Machine Learning (CE 40477)

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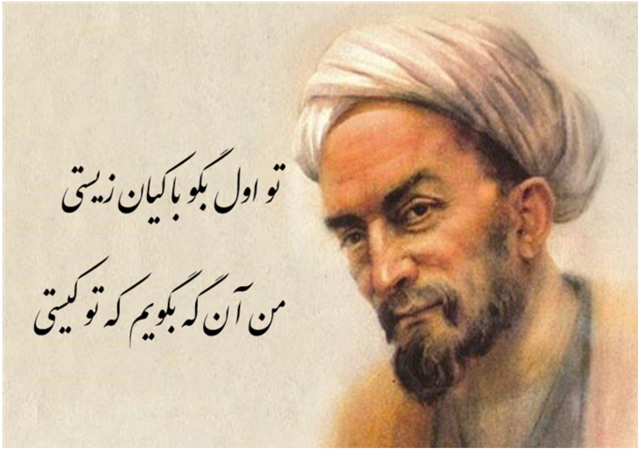
Parametric vs. non-parametric methods

- **Parametric** methods need to **find parameters** from data and then use the inferred parameters to decide on new data points
    - Learning: finding parameters from data
    - e.g., **Linear regression**, **Logistic regression**
- **Non-parametric** methods
    - Training examples are **explicitly** used
    - **Training phase** is **not required**
    - e.g., **k-Nearest neighbors (kNN)**
- Both supervised and unsupervised learning can be categorized into parametric and non-parametric methods

Non-parametric learners

- **Memory-based** or **Instance-based** learners
    - lazy learning: (almost) all the work at the test time
- Generic description:
    - Memorize training $(x^{(1)}, y^{(1)}), \dots, (x^{(n)}, y^{(n)})$
    - Given test x predict: $\hat{y} = f(x; x^{(1)}, y^{(1)}, \dots, x^{(n)}, y^{(n)})$
- f is typically expressed in terms of the similarity of the test samples x to the training samples $x^{(1)}, \dots, x^{(n)}$
- kNN is an instance-based learner

kNN concept



- First, tell me who you have lived with, Then, I will tell you who you are.

Figure adapted from https://setare.com

kNN

- K-NN classifier: $k \geq 1$ nearest neighbors
    - Label for x predicted by majority voting among its $k-NN$
- $k = 5$, $x = [x_1, x_2]$

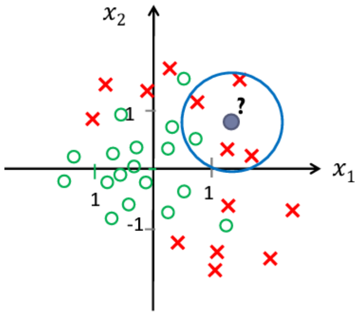


Figure adapted from M.Soleymani ML slides, Sharif University of Technology

kNN classifier

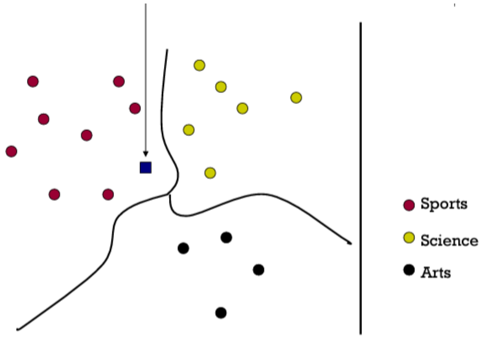
- Given
  - Training data $\{(x^{(1)}, y^{(1)}), \dots, (x^{(n)}, y^{(n)})\}$ are simply stored.
- To classify x:
  - Find k nearest training samples to x
  - Out of these k samples, identify the number of samples k_j belonging to class C_j $(j = 1, \dots, C)$.
  - Assign x to the class C_{j^*} where $j^* = \underset{j=1,\dots,c}{\arg\max}\ k_j$
- It can be considered as a **discriminative** method.

kNN classifier cont.

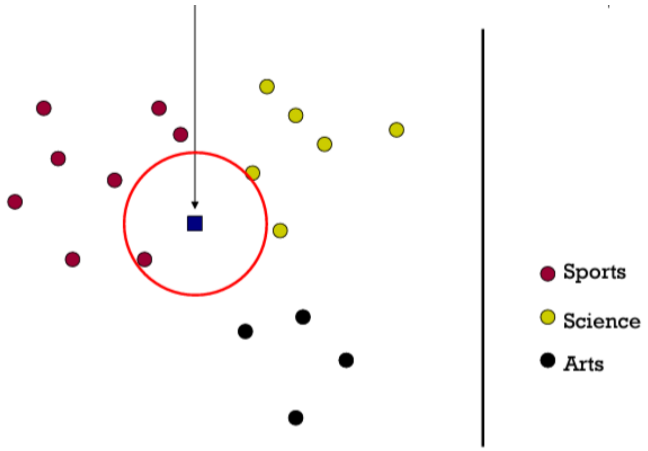
- With **kNN** we can obtain **non-linear** decision surfaces unlike the previous methods (linear and logistic regression)
- But note that this method could be prone to **outliers** or **noisy** data especially if:
  - We have **small dataset**
  - Our data is **low-dimensional**
  - We use a **small value of k** (like $k = 1$ is only determined by the nearest neighbor and could be misleading in many test cases.

