K nearest neighbor

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This slides are created based on the slides of the Sebastian Raschka for the introduction to machine learning course

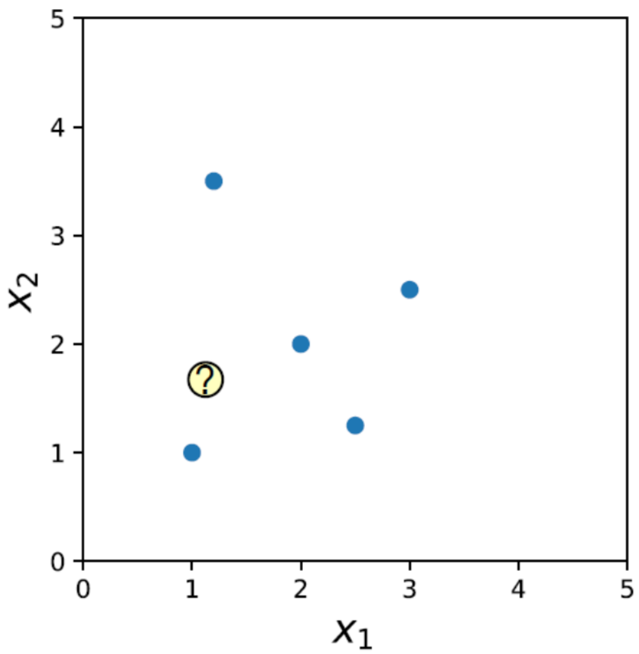
Topics

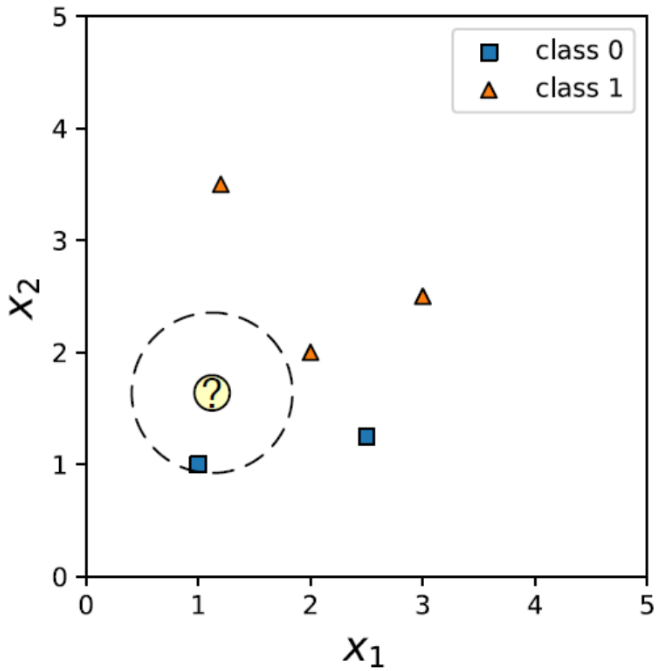
- **Intro to nearest neighbor models**
- Nearest neighbor decision boundary
- K-nearest neighbors
- Improving k-nearest neighbors: modifications and hyperparameters
- K-nearest neighbors in Python

1-Nearest Neighbor

1-Nearest Neighbor

- Task: predict the target / label of a new data point





- How? Look at most "similar" data point in training set

1-Nearest Neighbor Training Step

$$\langle \mathbf{x}^{[i]}, y^{[i]} \rangle \in \mathscr{D} \quad (|\mathscr{D}| = n)$$

How do we "train" the 1-NN model?

