Classification II: evaluation & tuning

Session learning objectives

By the end of the session, learners will be able to do the following:

- Describe what training, validation, and test data sets are and how they are used in classification.
- Split data into training, validation, and test data sets.
- Describe what a random seed is and its importance in reproducible data analysis.
- Set the random seed in Python using the `numpy.random.seed` function.
- Describe and interpret accuracy, precision, recall, and confusion matrices.

Session learning objectives cont’d

By the end of the session, learners will be able to do the following:

- Evaluate classification accuracy, precision, and recall in Python using a test set, a single validation set, and cross-validation.
- Produce a confusion matrix in Python.
- Choose the number of neighbors in a K-nearest neighbors classifier by maximizing estimated cross-validation accuracy.
- Describe underfitting and overfitting, and relate it to the number of neighbors in K-nearest neighbors classification.
- Describe the advantages and disadvantages of the K-nearest neighbors classification algorithm.

Evaluating performance

- Sometimes our classifier might make the wrong prediction.
- A classifier does not need to be right 100% of the time to be useful, though we don't want the classifier to make too many wrong predictions.
- How do we measure how "good" our classifier is?

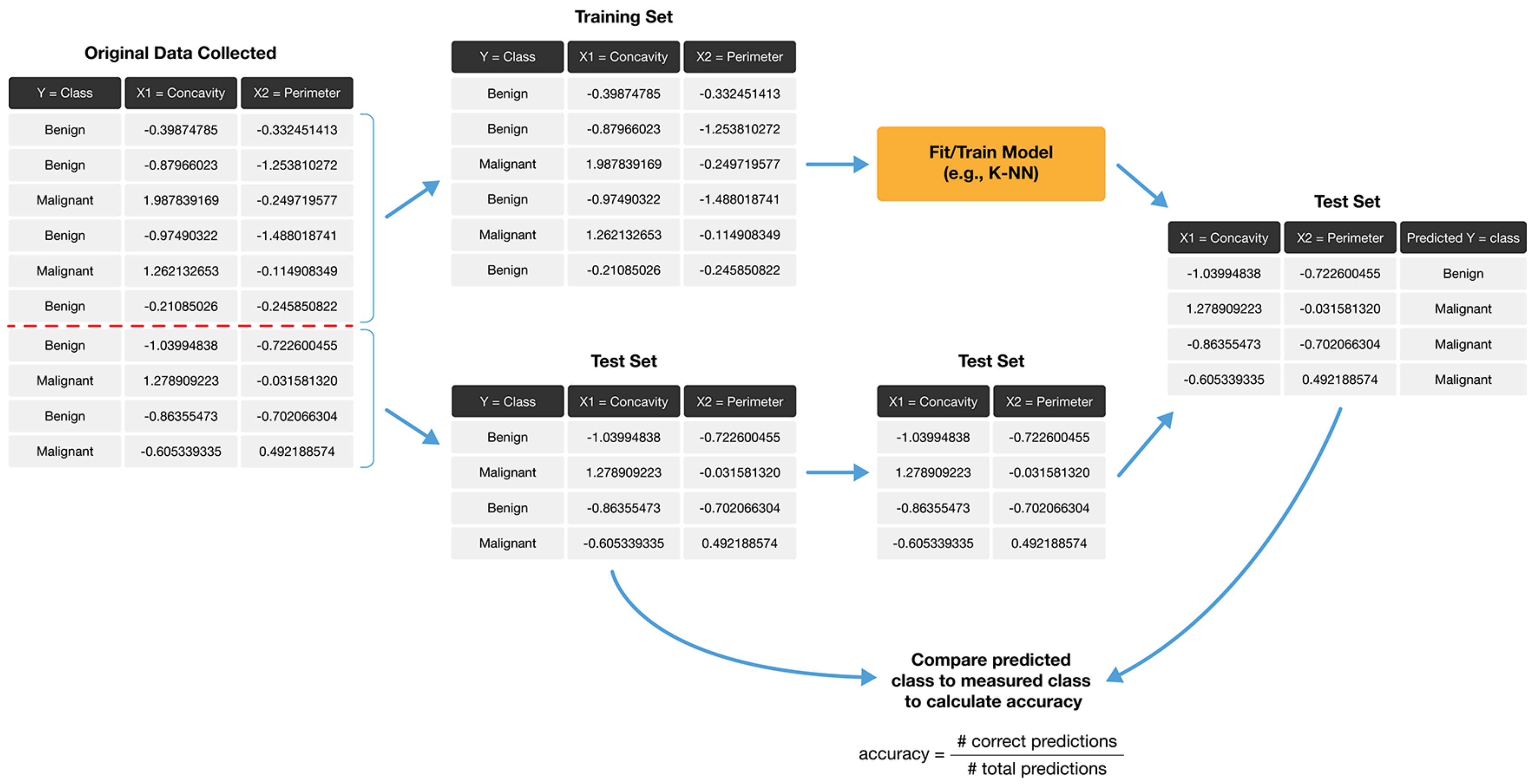
Data splitting

- The trick is to split the data into a **training set** and **test set**.
- Only the **training set** when building the classifier.
- To evaluate the performance of the classifier, we first set aside the labels from the **test set**, and then use the classifier to predict the labels in the **test set**.
- If our predictions match the actual labels for the observations in the **test set**, then we have some confidence that our classifier might also accurately predict the class labels for new observations without known class labels.

