Fundamentals of Artificial Intelligence

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TE HERENGA WAKA

COMP307/AIML420
ML: kNN and K-fold CV

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Outline

- **K-Nearest Neighbor (kNN)**
  - Classification (Supervised Learning)
  - Basic NN (1-NN)
  - Distance metrics
- **K-Fold Cross Validation (CV)**
  - Evaluation
  - Why? Revisiting generalization
  - Leave-one out
- **Evaluation Metrics**
  - Why should we care about them?

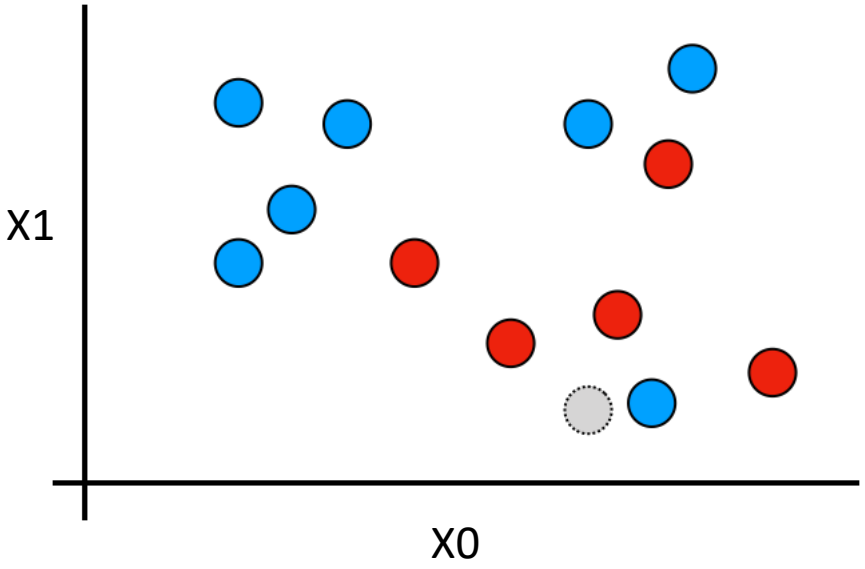
K-Nearest Neighbor

- One of the most intuitive ML algorithms
- Classic example of Lazy Learning (or case-based learning)
- **K** refers to the number of neighbors considered
- Requires a distance metric

The basic algorithm

- **Training:** store all training instances
- **Predicting:** The most **common** class label among the **k** instances **closer** to a **new instance** determines its label

1-NN



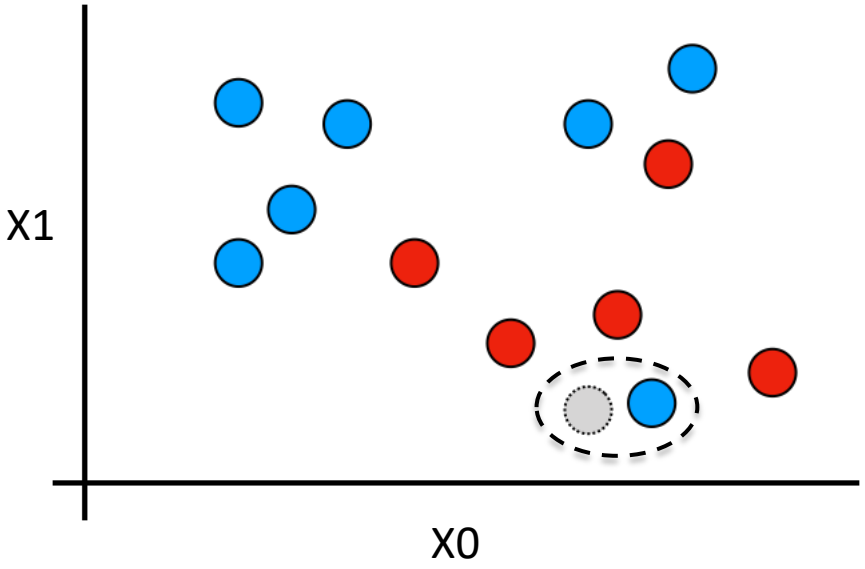
Suppose a binary classification problem: blue and red circles

There are two input features X0 and X1

We want to classify the "unknown" gray instance

- **Training:** The training data is shown above (all the red and blue circles)
- We don't know the class for the gray instance.