To train the 1-NN model, we simply "remember" the training dataset

1-Nearest Neighbor Prediction Step

closest_point := None

closest_distance := ∞

query point

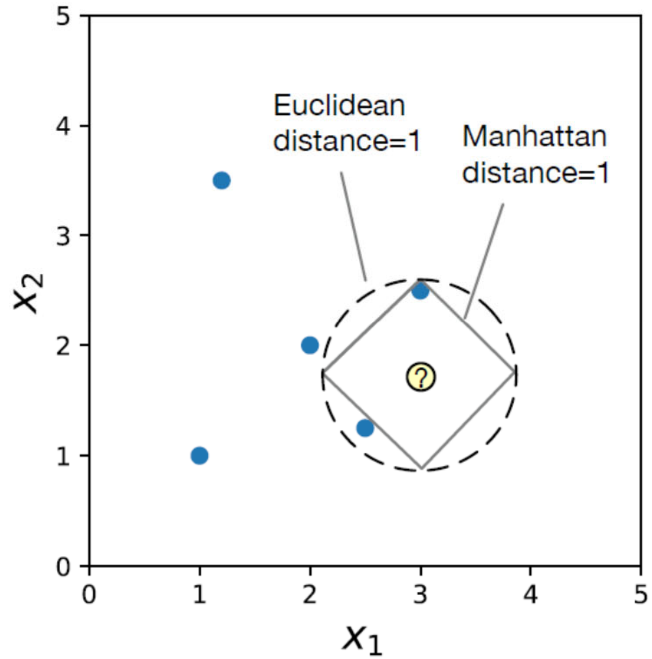
- for $i = 1, \ldots, n$:
  - current_distance := $d(\mathbf{x}^{[i]}, \mathbf{x}^{[q]})$
  - if current_distance < closest_distance:
    - closest_distance := current_distance
    - closest_point := $\mathbf{x}^{[i]}$
- return f(closest_point)

Which Point is Closest to ? ?

- Depends on the Distance Measure!
- Commonly used: Euclidean Distance

$$d(\mathbf{x}^{[a]}, \mathbf{x}^{[b]}) = \sqrt{\sum_{j=1}^{m} \left(x_j^{[a]} - x_j^{[b]}\right)^2}$$

- Other metrics : Manhatan distance
-



Some Common Continuous Distance Measures

- Euclidean

- Manhattan

- Minkowski: $d(\mathbf{x}^{[a]}, \mathbf{x}^{[b]}) = \left[\sum_{j=1}^{m} \left(\left| x_j^{[a]} - x_j^{[b]} \right| \right)^p \right]^{\frac{1}{p}}$