Splitting the data into training and testing sets

Prediction accuracy

$$\text{accuracy} = \frac{\text{number of correct predictions}}{\text{total number of predictions}}$$



Fit/Train Model (e.g., K-NN)
Compare predicted class to measured class to calculate accuracy

Original Data Collected

Y = Class	X1 = Concavity	X2 = Perimeter
Benign	-0.39874785	-0.332451413
Benign	-0.87966023	-1.253810272
Malignant	1.987839169	-0.249719577
Benign	-0.97490322	-1.488018741
Malignant	1.262132653	-0.114908349
Benign	-0.21085026	-0.245850822
Benign	-1.03994838	-0.722600455
Malignant	1.278909223	-0.031581320
Benign	-0.86355473	-0.702066304
Malignant	-0.605339335	0.492188574

Training Set

Y = Class	X1 = Concavity	X2 = Perimeter
Benign	-0.39874785	-0.332451413
Benign	-0.87966023	-1.253810272
Malignant	1.987839169	-0.249719577
Benign	-0.97490322	-1.488018741
Malignant	1.262132653	-0.114908349
Benign	-0.21085026	-0.245850822

Test Set

Y = Class	X1 = Concavity	X2 = Perimeter
Benign	-1.03994838	-0.722600455
Malignant	1.278909223	-0.031581320
Benign	-0.86355473	-0.702066304
Malignant	-0.605339335	0.492188574

Test Set

X1 = Concavity	X2 = Perimeter
-1.03994838	-0.722600455
1.278909223	-0.031581320
-0.86355473	-0.702066304
-0.605339335	0.492188574

Test Set

X1 = Concavity	X2 = Perimeter	Predicted Y = class
-1.03994838	-0.722600455	Benign
1.278909223	-0.031581320	Malignant
-0.86355473	-0.702066304	Malignant
-0.605339335	0.492188574	Malignant

$$\text{accuracy} = \frac{\text{\# correct predictions}}{\text{\# total predictions}}$$

Is knowing accuracy enough?

- Example accuracy calculation:

$$\text{accuracy} = \frac{\text{number of correct predictions}}{\text{total number of predictions}} = \frac{58}{65} = 0.892$$

- Prediction accuracy only tells us how often the classifier makes mistakes in general, but does not tell us anything about the *kinds* of mistakes the classifier makes.
- The **confusion matrix** tells a more complete story.

Example confusion matrix for the breast cancer data:

	Predicted Malignant	Predicted Benign
Actually Malignant	1	3
Actually Benign	4	57

- **True Positive:** A malignant observation that was classified as malignant (top left).
- **False Positive:** A benign observation that was classified as malignant (bottom left).
- **True Negative:** A benign observation that was classified as benign (bottom right).
- **False Negative:** A malignant observation that was classified as benign (top right).

Precision & recall

- *Precision* quantifies how many of the positive predictions the classifier made were actually positive.

$$\text{precision} = \frac{\text{number of correct positive predictions}}{\text{total number of positive predictions}}$$

- *Recall* quantifies how many of the positive observations in the test set were identified as positive.

$$\text{recall} = \frac{\text{number of correct positive predictions}}{\text{total number of positive test set observations}}$$

Precision and recall for the breast cancer data set example

	Predicted Malignant	Predicted Benign
Actually Malignant	1	3
Actually Benign	4	57

$$\text{precision} = \frac{1}{1+4} = 0.20, \quad \text{recall} = \frac{1}{1+3} = 0.25$$

> So even with an accuracy of 89%, the precision and recall of the classifier were both relatively low. For this data analysis context, recall is particularly important: if someone has a malignant tumor, we certainly want to identify it. A recall of just 25% would likely be unacceptable!

Randomness and seeds

- Our data analyses will often involve the use of randomness
- We use randomness any time we need to make a decision in our analysis that needs to be fair, unbiased, and not influenced by human input (e.g., splitting into training and test sets).
- However, the use of randomness runs counter to one of the main tenets of good data analysis practice: reproducibility…
- The trick is that in Python—and other programming languages—randomness is not actually random! Instead, Python uses a random number generator that produces a sequence of numbers that are completely determined by a seed value.
- Once you set the seed value, everything after that point may look random, but is actually totally reproducible.

Setting the seed in Python

Let's say we want to make a series object containing the integers from 0 to 9. And then we want to randomly pick 10 numbers from that list, but we want it to be reproducible.

```python
import numpy as np
import pandas as pd

np.random.seed(1)

nums_0_to_9 = pd.Series([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])

random_numbers1 = nums_0_to_9.sample(n=10).to_list()
random_numbers1
```

```
[2, 9, 6, 4, 0, 3, 1, 7, 8, 5]
```

You can see that `random_numbers1` is a list of 10 numbers from 0 to 9 that, from all appearances, looks random. If we run the `sample` method again, we will get a fresh batch of 10 numbers that also look random.

```python
random_numbers2 = nums_0_to_9.sample(n=10).to_list()
random_numbers2
```

```
[9, 5, 3, 0, 8, 4, 2, 1, 6, 7]
```

Setting the seed in Python (cont’d)

If we choose a different value for the seed—say, 4235—we obtain a different sequence of random numbers:

```python
# seed was 1 on the last slide when we generated this list
random_numbers1
```

```
[2, 9, 6, 4, 0, 3, 1, 7, 8, 5]
```

```python
np.random.seed(4235)
random_numbers1_different = nums_0_to_9.sample(n=10).to_list()

random_numbers1
random_numbers1_different
```