1-NN



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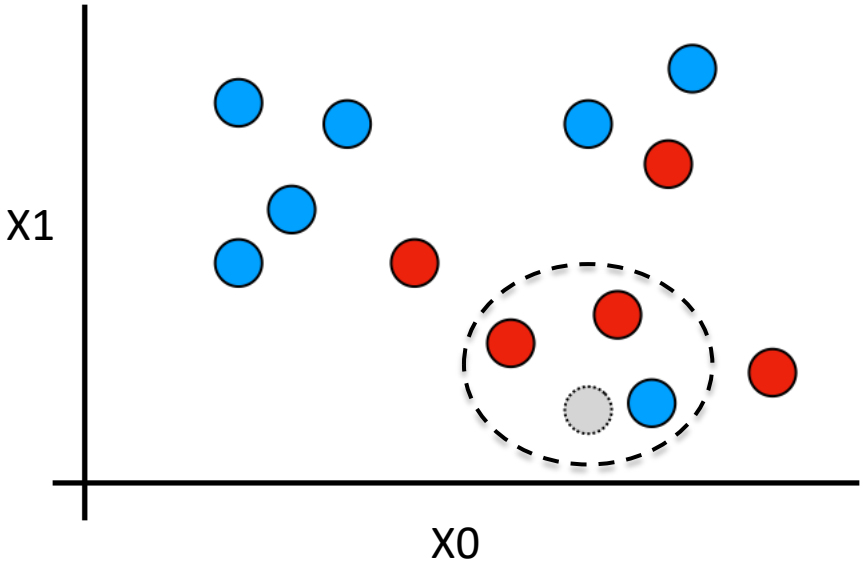
- **Prediction:** Find the closest neighbor in the training set to the gray inst.
  - The blue instance is the closest neighbor (prediction = blue)

k-NN



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- **Prediction:** Find the closest neighbors in the training set to the gray inst.
  - Assuming **k = 3**, there are 1 blue and 2 red as nearest neighbors (prediction = red)

Distance

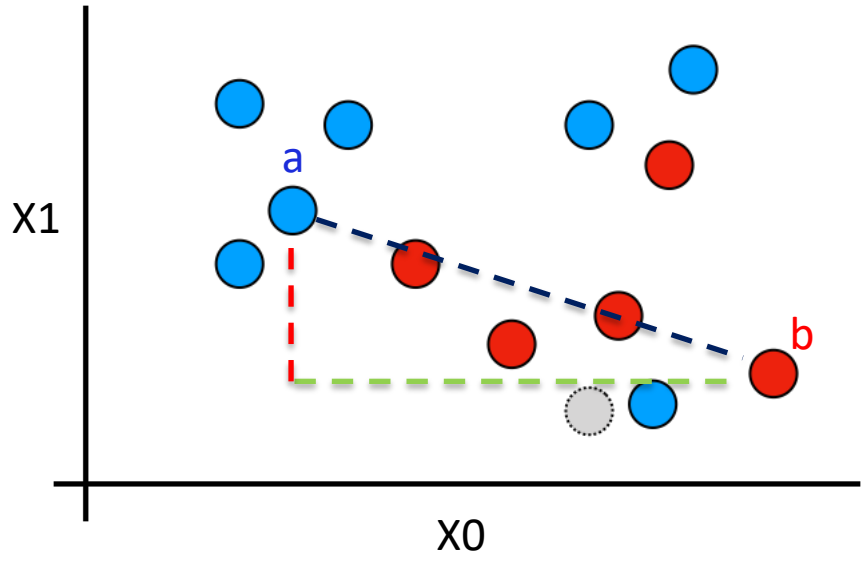
- The notion of “distance” is crucial for kNN (and other ML algorithms)