- Cosine similarity

Some Discrete Distance Measures

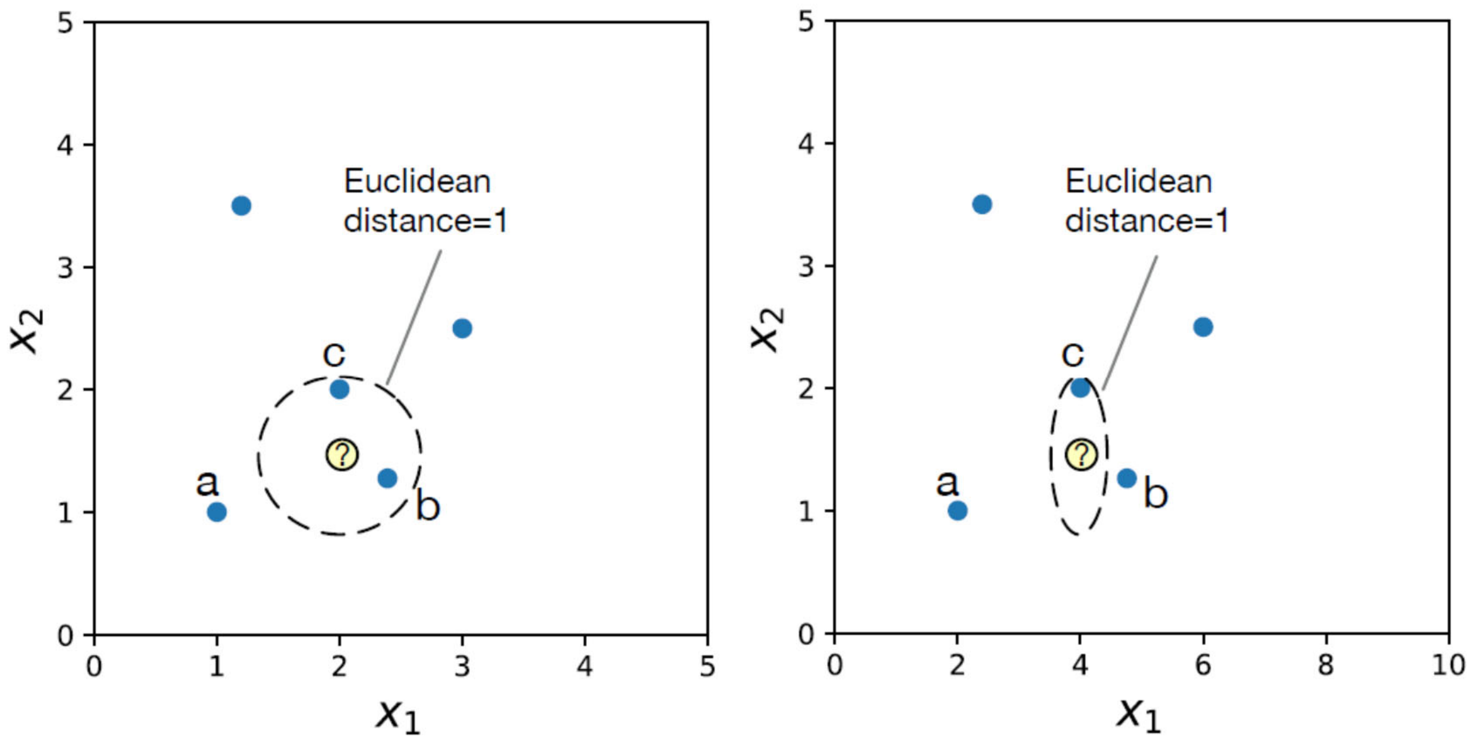
Hamming distance: $d(\mathbf{x}^{[a]}, \mathbf{x}^{[b]}) = \sum_{j=1}^{m} \left| x_j^{[a]} - x_j^{[b]} \right|$ where $x_j \in \{0,1\}$

Jaccard/Tanimoto similarity:

$$J(A, B) = \frac{|A \cap B|}{|A \cup B|} = \frac{|A \cap B|}{|A| + |B| - |A \cap B|}$$

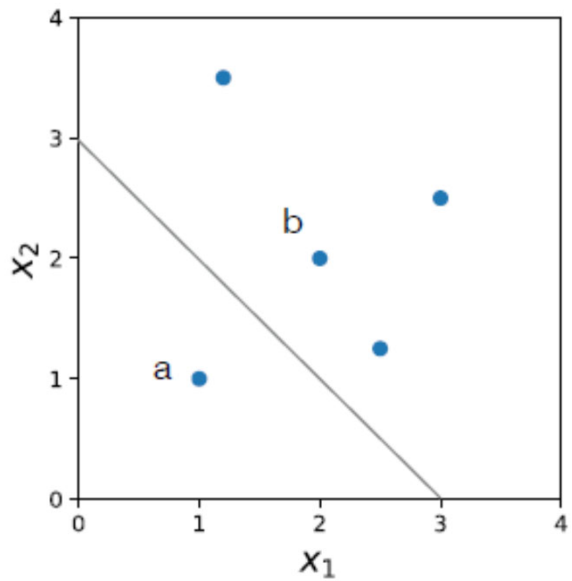
Dice: $D(A, B) = \frac{2|A \cap B|}{|A| + |B|}$

