

Lecture 12

Evaluating Regression Models

- ① Recap
- ② Measuring Error
- ③ Estimating Test Error
- ④ Cross-Validation

1 Recap

2 Measuring Error

3 Estimating Test Error

4 Cross-Validation

Training and Test Data

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```
import pandas as pd

df = pd.read_csv("https://dlsun.github.io/pods/data/bordeaux.csv",
                  index_col="year")
df_train = df.loc[:1980].copy()
df_test = df.loc[1981:].copy()
```

Purpose:

To train the model using data up to 1980 and predict outcomes for the years after 1981.

Training and Test Data

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df_train = df.loc[:1980].copy()
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```

Let's separate the inputs X from the labels y .

```
X_train = df_train[["win", "summer"]]
y_train = df_train["price"]

X_test = df_test[["win", "summer"]]
```

Selects winter rainfall (`win`) and summer temperature (`summer`) as input features for training.

Selects price as the target variable for training.

Selects the same input features for the test set.

price is not included because it is unknown and will be predicted

K- Nearest Neighbors

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

pipeline = make_pipeline(
    StandardScaler(),
    KNeighborsRegressor(n_neighbors=5))
pipeline.fit(X=X_train, y=y_train)
pipeline.predict(X=X_test)
```

Scale the inputs → train a KNN regression model → predict prices for unseen years.

A pipeline in machine learning is a structure that runs multiple steps together as if they were a single model.

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array([35.8, 54. , 52.2, 18.4, 35.6, 13.2, 37. , 51.4, 36.6, 36.6, 40.6])
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```

Today: How do we know if this model is any good?

1 Recap

2 Measuring Error

3 Estimating Test Error

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If the true labels are y_1, \dots, y_n and our model predicts $\hat{y}_1, \dots, \hat{y}_n$, how do we measure how well our model did?

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Calculating MSE or MAE requires data where true labels are known. Where can we find such data?

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Remember, we are predicting the price of wine. So the model is off by 207.24 square dollars on average.

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Remember, we are predicting the price of wine. So the model is off by 207.24 square dollars on average.

The square root is easier to interpret. The model is off by $\sqrt{207.24} \approx \$14.40$ on average. This is called the **RMSE**.

Root Mean Squared Error

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A 1-nearest neighbor model will always be perfect on the training data. But is it necessarily the best model?

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In general, test error > training error.

Training error = error on the data the model was trained on

Test error = error on new, unseen data

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Now: How do we estimate the test error?

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Validation Set

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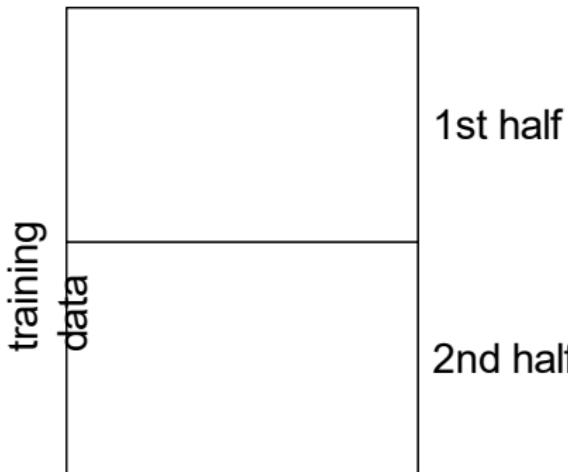
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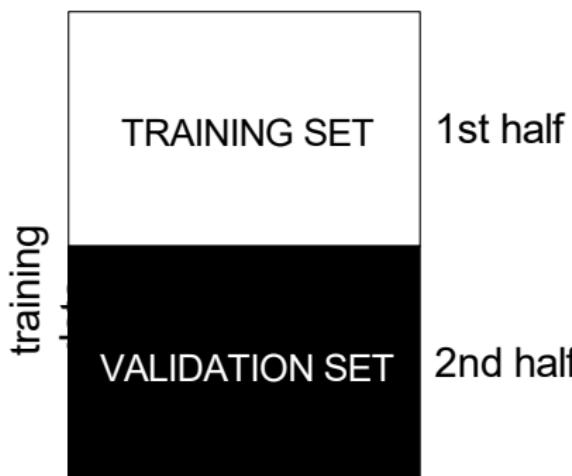
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Implementing the Validation Set

Let's implement this idea in a Colab!