- Most popular one is the Euclidean distance
  - Given two feature vectors **a** and **b** with **continuous values**

$$d(a,b) = \sqrt{\sum_{i=1}^{n}(a_i - b_i)^2} = \sqrt{(a_1 - b_1)^2 + (a_2 - b_2)^2 + \cdots + (a_n - b_n)^2}$$

Euclidean Distance Example

$$d(a,b) = \sqrt{\sum_{i=1}^{n}(a_i - b_i)^2} = \sqrt{(a_1 - b_1)^2 + (a_2 - b_2)^2 + \cdots + (a_n - b_n)^2}$$



$$d(a,b) = \sqrt{(a_{X0} - b_{X0})^2 + (a_{X1} - b_{X1})^2}$$

More on distances

- We often “normalize” the input data, so that values from all features are within the same range (0,1)
- A common normalization technique is Min-Max normalization

$$x' = \frac{x - x_{min}}{x_{max} - x_{min}}$$ where x is a feature

- We can apply this directly inside the Euclidean distance calculation:

$$d(a,b) = \sqrt{\sum_{i=1}^{n} \frac{(a_i - b_i)^2}{R_i^2}}$$ assuming R_i as the range for feature X_i

i.e. x_{max} - x_{min}

Considerations about kNN

- **Training** and **Predicting**
  - In most ML algorithms training is costly, but predicting is efficient*
  - What about kNN?
- **Nominal features** can be difficult to handle
- **High-dimensional data**: distance may lose meaning
- How to choose **k**? Try to **avoid ties**
- The distances can be used to **weight neighbors**
- kNN can be easily adapted for **regression**

Evaluation strategy (k-fold CV)

- Evaluation is utterly important. **Why?**

- Should the training data be used to evaluate the predictive performance?
  - Remember generalization?

Yes? No? Why?