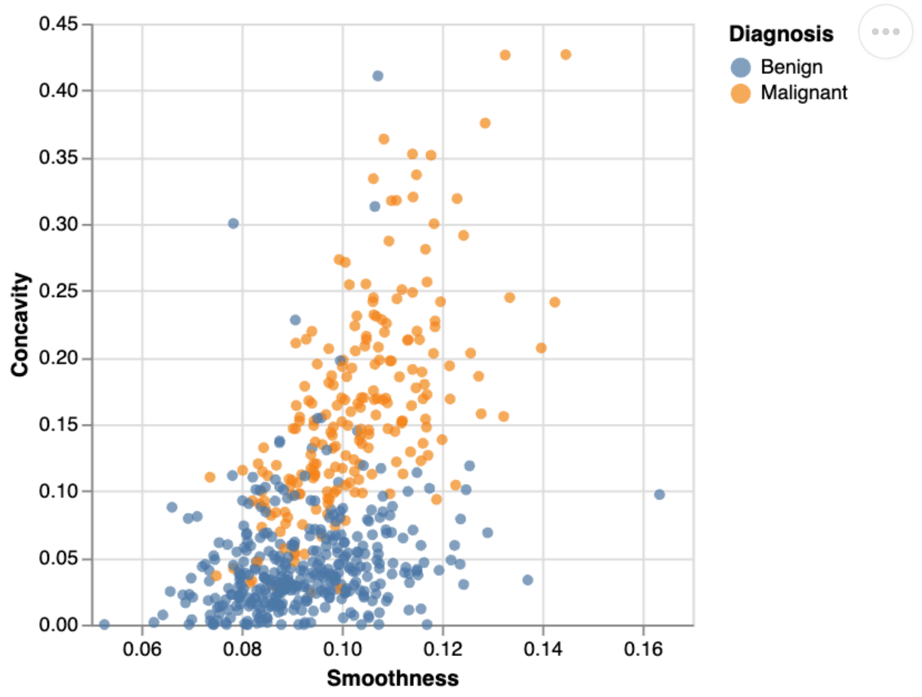
```
[6, 7, 2, 3, 5, 9, 1, 4, 0, 8]
```

Back to the breast cancer data set example

```python
# load packages
import altair as alt
import pandas as pd
from sklearn import set_config

# Output dataframes instead of arrays
set_config(transform_output="pandas")

# set the seed
np.random.seed(3)

# load data
cancer = pd.read_csv("data/wdbc_unscaled.csv")
# re-label Class "M" as "Malignant", and Class "B" as "Benign"
cancer["Class"] = cancer["Class"].replace({
    "M" : "Malignant",
    "B" : "Benign"
})
```

Breast cancer data

```python
perim_concav = alt.Chart(cancer).mark_circle().enc
    x=alt.X("Smoothness").scale(zero=False),
    y="Concavity",
    color=alt.Color("Class").title("Diagnosis")
)
```



Create the train / test split

- **Before** fitting any models, or doing exploratory data analysis, it is critical that you split the data into training and test sets.
- Typically, the training set is between 50% and 95% of the data, while the test set is the remaining 5% to 50%.
- The `train_test_split` function from `scikit-learn` handles the procedure of splitting the data for us.
- Use `shuffle=True` to remove the influence of order in the data set.
- Set the `stratify` parameter to be the response variable to ensure the same proportion of each class ends up in both the training and testing sets.

Splitting the breast cancer data set

- Split the data so 75% are in the training set, and 25% in the test set
- Data are shuffled
- Split is stratified on the `Class` variable

```python
from sklearn.model_selection import train_test_split

cancer_train, cancer_test = train_test_split(
    cancer, train_size=0.75, stratify=cancer["Class"]
)
```

Checking the splits

- We can use `.info()` to look at the splits
- Let's look at the training split (in practice you look at both)

```
cancer_train.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Index: 426 entries, 196 to 296
Data columns (total 12 columns):
 #   Column             Non-Null Count  Dtype  
---  ------             --------------  -----  
 0   ID                 426 non-null    int64  
 1   Class              426 non-null    object 
 2   Radius             426 non-null    float64
 3   Texture            426 non-null    float64
 4   Perimeter          426 non-null    float64
 5   Area               426 non-null    float64
 6   Smoothness         426 non-null    float64
 7   Compactness        426 non-null    float64
 8   Concavity          426 non-null    float64
 9   Concave_Points     426 non-null    float64
 10  Symmetry           426 non-null    float64
 11  Fractal_Dimension  426 non-null    float64
dtypes: float64(10), int64(1), object(1)
memory usage: 43.3+ KB
```

Checking the splits

- We can use the `value_counts` method with the `normalize` argument set to `True` to find the percentage of malignant and benign classes in `cancer_train`.
- We can see our class proportions were roughly preserved when we split the data.

```
cancer_train["Class"].value_counts(normalize=True)
```

```
Class
Benign       0.626761
Malignant    0.373239
Name: proportion, dtype: float64
```

Preprocessing with data splitting

- Many machine learning models are sensitive to the scale of the predictors, and even if not, comparison of importance of features for prediction after fitting requires scaling.
- When preprocessing the data (scaling is part of this), it is critical that we use **only the training set** in creating the mathematical function to do this.
- If this is not done, we will get overly optimistic test accuracy, as our test data will have influenced our model.
- After creating the preprocessing function, we can then apply it separately to both the training and test data sets.

Preprocessing with `scikit-learn`

- `scikit-learn` helps us handle this properly as long as we wrap our analysis steps in a `Pipeline`.
- Specifically, we construct and prepare the preprocessor using `make_column_transformer`:

```python
from sklearn.preprocessing import StandardScaler
from sklearn.compose import make_column_transformer, make_column_selector

cancer_preprocessor = make_column_transformer(
    (StandardScaler(), ["Smoothness", "Concavity"]),
)
```

Train the classifier

Predict the labels in the test set

Now that we have a K-nearest neighbors classifier object, we can use it to predict the class labels for our test set:

```python
cancer_test["predicted"] = knn_pipeline.predict(cancer_test[["Smoothness", "Concavity"]])
print(cancer_test[["ID", "Class", "predicted"]])
```

```
           ID      Class  predicted
116    864726     Benign  Malignant
146    869691  Malignant  Malignant
..        ...        ...        ...
281   8912055     Benign     Benign
15   84799002  Malignant  Malignant

[143 rows x 3 columns]
```

Evaluate performance

To evaluate the model, we will look at:

- accuracy
- precision
- recall
- confusion matrix
- compare to baseline model (majority classifier)

All of these together, will help us develop a fuller picture of how the model is performing, as opposed to only evaluating the model based on a single metric or table.

Accuracy, precision and recall

```python
knn_pipeline.score(
    cancer_test[["Smoothness", "Concavity"]],
    cancer_test["Class"]
)
```

```
0.8951048951048951
```

```python
from sklearn.metrics import recall_score, precision_score

precision_score(
    y_true=cancer_test["Class"],
    y_pred=cancer_test["predicted"],
    pos_label="Malignant"
)
```

```
np.float64(0.8275862068965517)
```

```python
recall_score(
    y_true=cancer_test["Class"],
    y_pred=cancer_test["predicted"],
    pos_label="Malignant"
)
```

```
np.float64(0.9056603773584906)
```

Confusion matrix

- We can look at the *confusion matrix* for the classifier using the `crosstab` function from `pandas`.
- The `crosstab` function takes two arguments: the actual labels first, then the predicted labels second.
- Note that `crosstab` orders its columns alphabetically, but the positive label is still `Malignant`, even if it is not in the top left corner as in the table shown earlier.

```
pd.crosstab(
    cancer_test["Class"],
    cancer_test["predicted"]
)
```

predicted	**Benign**	**Malignant**
Class		
Benign	80	10
Malignant	5	48

Critically analyze performance

- Is 90% accuracy, a precision of 83% and a recall of 91% good enough?
- To get a sense of scale, we often compare our model to a baseline model. In the case of classification, this would be the majority classifier (*always* guesses the majority class label from the training data).
- For the breast cancer training data, the baseline classifier's accuracy would be 63%

```
cancer_train["Class"].value_counts(normalize=True)
```

```
Class
Benign       0.626761
Malignant    0.373239
Name: proportion, dtype: float64
```

- So we do see that our model is doing a LOT better than the baseline, which is great, but considering our application domain is in cancer diagnosis, we still have a ways to go...
- Analyzing model performance really depends on your application!

