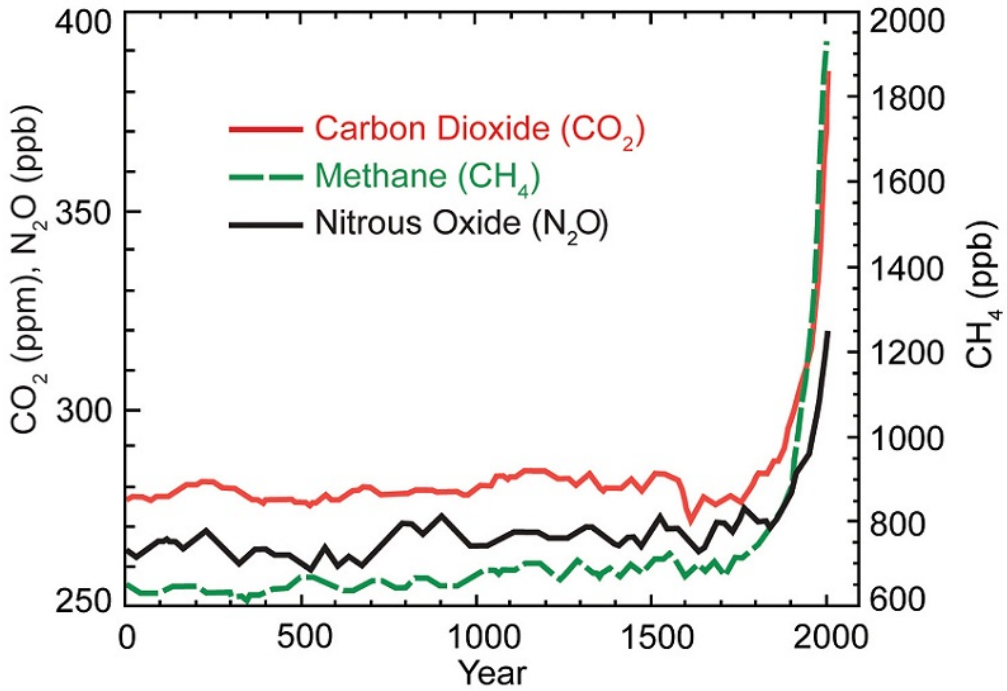
Model Selection and Hyperparameter Tuning

Dennis Sun (modified by Jonathan Taylor)
Stanford University

DATASCI 112

May 1, 2026



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

1 Recap

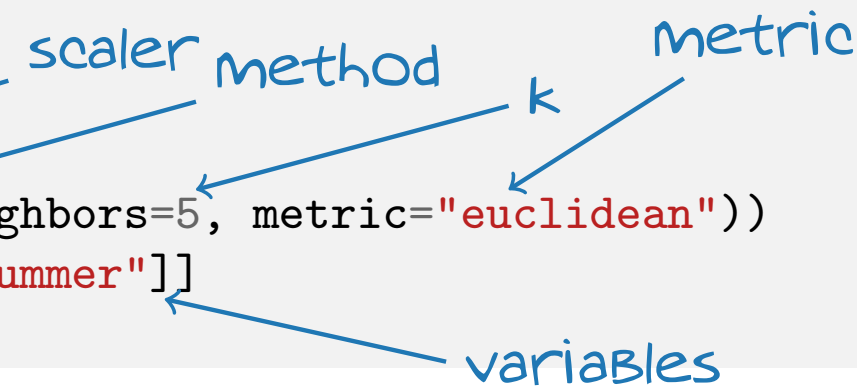
2 Model Selection and Hyperparameter Tuning

3 Grid Search

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(
    StandardScaler(),
    KNeighborsRegressor(n_neighbors=5, metric="euclidean"))
X_train = df_train[["win", "summer"]]
y_train = df_train["price"]
```



The right way to evaluate machine learning models is *test error*, which is estimated using cross-validation

```
from sklearn.model_selection import cross_val_score
scores = cross_val_score(
    pipeline,
    X=X_train, y=y_train,
    scoring="neg_mean_squared_error",
    cv=4)
-scores.mean()
```