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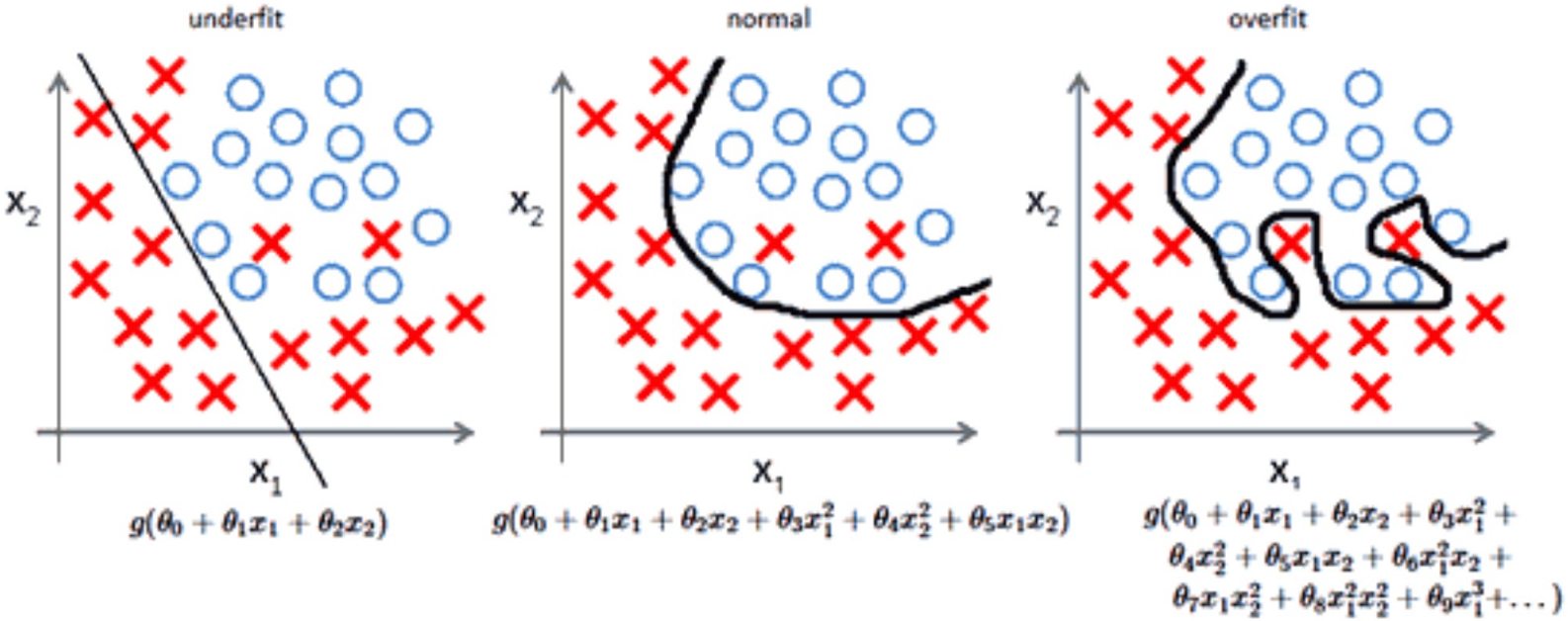
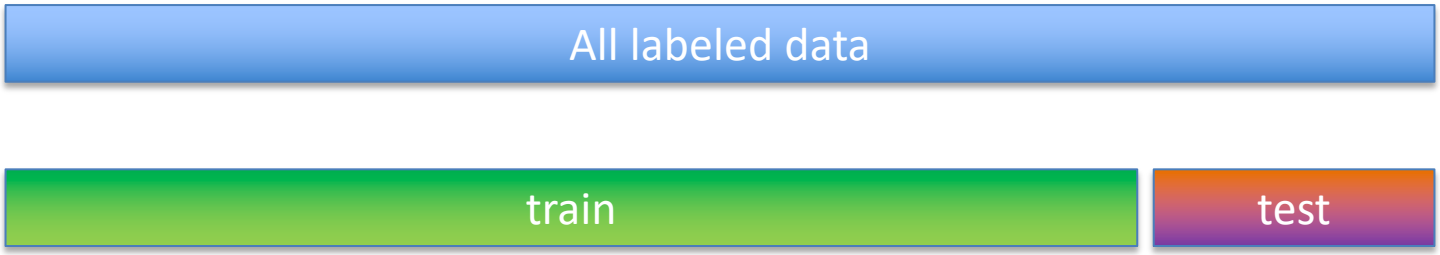


Evaluation strategy (k-fold CV)

Holdout evaluation

- To address overfitting, we can evaluate using data that was not used for training (i.e. test data)



- The aim is to evaluate the model's ability to **generalize** to new and unseen data by testing it with previously unused data.

Why k-fold cross validation?

- What are the main **limitations** of the *Holdout Evaluation*?