Tuning the classifier

- Most predictive models in statistics and machine learning have parameters (a number you have to pick in advance that determines some aspect of how the model behaves).
- For our working example, K-nearest neighbors classification algorithm, K is a parameter that we have to pick that determines how many neighbors participate in the class vote.
- How do we choose K, or any parameter for other models?
- **Data splitting**!

Validation set

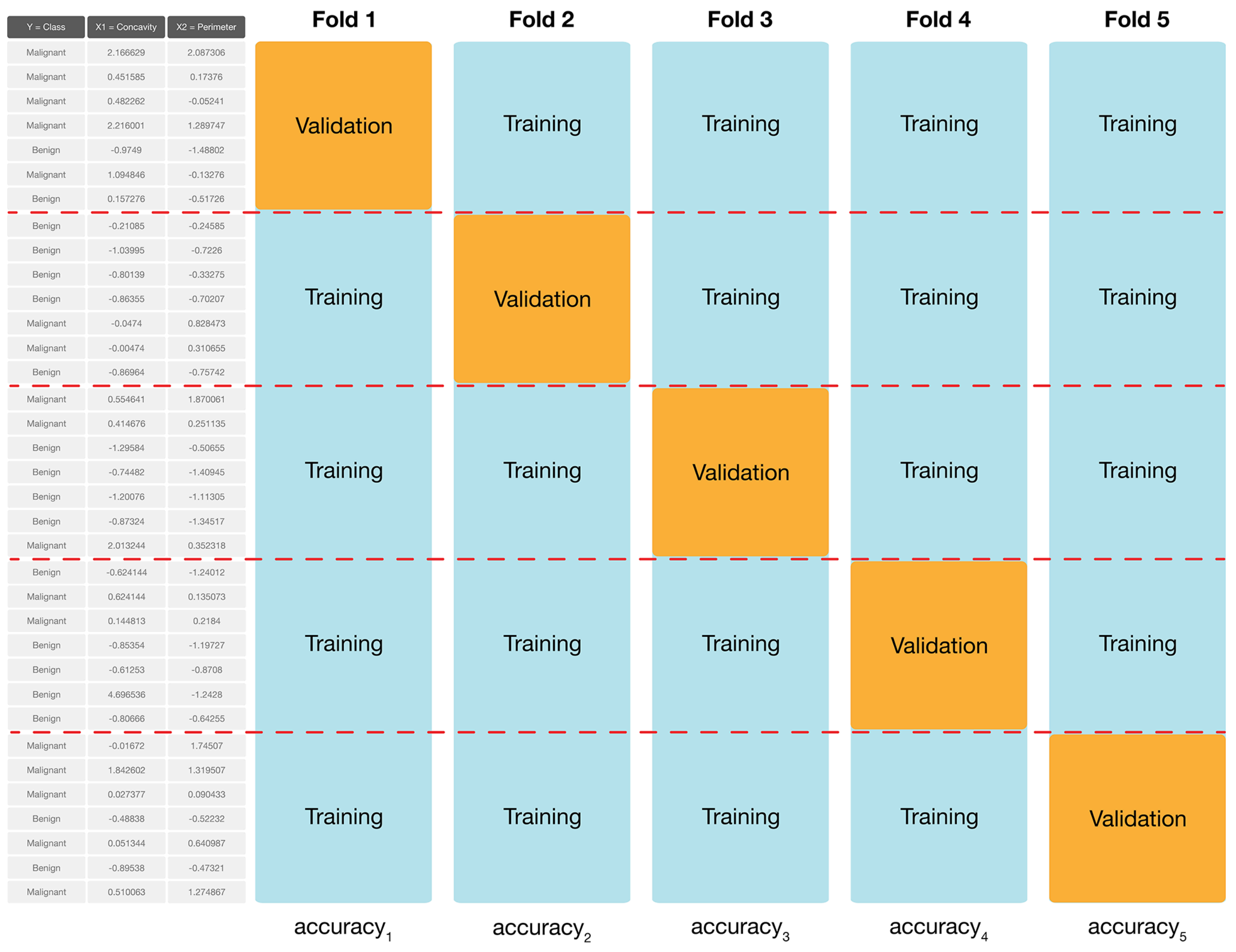
- Cannot use the test set to choose the parameter!
- But we can split the training set into two partitions, a traning set and a validation set.
- For each parameter value we want to assess, we can fit on the training set, and evaluate on the validation set.
- Then after we find the best value for our parameter, we can refit the model with the best parameter on the entire training set and then evaluate our model on the test set.

Can we do better?

- Depending on how we split the data into the training and validation sets, we might get a lucky split (or an unlucky one) that doesn't give us a good estimate of the model's true accuracy.
- In many cases, we can do better by making many splits, and averaging the accuracy scores to get a better estimate.
- We call this cross-validation.