Feature Scaling



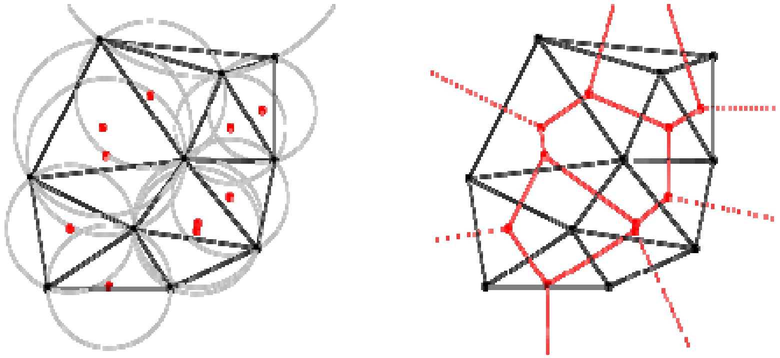
Nearest Neighbor Decision Boundary

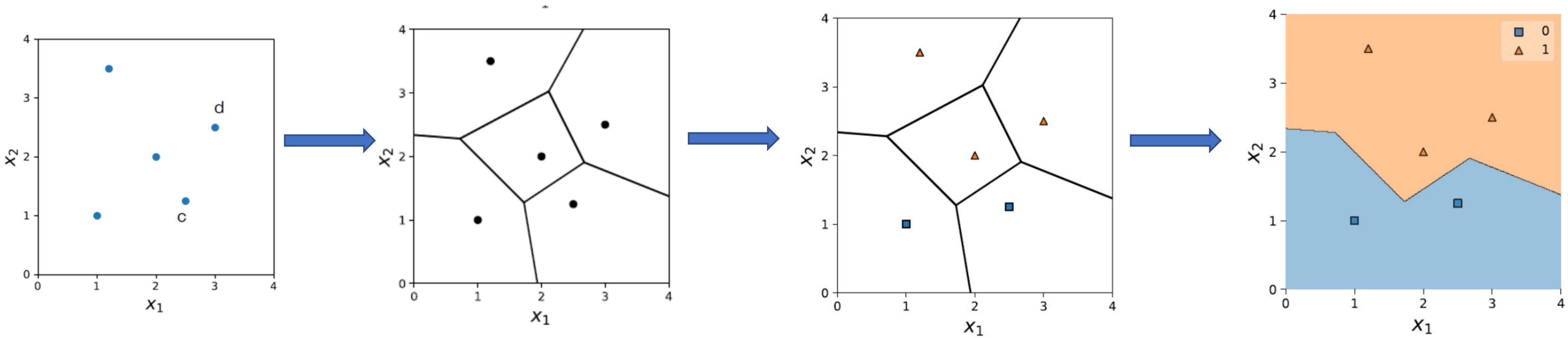
Decision Boundary Between (a) and (b)