1 Recap

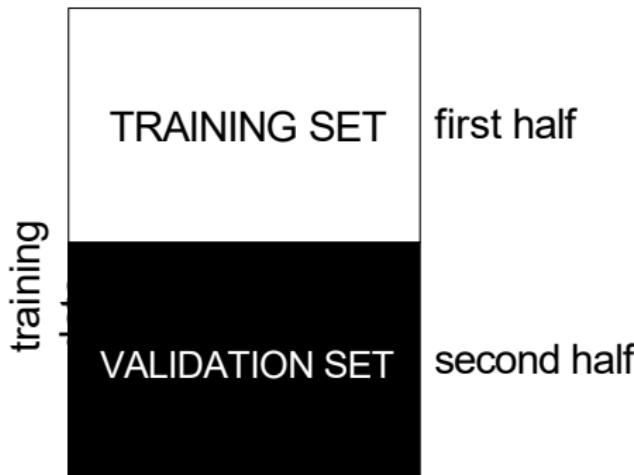
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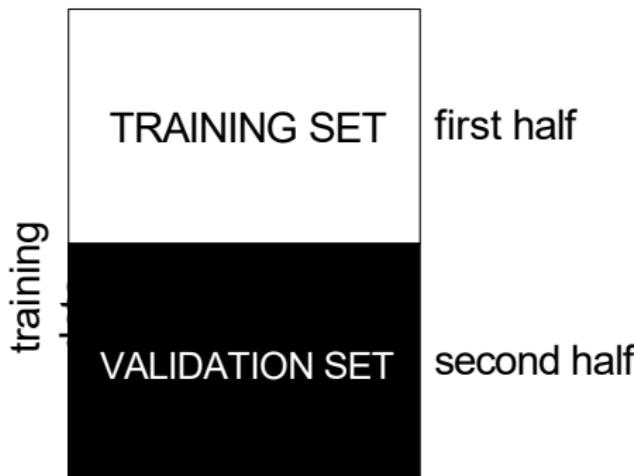
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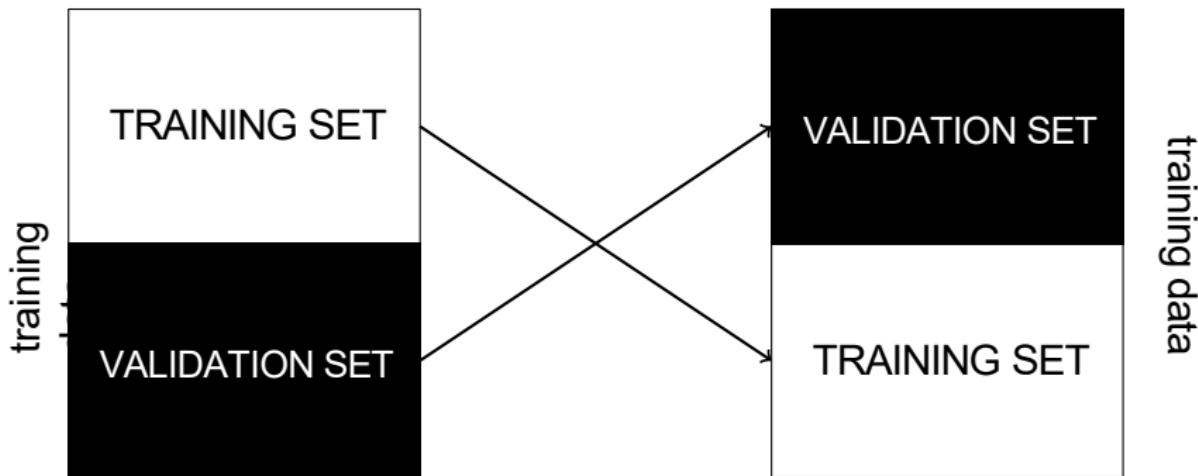
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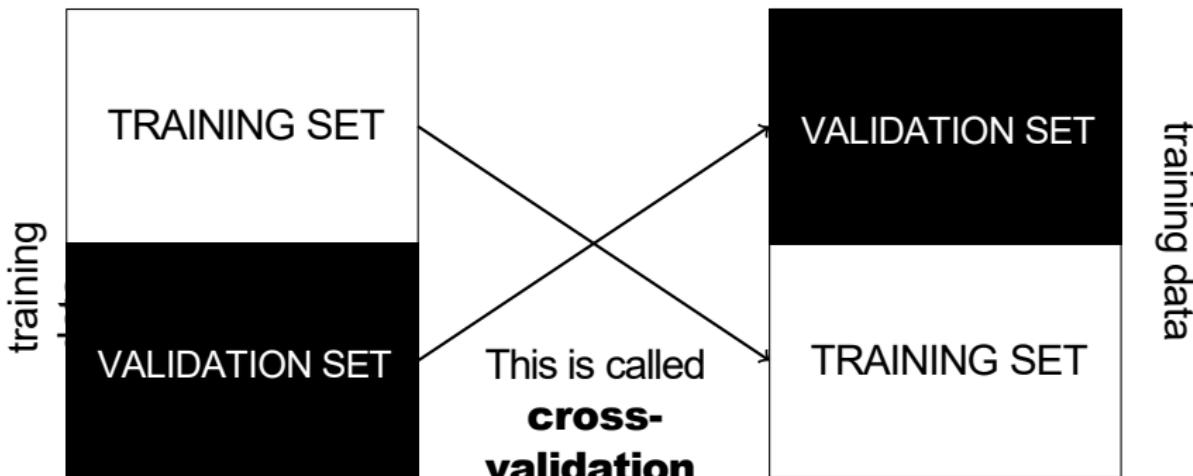
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Implementing Cross-Validation from Scratch

Previously, we fit the model to the training set and evaluated the predictions on the validation set.