Cross-validation

An example of 5-fold cross-validation:



Y = Class	X1 = Concavity	X2 = Perimeter
Malignant	2.166629	2.087306
Malignant	0.451585	0.17376
Malignant	0.482262	-0.05241
Malignant	2.216001	1.289747
Benign	-0.9749	-1.48802
Malignant	1.094846	-0.13276
Benign	0.157276	-0.51726
Benign	-0.21085	-0.24585
Benign	-1.03995	-0.7226
Benign	-0.80139	-0.33275
Benign	-0.86355	-0.70207
Malignant	-0.0474	0.828473
Malignant	-0.00474	0.310655
Benign	-0.86964	-0.75742
Malignant	0.554641	1.870061
Malignant	0.414676	0.251135
Benign	-1.29584	-0.50655
Benign	-0.74482	-1.40945
Benign	-1.20076	-1.11305
Benign	-0.87324	-1.34517
Malignant	2.013244	0.352318
Benign	-0.624144	-1.24012
Malignant	0.624144	0.135073
Malignant	0.144813	0.2184
Benign	-0.85354	-1.19727
Benign	-0.61253	-0.8708
Benign	4.696536	-1.2428
Benign	-0.80666	-0.64255
Malignant	-0.01672	1.74507
Malignant	1.842602	1.319507
Malignant	0.027377	0.090433
Benign	-0.48838	-0.52232
Malignant	0.051344	0.640987
Benign	-0.89538	-0.47321
Malignant	0.510063	1.274867

$$\text{cross validation accuracy} = \frac{\text{accuracy}_1 + \text{accuracy}_2 + \text{accuracy}_3 + \text{accuracy}_4 + \text{accuracy}_5}{\text{\#folds}}$$

Cross-validation in `scikit-learn`

Parameter value selection

- Since cross-validation helps us evaluate the accuracy of our classifier, we can use cross-validation to calculate an accuracy for each value of our parameter, here K, in a reasonable range,
- Then we pick the value of K that gives us the best accuracy, and refit the model with our parameter on the training data, and then evaluate on the test data.
- The `scikit-learn` package collection provides built-in functionality, named `GridSearchCV`, to automatically handle the details for us.

Parameter value selection

```python
knn = KNeighborsClassifier() #don't specify the number of neighbours
cancer_tune_pipe = make_pipeline(cancer_preprocessor, knn)

parameter_grid = {
    "kneighborsclassifier__n_neighbors": range(1, 100, 5),
}

from sklearn.model_selection import GridSearchCV

cancer_tune_grid = GridSearchCV(
    estimator=cancer_tune_pipe,
    param_grid=parameter_grid,
    cv=10
)
```

Parameter value selection

Now we use the fit method on the `GridSearchCV` object to begin the tuning process.

```python
cancer_tune_grid.fit(
    cancer_train[["Smoothness", "Concavity"]],
    cancer_train["Class"]
)
accuracies_grid = pd.DataFrame(cancer_tune_grid.cv
accuracies_grid.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 20 entries, 0 to 19
Data columns (total 19 columns):
 #   Column                                   Non-Null
Count  Dtype
---  ------                                   --------
------  -----
 0   mean_fit_time                            20 non-
null     float64
 1   std_fit_time                             20 non-
null     float64
 2   mean_score_time                          20 non-
null     float64
 3   std_score_time                           20 non-
null     float64
 4   param_kneighborsclassifier__n_neighbors  20 non-
null     int64
 5   params                                   20 non-
null     object
 6   split0_test_score                        20 non-
null     float64
 7   split1_test_score                        20 non-
```

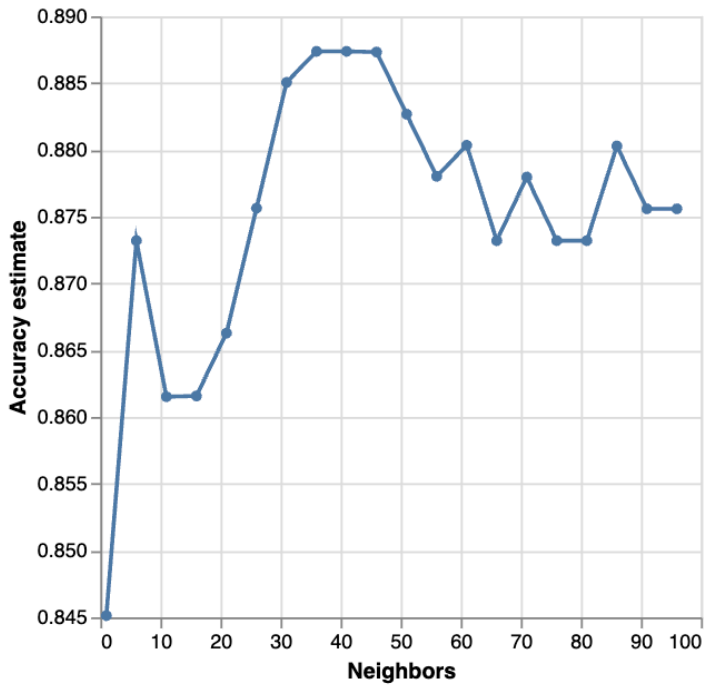
Parameter value selection

```python
accuracies_grid["sem_test_score"] = accuracies_grid["std_test_score"] / 10**(1/2)
accuracies_grid = (
    accuracies_grid[[
        "param_kneighborsclassifier__n_neighbors",
        "mean_test_score",
        "sem_test_score"
    ]]
    .rename(columns={"param_kneighborsclassifier__n_neighbors": "n_neighbors"})
)
print(accuracies_grid)
```

```
    n_neighbors  mean_test_score  sem_test_score
0             1         0.845127        0.019966
1             6         0.873200        0.015680
..          ...              ...             ...
18           91         0.875581        0.012967
19           96         0.875581        0.008193

[20 rows x 3 columns]
```

Visualize paramter value selection

```python
accuracy_vs_k = (
    alt.Chart(accuracies_grid)
    .mark_line(point=True)
    .encode(
        x=alt.X("n_neighbors")
        .title("Neighbors"),
        y=alt.Y("mean_test_score")
        .scale(zero=False)
        .title("Accuracy estimate")
    )
)
```



Best parameter value

We can also obtain the number of neighbours with the highest accuracy programmatically by accessing the `best_params_` attribute of the fit `GridSearchCV` object.

```python
cancer_tune_grid.best_params_
```