Decision Boundary of 1-NN

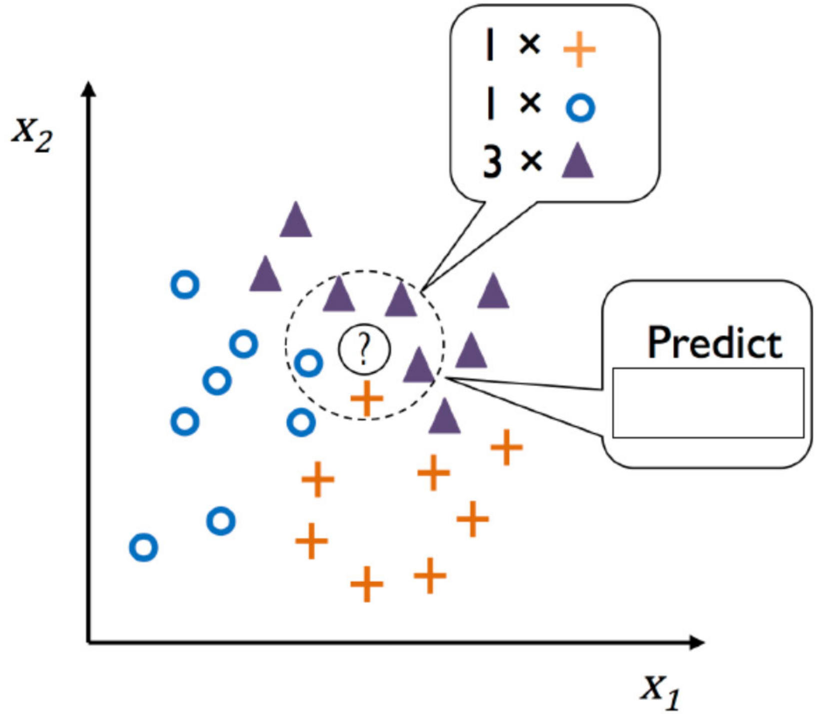
Using Delaunay triangulation

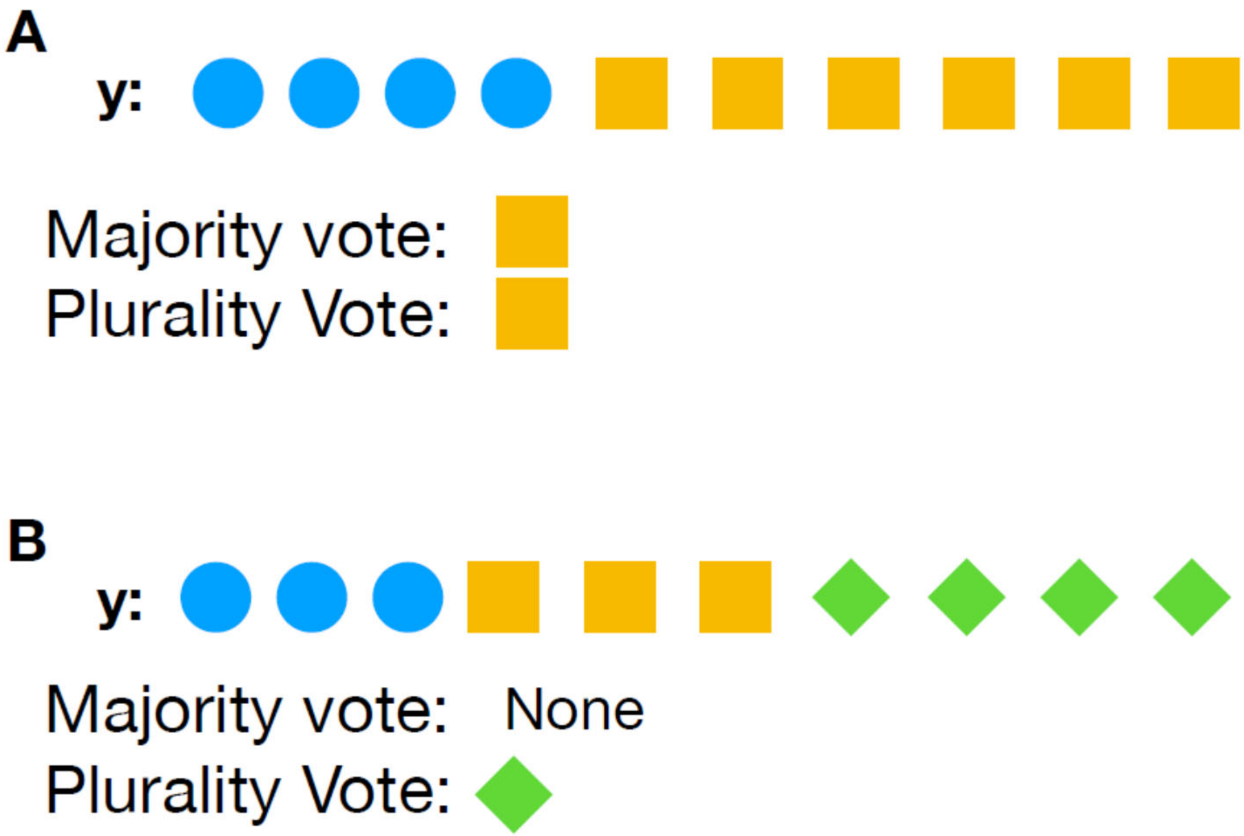




K nearest neighbour

k-Nearest Neighbors




A
y:
Majority vote:
Plurality Vote:
B
y:
Majority vote: None
Plurality Vote:

kNN for Classification

$$\mathcal{D}_k = \{\langle \mathbf{x}^{[1]}, f(\mathbf{x}^{[1]}) \rangle, \ldots, \langle \mathbf{x}^{[k]}, f(\mathbf{x}^{[k]}) \rangle\} \quad \mathcal{D}_k \subseteq \mathcal{D}$$

$$h(\mathbf{x}^{[q]}) = arg \max_{y \in \{1,\ldots,t\}} \sum_{i=1}^{k} \delta(y, f(\mathbf{x}^{[i]}))$$

$$\delta(a, b) = \begin{cases} 1, & \textbf{if } a = b, \\ 0, & \textbf{if } a \neq b. \end{cases}$$

$$h(\mathbf{x}^{[t]}) = \textbf{mode}\left(\{f(\mathbf{x}^{[1]}), \ldots, f(\mathbf{x}^{[k]})\}\right)$$