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pipeline.fit(X_train_set, y_train_set)  
y_val_set_ = pipeline.predict(X_val_set)  
mean_squared_error(y_val_set, y_val_set_)
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195.71428571428572

Train the model → predict on validation data → evaluate prediction error using MSE.

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Train on validation data → predict training data → measure error with MSE.

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Wow, the estimates can be quite different!

To come up with one overall estimate of the test error, we can average them.

```
(195.71 + 306.92) / 2
```

251.315

K-Fold Cross Validation

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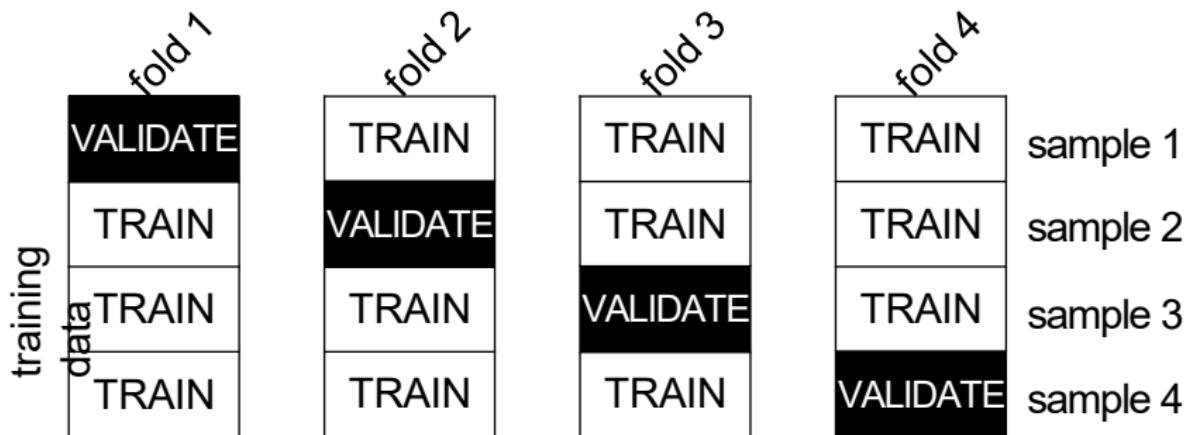
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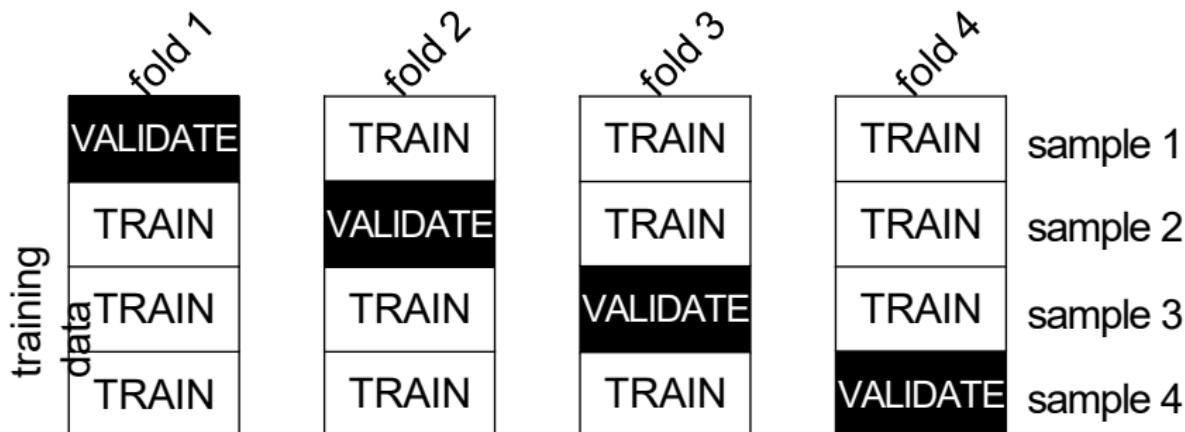


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This way, we use $1 - 1/K$ of the data for training.

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from sklearn.model_selection import cross_val_score
scores = cross_val_score(
    pipeline,
    X=df_train[["win", "summer"]],
    y=df_train["price"],           # this is all of the training data!
    scoring="neg_mean_squared_error", # higher is better for a score
    cv=4)
scores
```

cv = 4: Performs 4-fold cross-validation
Training data is split into 4 parts.
Each part is used once as validation data.

scores shows how well the model predicts wine prices across 4 different train-validation splits.

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262.7142857142857

RMSE ≈ 16.21 (modelin tahmin ettiği şarap fiyatlarının gerçek fiyatlardan ortalama olarak yaklaşık 16.2 birim saplığı anlamına gelir.)