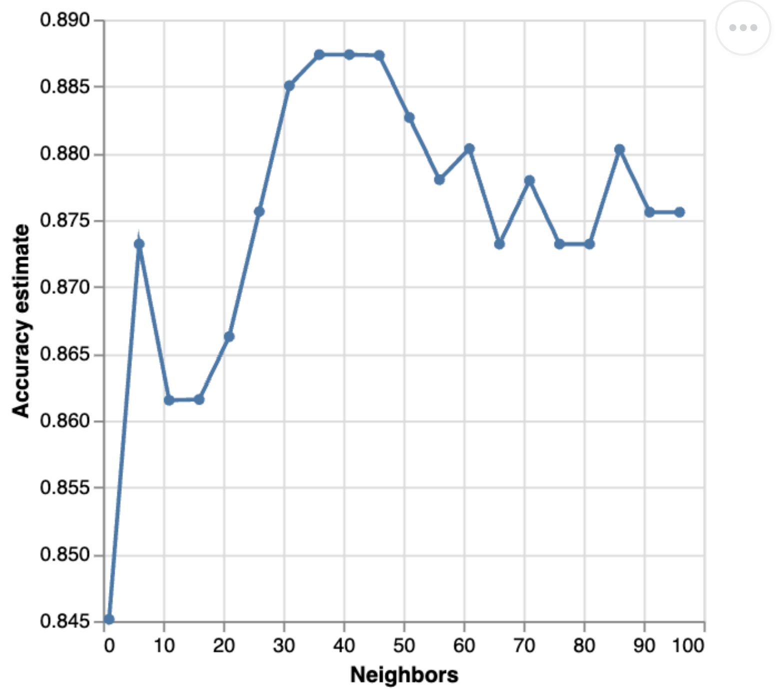
```
{'kneighborsclassifier__n_neighbors': 36}
```

Best parameter value

Do we use K = 36?

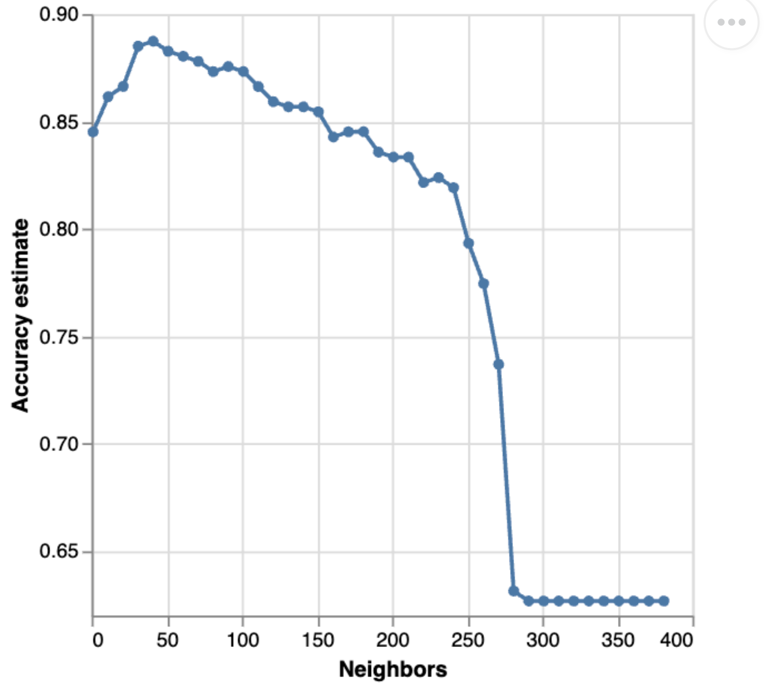
Generally, when selecting a parameters, we are looking for a value where:

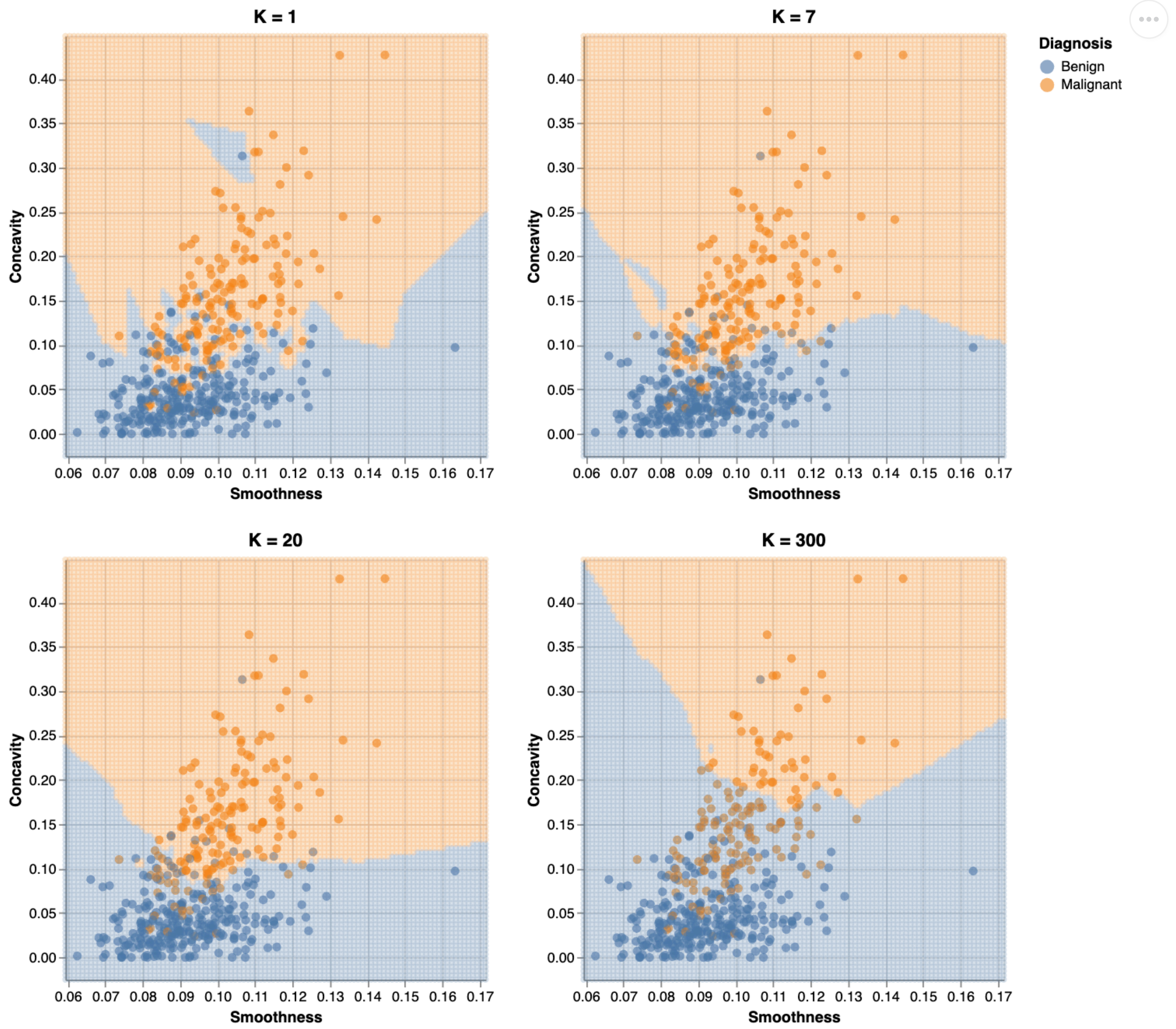
- we get roughly optimal accuracy
- changing the value to a nearby one doesn't change the accuracy too much
- the cost of training the model is not prohibitive