*k*NN for Regression

$$\mathscr{D}_k = \{\langle \mathbf{x}^{[1]}, f(\mathbf{x}^{[1]})\rangle, \ldots, \langle \mathbf{x}^{[k]}, f(\mathbf{x}^{[k]})\rangle\} \quad \mathscr{D}_k \subseteq \mathscr{D}$$

$$h(\mathbf{x}^{[t]}) = \frac{1}{k}\sum_{i=1}^{k} f(\mathbf{x}^{[i]})$$

Distance-weighted *k*NN

$$h(\mathbf{x}^{[t]}) = arg \max_{j \in \{1,...,p\}} \sum_{i=1}^{k} w^{[i]} \delta(j, f(\mathbf{x}^{[i]}))$$

$$w^{[i]} = \frac{1}{d(\mathbf{x}^{[i]}, \mathbf{x}^{[t]})^2}$$

Nearest Neighbor Search

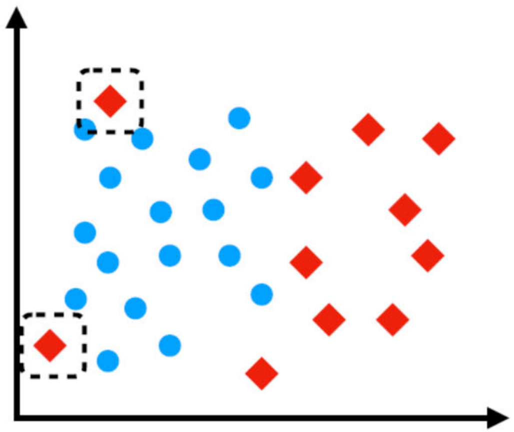
$\mathcal{D}_k := \{\}$

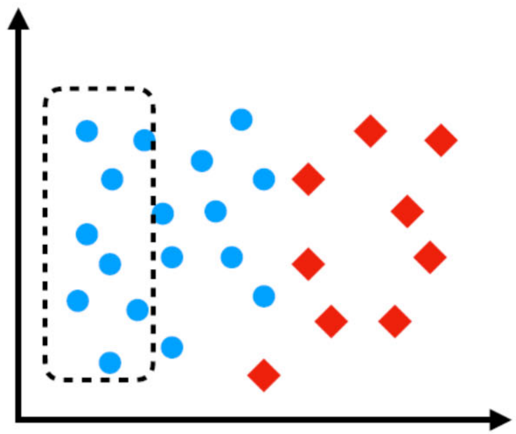
while $|\mathcal{D}_k| <$ k:

- $\texttt{closest\_distance} := \infty$
- for $i = 1, ..., n, \quad \forall i \notin \mathcal{D}_k$:
  - $\texttt{current\_distance} := d(\mathbf{x}^{[i]}, \mathbf{x}^{[q]})$
  - if $\texttt{current\_distance} < \texttt{closest\_distance}$:
    * $\texttt{closest\_distance} := \texttt{current\_distance}$
    * $\texttt{closest\_point} := \mathbf{x}^{[i]}$
- add $\texttt{closest\_point}$ to $\mathcal{D}_k$