```
375.27166666666665
```

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

1 Recap

2 Model Selection and Hyperparameter Tuning

3 Grid Search

Two Related Problems

Model Selection refers to the choice of:

- which input features to include (e.g., winter rainfall, summer temperature)
- what preprocessing to do (e.g., scaler)
- what machine learning method to use (e.g., k-nearest neighbors)

Hyperparameter Tuning refers to the choice of parameters in the machine learning method.
For k-nearest neighbors, hyperparameters include:

- k
- metric (e.g., Euclidean distance)

The distance isn't important. People will typically use cross-validation and pick the model / hyperparameter with the smallest test error.

Example of Model Selection

Which input features should we include?

- winter rain, summer temp
- winter rain, summer temp, harvest rain
- winter rain, summer temp, harvest rain, Sept. temp

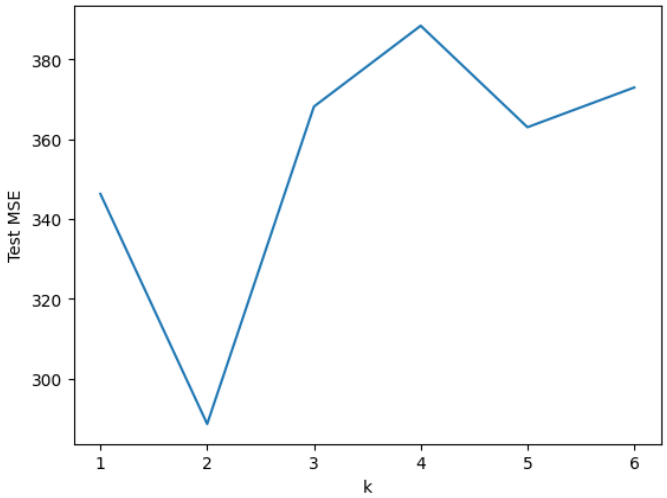
```
for features in [["win", "summer"],
                 ["win", "summer", "har"],
                 ["win", "summer", "har", "sep"]]:
  scores = cross_val_score(
      pipeline,
      X=df_train[features],
      y=df_train["price"],
      scoring="neg_mean_squared_error",
      cv=4)
  print(features, -scores.mean())
```