Under/Overfitting

- What happens if we keep increasing the number of neighbors K?
- The cross-validation accuracy estimate actually starts to decrease!




K = 1
K = 7
K = 20
K = 300
Concavity
Smoothness
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
0.06
0.07
0.08
0.09
0.10
0.11
0.12
0.13
0.14
0.15
0.16
0.17
Diagnosis
● Benign
● Malignant

Evaluating on the test set

- Before we evaluate on the test set, we need to refit the model using the best parameter(s) on the entire training set
- Luckily, `scikit-learn` does it for us automatically!
- To make predictions and assess the estimated accuracy of the best model on the test data, we can use the `score` and `predict` methods of the fit `GridSearchCV` object.

```
cancer_test["predicted"] = cancer_tune_grid.predic
    cancer_test[["Smoothness", "Concavity"]]
)
```

Evaluating on the test set

We can then pass those predictions to the `precision`, `recall`, and `crosstab` functions to assess the estimated precision and recall, and print a confusion matrix.

```python
cancer_tune_grid.score(
    cancer_test[["Smoothness", "Concavity"]],
    cancer_test["Class"]
)
```

```
0.9090909090909091
```

```python
precision_score(
    y_true=cancer_test["Class"],
    y_pred=cancer_test["predicted"],
    pos_label='Malignant'
)
```

```
np.float64(0.8846153846153846)
```

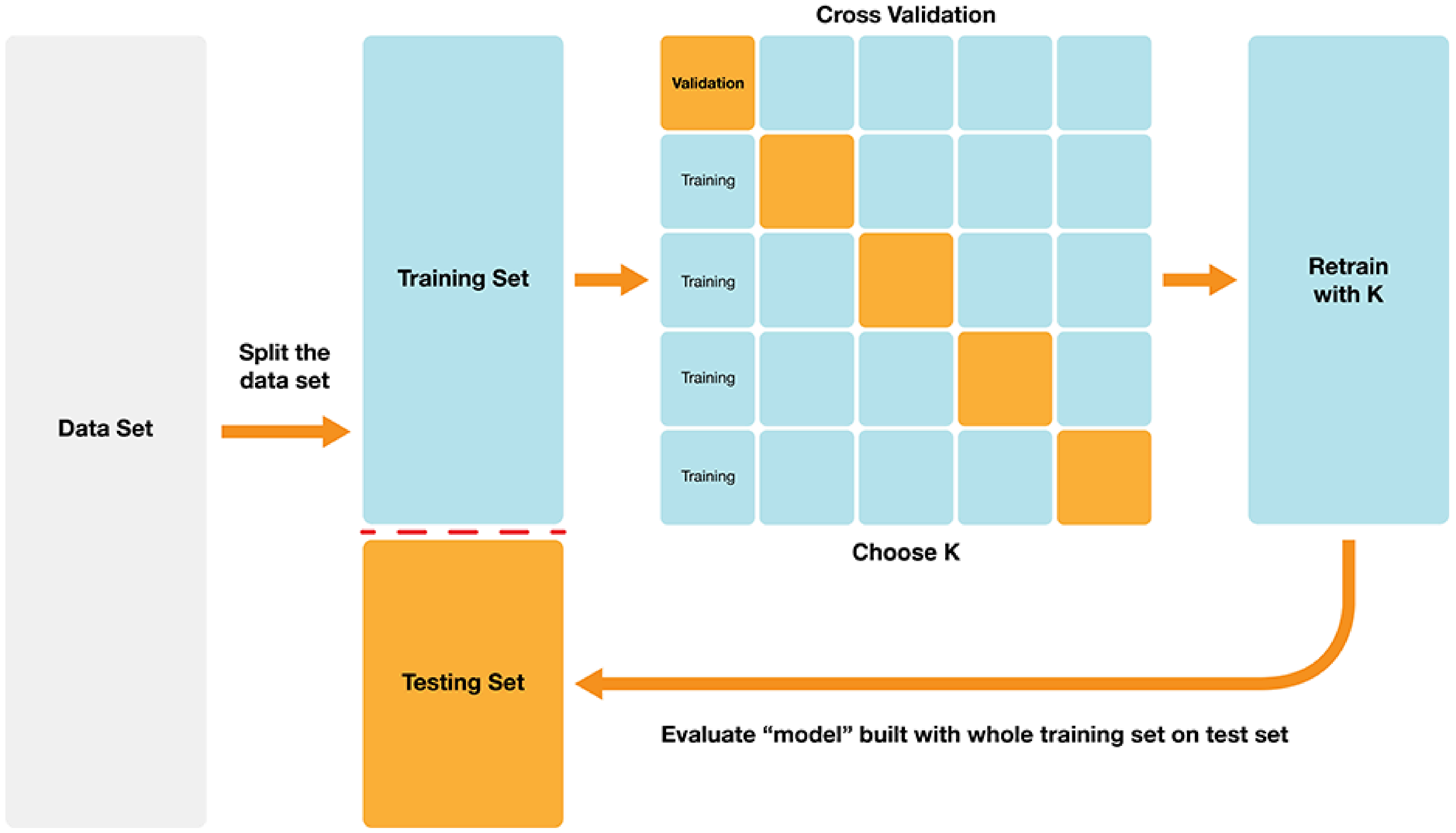
```python
recall_score(
    y_true=cancer_test["Class"],
    y_pred=cancer_test["predicted"],
    pos_label='Malignant'
)
```

```
np.float64(0.8679245283018868)
```

```python
conf_matrix = pd.crosstab(
    cancer_test["Class"],
    cancer_test["predicted"]
)
print(conf_matrix)
```

```
predicted  Benign  Malignant
Class
Benign         84          6
Malignant       7         46
```