Improving Computational Performance

- Pruning



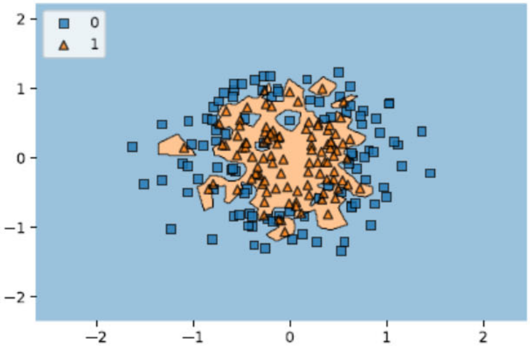


Hyperparameter

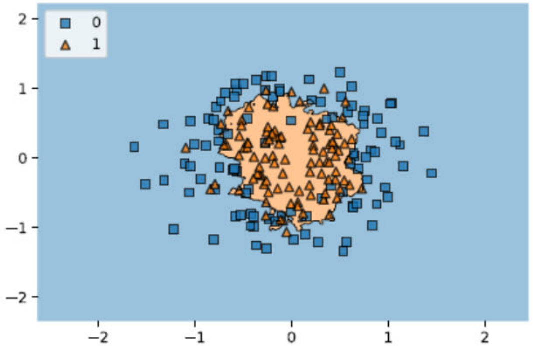
Value of k

$$k \in \{1,3,7\}$$

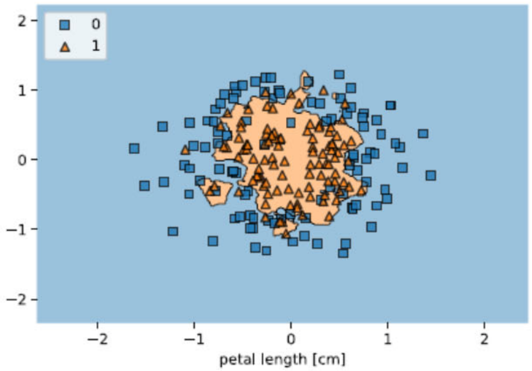
$k = \_$



$k = \_$



$k = \_$



How to choose the value of K

- **Cross-Validation**
  - try different values of K and evaluate the performance of the model using metrics like accuracy, precision, recall, or F1 score
- **Odd vs. Even K**
  - It is generally recommended to use an odd value for K to avoid ties in voting
- **Rule of Thumb**
  - A common rule of thumb is to set K to the square root of the total number of samples in your dataset. This is a good starting point but may not always be the optimal choice.

How to choose the value of K

- **Domain Knowledge**
  - Depending on the characteristics of your dataset and problem domain, you may have insights that can guide you in choosing an appropriate value of K. For example, if you know that the decision boundaries are complex, you may want to choose a smaller value of K.

```
[ ] from sklearn.datasets import load_iris
    from sklearn.model_selection import train_test_split
    from sklearn.neighbors import KNeighborsClassifier
```

```
[ ] iris = load_iris()
    X, y = iris.data[:, 2:], iris.target
    X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3,

                                                         shuffle=True)
```

```
[ ] knn_model = KNeighborsClassifier(n_neighbors=3)
    knn_model.fit(X_train, y_train)

    y_pred = knn_model.predict(X_test)
```

```
[ ] num_correct_predictions = (y_pred == y_test).sum()
    accuracy = (num_correct_predictions / y_test.shape[0]) * 100

    # print('Test set accuracy: %.2f%%' % accuracy)

    print(f'Test set accuracy: {accuracy:.2f}%')
```

```
Test set accuracy: 95.56%
```

```python
mean_scores = []
for k in range (1,11) :
  knn_model = KNeighborsClassifier(n_neighbors = k)
  knn_model.fit(X_train, y_train)

  scores = cross_val_score(knn_model, X_train, y_train, cv = 5)
  mean_scores.append(scores.mean())

ck = np.argmax(mean_scores)
print(ck)
knn_model = KNeighborsClassifier(n_neighbors = ck+1)
knn_model.fit(X_train, y_train)

y_pred = knn_model.predict(X_test)

num_correct_predictions = (y_pred == y_test).sum()
accuracy = (num_correct_predictions / y_test.shape[0]) * 100

# print('Test set accuracy: %.2f%%' % accuracy)

print(f'Test set accuracy: {accuracy:.2f}%')
```

```
4
Test set accuracy: 97.78%
```