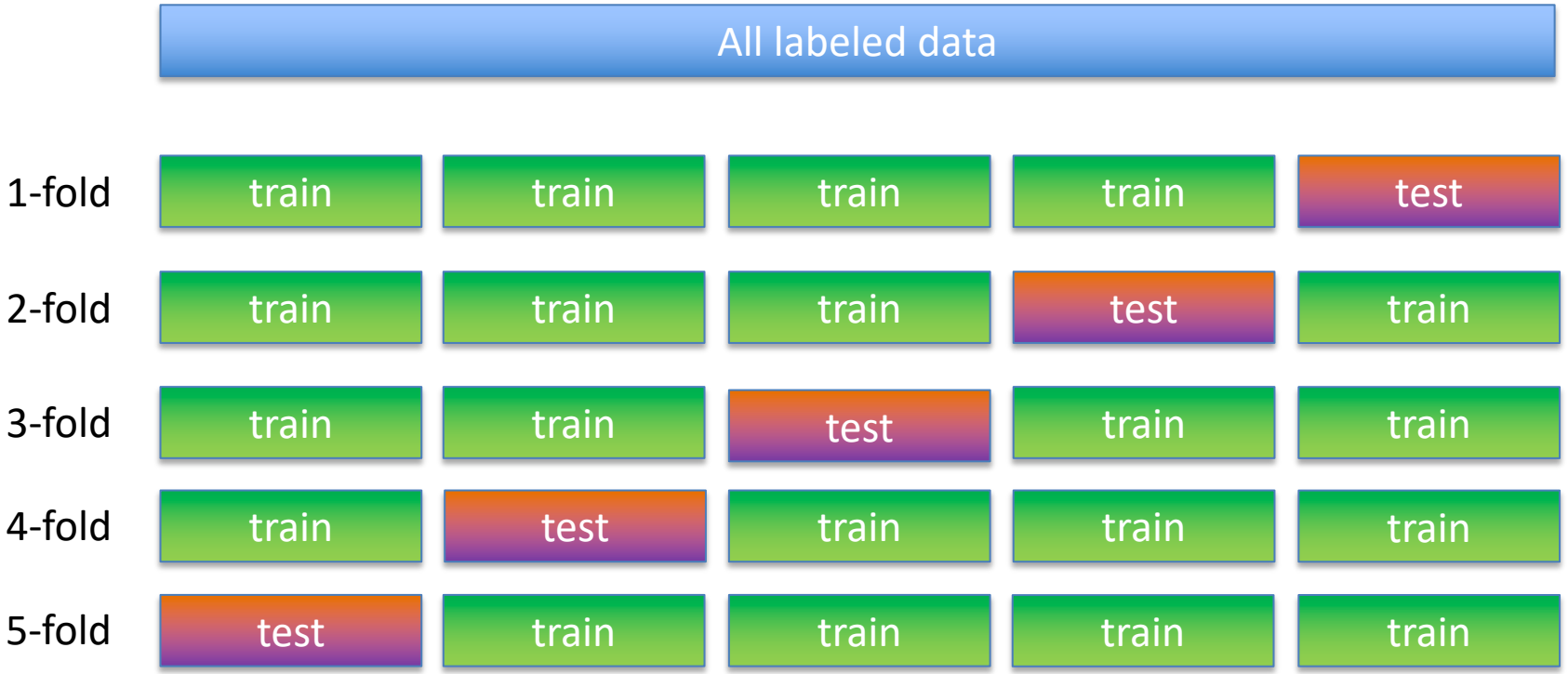
Why k-fold cross validation?

- What are the main **limitations** of the *Holdout Evaluation*?
  - Holdout evaluation **may be biased** if the testing dataset is **not representative of the overall population**
  - Having a **small dataset** results in a smaller test set, which can **lower our confidence** in the experimental results

K-fold cross validation can help us mitigate these limitations!

k-fold cross validation

- Create k train and test sets, e.g. 5-fold CV



k-fold cross validation

- k-fold CV allows us to make **efficient use of the available data** by using each data point for both training and testing, leading to a better estimate of model performance

- **More reliable estimate of performance** especially when the dataset is small or there is a high variance in the data

- **Reduces the risk of overfitting**, as it tests the model on multiple independent test sets, preventing the model from becoming too specific to the training data

k-fold cross validation

- **Leave-one out:** Extreme case of k-fold CV
  - Create as many test sets as there are data points, each test set contains only one instance
  - It can be useful when the dataset is very small
  - Computationally intensive
  - Can lead to overfitting in some cases

- In overall, we use 5-fold CV or 10-fold CV
  - It depends on the computational resources available
  - More folds leads to more confidence on the results