```
['win', 'summer'] 375.27166666666665
['win', 'summer', 'har'] 363.04047619047617
['win', 'summer', 'har', 'sep'] 402.4507142857142
```

Example of Hyperparameter Tuning

What is the best value of k?

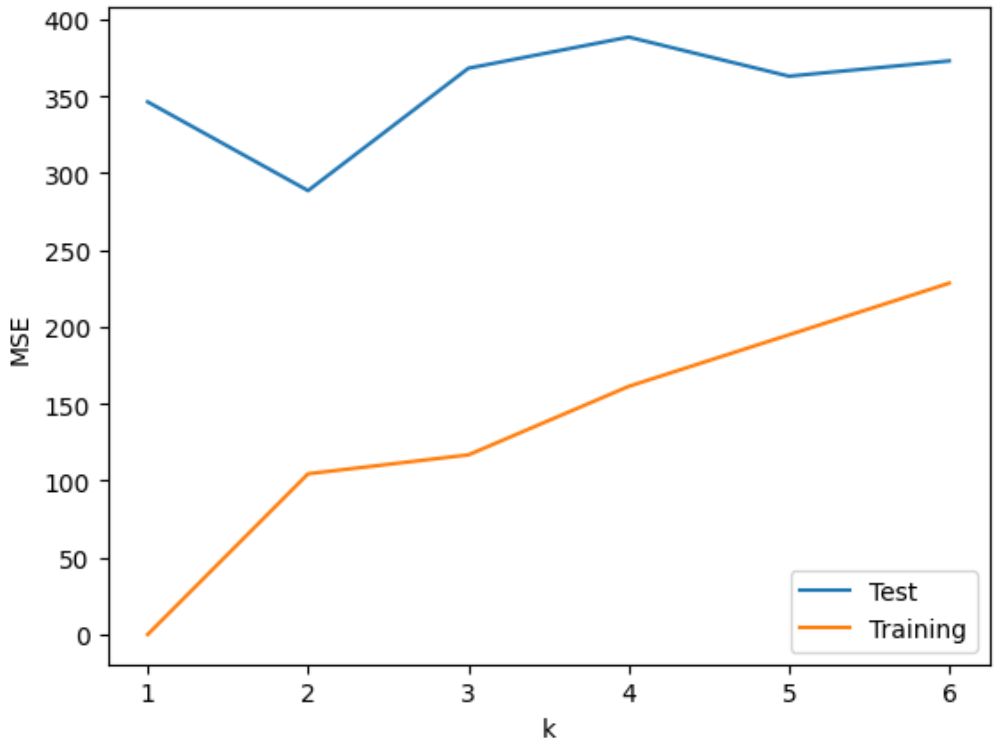
```
ks, test_mses = range(1, 7), []
for k in ks:
  pipeline = make_pipeline(
      StandardScaler(),
      KNeighborsRegressor(n_neighbors=k, metric="euclidean"))
  scores = cross_val_score(
      pipeline, X_train, y_train,
      scoring="neg_mean_squared_error", cv=4)
pd.Series(test_mses, index=ks).plot.line()
```



The best value of k is 2.

Training vs. Test Error

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



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

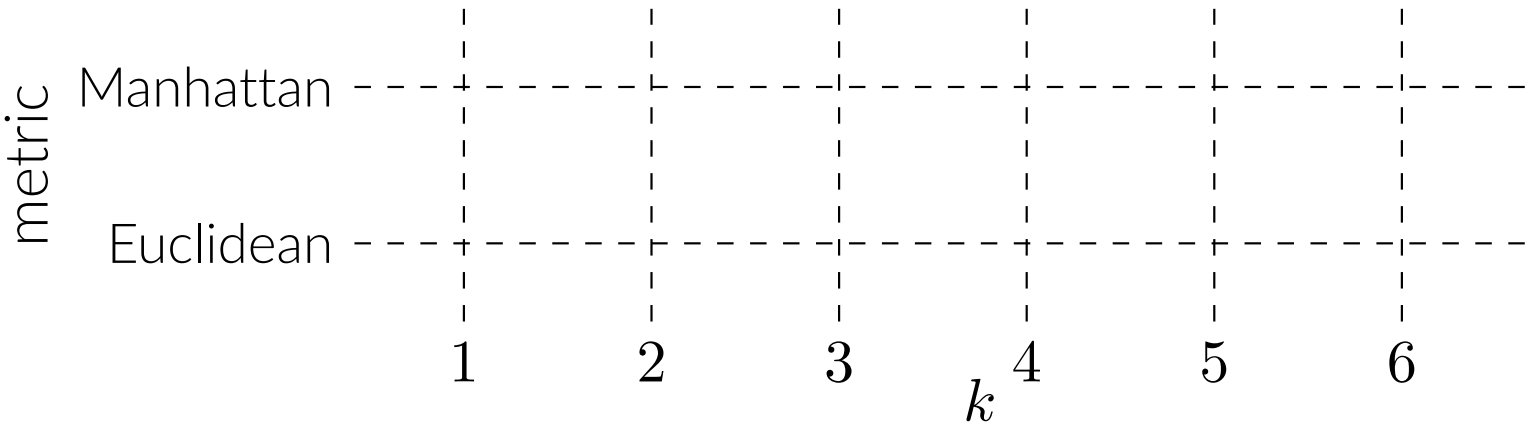
2 Model Selection and Hyperparameter Tuning

3 Grid Search

Grid Search

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

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



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?

There were 5 input features in the original data (summer temp, harvest rainfall, winter rainfall, Sept. temperature, age).
How many combinations of features would we need to try?

$2^5 = 32$

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

- 6 choices of k
- 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!

Heuristics for Parameter Tuning

For large data sets, it is impossible to try every combination of models and parameters.

So instead we use *heuristics*, which do not guarantee the best model but tend to work well in practice.

- **randomized search**: try random combinations of parameters, implemented in Scikit-Learn as `RandomizedSearchCV`.
- **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,
  - cycle through the parameters.

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!