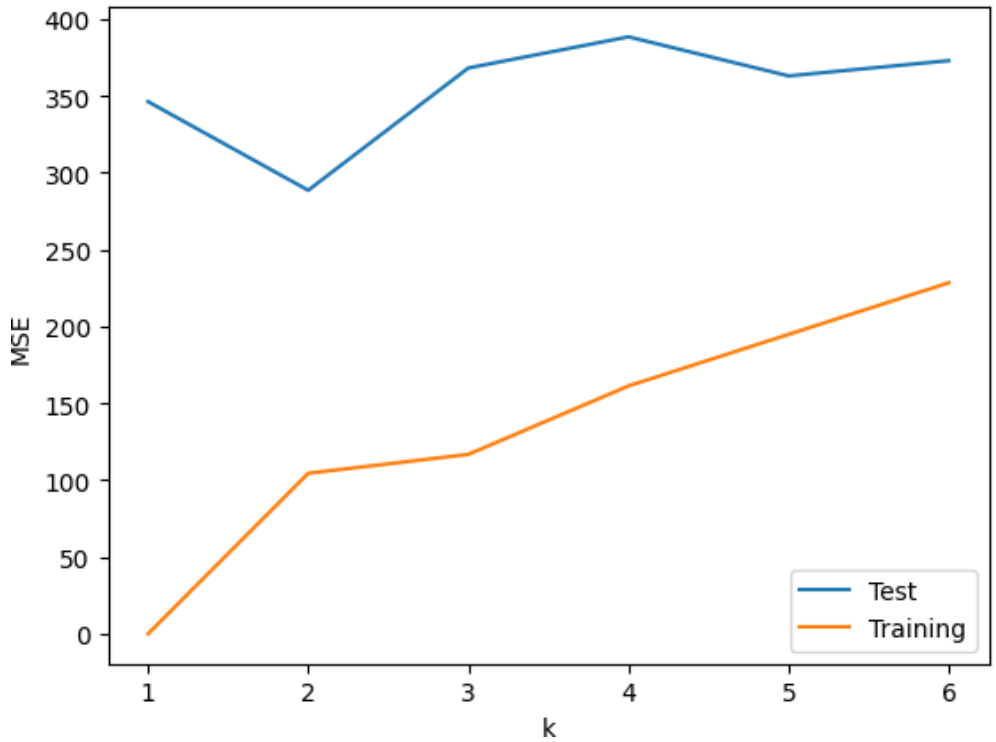

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In other words, the $k = 1$ model has **overfit** to the training data.

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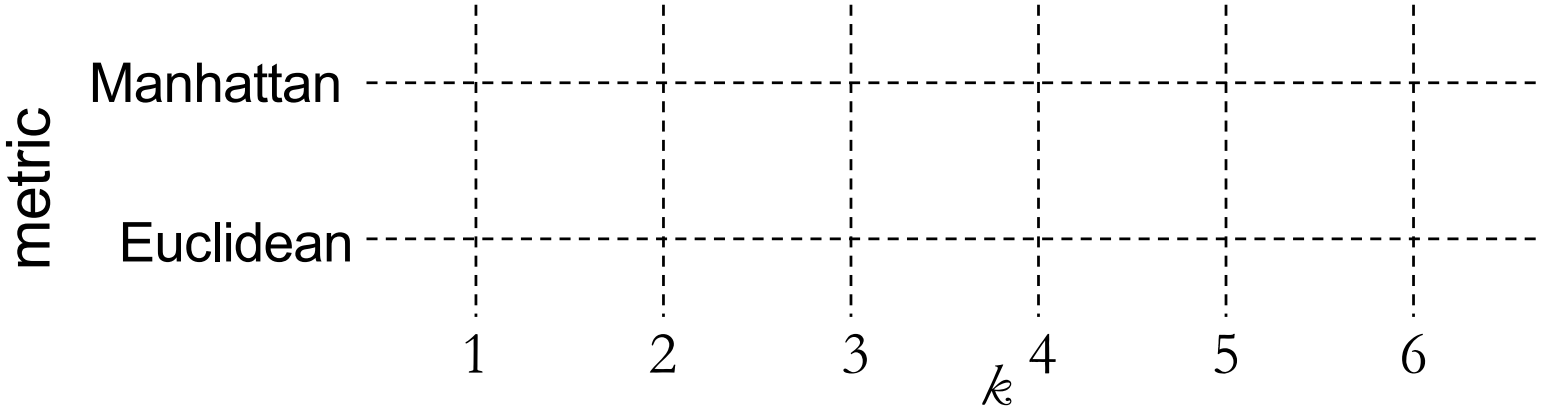

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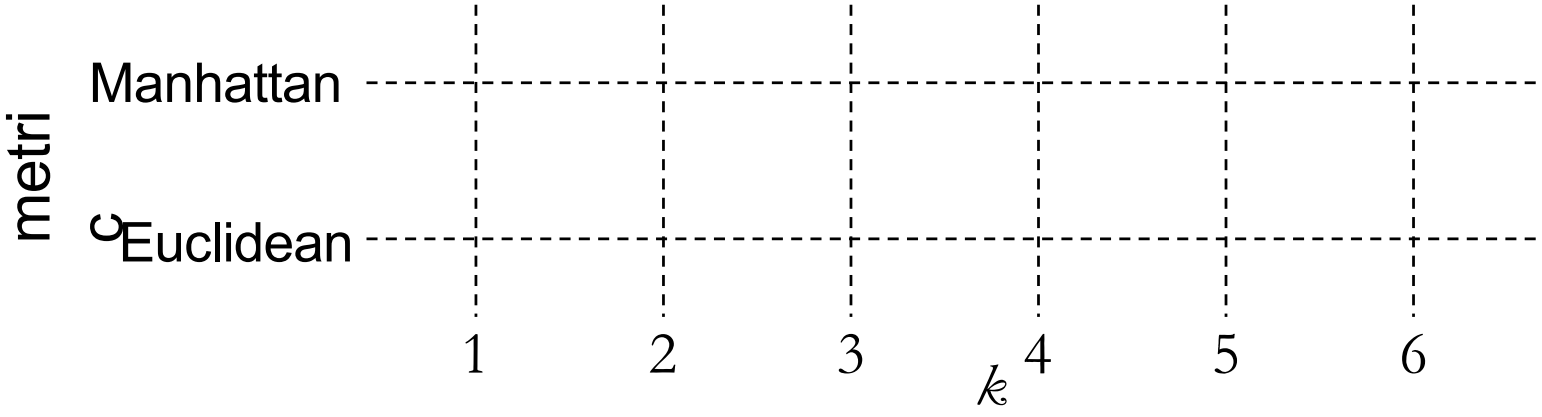

Scikit-Learn's `GridSearchCV` automates the creation of a grid with all combinations.

Grid Search in Scikit-Learn

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

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

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- 2 choices of distance metric (Euclidean, Manhattan)
- 2 choices of scaler (StandardScaler, MinMaxScaler)

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

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

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