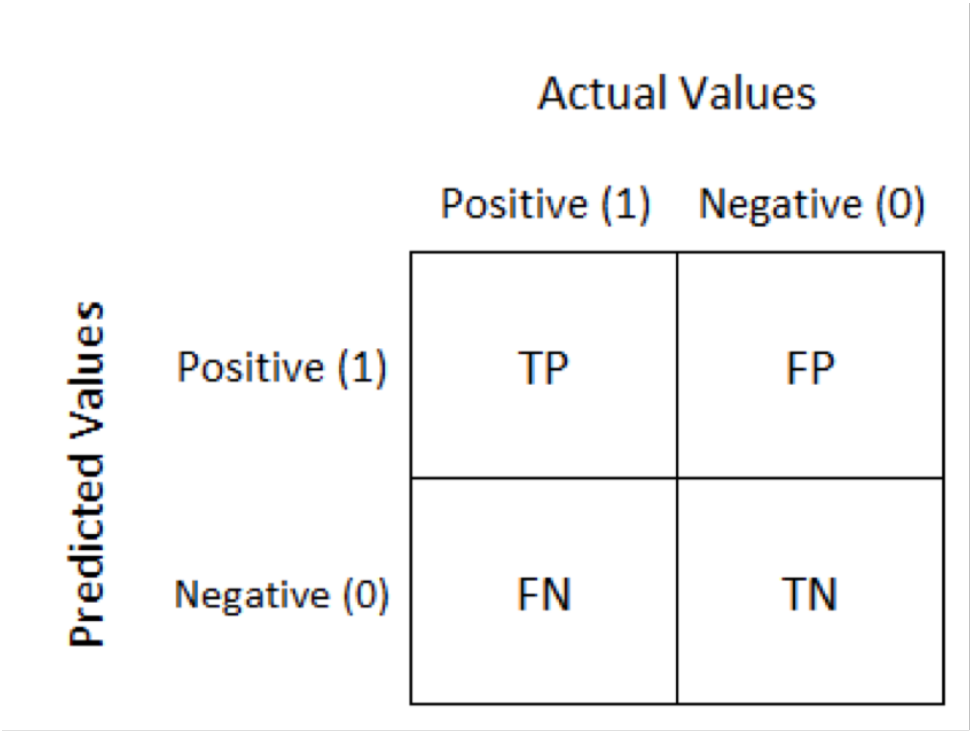
- Stratified k-fold CV
  - take into account the distribution of the class labels

Evaluation Metrics

- Evaluation strategy vs Evaluation Metric
  - Examples:
    - Strategy: 10-fold CV
    - Metric: Accuracy
  - The strategy is how we do it, the metric is what we observe

- Different metrics for different tasks and problems
  - Choosing the correct evaluation metric is very important
  - The task at hand (classification or regression?)
  - The problem characteristics (much more instances of one class?)

Evaluation Metrics



Confusion matrix

TP: True Positive; FP: False Positive;
FN: False Negative; TN: True Negative

There are several metrics…

- Accuracy
- Precision
- Recall
- F1-score
- Kappa
- …

How important is the metric definition?

Evaluation Metrics

Example

- Problem: classify instances as **SPAM (negative)** or **HAM (positive)**; test data contains 100 instances;
- Suppose an algorithm obtains 95% accuracy. Is this good?

Accuracy = (TP+TN) / (TP+TN+FN+FP)

Evaluation Metrics

Example

- Problem: classify instances as **SPAM (negative)** or **HAM (positive)**; test data contains 100 instances;
- Suppose an algorithm obtains 95% accuracy. Is this good?

What if 95 of the instances in the test data are **SPAM?**

Accuracy = (TP+TN) / (TP+TN+FN+FP)

Evaluation Metrics

Example

- Problem: classify instances as **SPAM (negative)** or **HAM (positive)**; test data contains 100 instances;
- Suppose an algorithm obtains 95% accuracy. Is this good?

What if 95 of the instances in the test data are **SPAM?**

It depends

Accuracy = (TP+TN) / (TP+TN+FN+FP)

Evaluation Metrics

- **Accuracy** does not tell us anything about how accurate the model is in predicting one specific class. In our example, we would like to know if the model can correctly predict **HAM** (positive class)

- Given that 95 of 100 test instances are **SPAM** and the accuracy is 95% it is likely that the model is simply always predicting **SPAM** (negative class)

- In these situations, we need to use more suitable metrics. In our example, we could use **recall***

* recall = TP / (TP+FN)

Summary

- **kNN** is a simple yet powerful **supervised learning** method
- K-fold CV is the *de facto* **evaluation strategy** in ML
- The **evaluation metric** is independent of the evaluation strategy and it is very important to choose it wisely

Coming up next…

- ML examples (Tutorial this week)
- Decision trees (Next lecture)