Summary



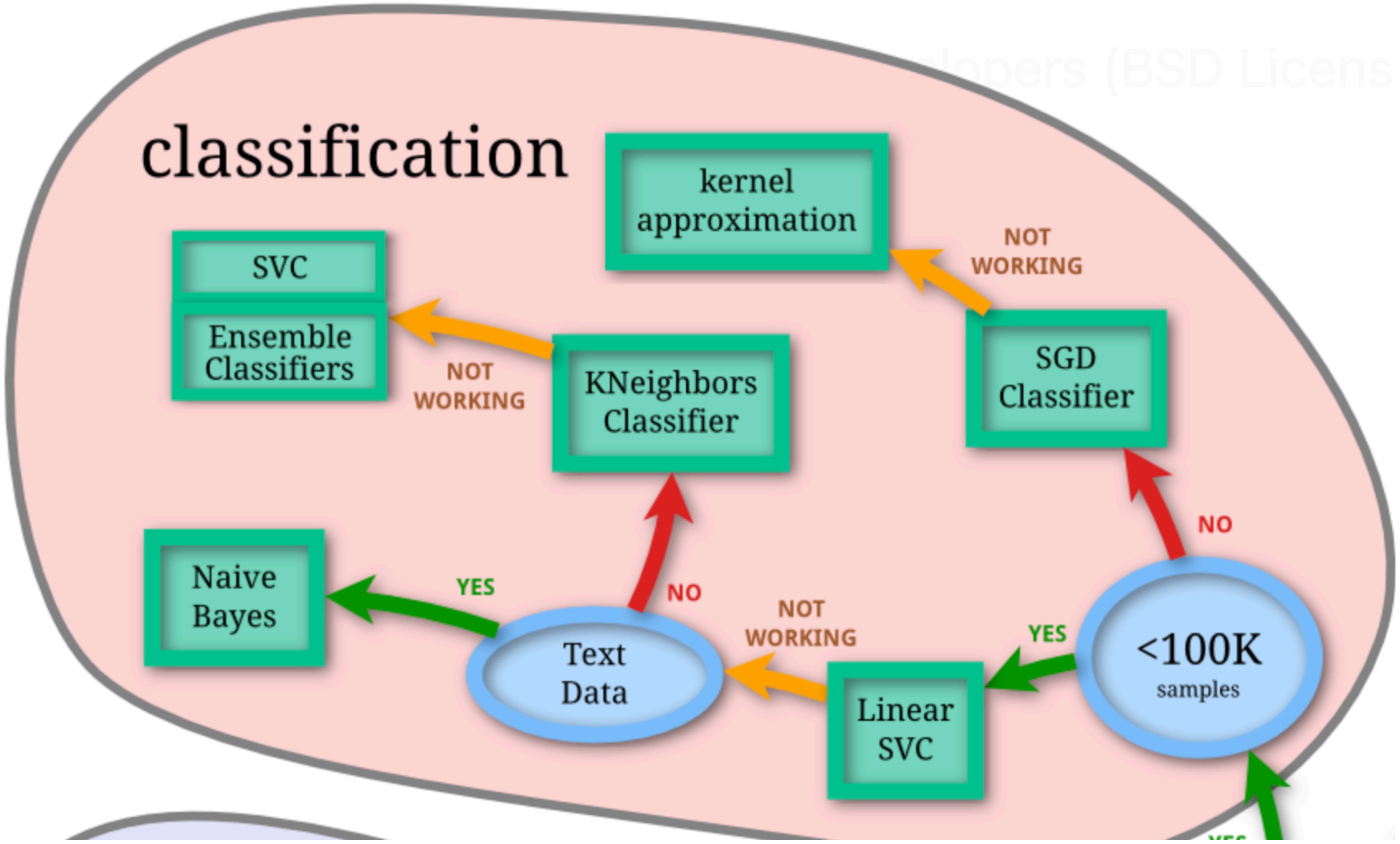
Data Set
Split the data set
Training Set
Testing Set
Cross Validation
Validation
Training
Training
Training
Training
Choose K
Retrain with K
Evaluate "model" built with whole training set on test set

K-nearest neighbors classification algorithm

Strengths: K-nearest neighbors classification ::: {.nonincremental} 1. is a simple, intuitive algorithm, 2. requires few assumptions about what the data must look like, and 3. works for binary (two-class) and multi-class (more than 2 classes) classification problems. :::

Weaknesses: K-nearest neighbors classification ::: {.nonincremental} 1. becomes very slow as the training data gets larger, 2. may not perform well with a large number of predictors, and 3. may not perform well when classes are imbalanced. :::

Other classification algorithms



`scikit-learn` *classification documentation:* *https://scikit-learn.org/stable/supervised_learning.html*

Additional resources

- The Classification II: evaluation & tuning chapter of Data Science: A First Introduction (Python Edition) by Tiffany Timbers, Trevor Campbell, Melissa Lee, Joel Ostblom, Lindsey Heagy contains all the content presented here with a detailed narrative.
- The `scikit-learn` website is an excellent reference for more details on, and advanced usage of, the functions and packages in the past two chapters. Aside from that, it also offers many useful tutorials to get you started.
- *An Introduction to Statistical Learning* {cite:p}`james2013introduction` provides a great next stop in the process of learning about classification. Chapter 4 discusses additional basic techniques for classification that we do not cover, such as logistic regression, linear discriminant analysis, and naive Bayes.

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