kNN example

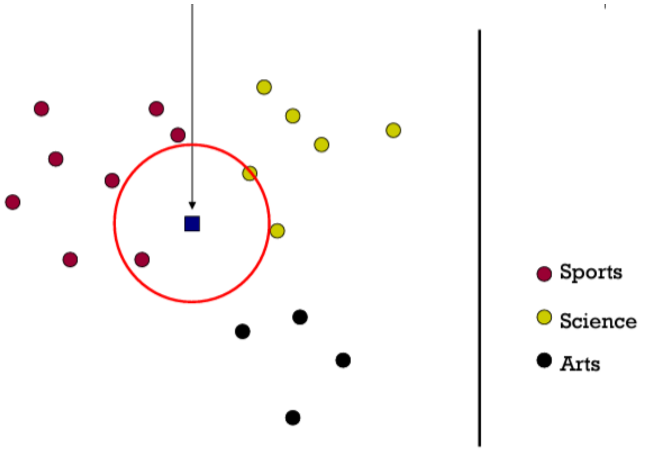
- We want to classify a new document and put it into one of three categories by studying its neighbor samples



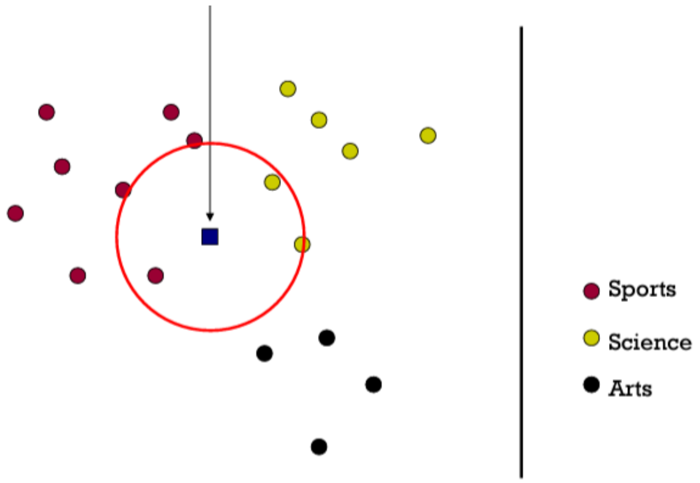
1-Nearest neighbor classifier



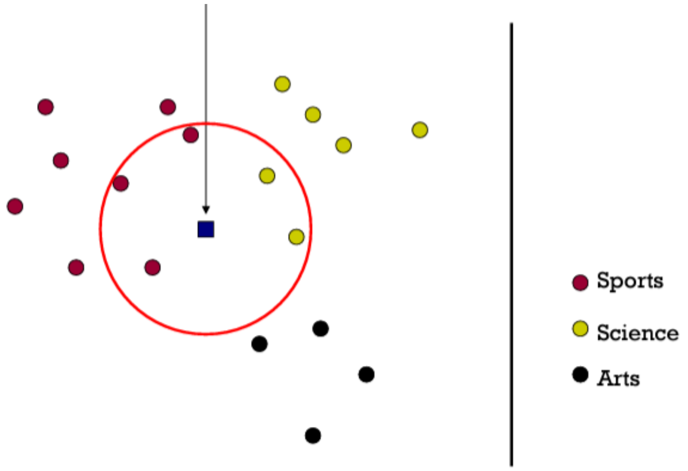
2-Nearest neighbor classifier



3-Nearest neighbor classifier



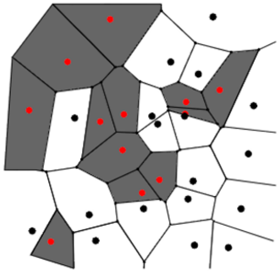
5-Nearest neighbor classifier



Figures for this example were adapted from E. Xing, "Theory of classification and nonparametric classifier." Lecture notes

Voronoi tessellation

- Voronoi tessellation:
  - Each cell consists of all points closer to a given training point than to any other training points
  - All points in a cell are labeled by the category of the corresponding training point



[Duda, Hurt, and Strok's Book]

Voronoi tessellation

- 1NN plot is a Voronoi tessellation

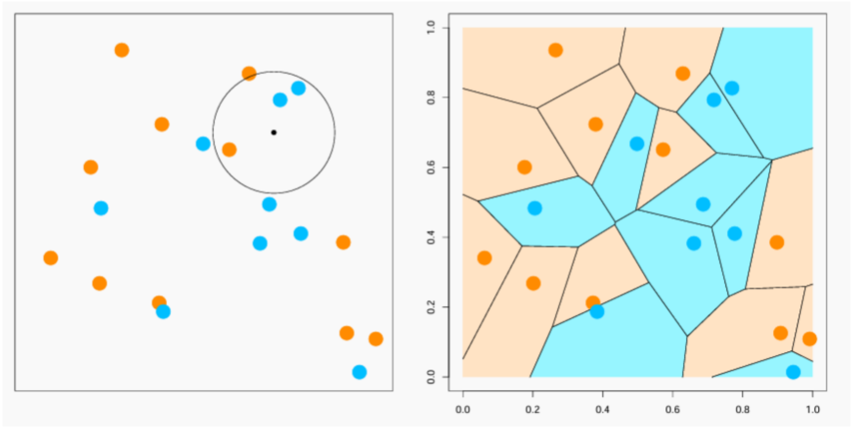
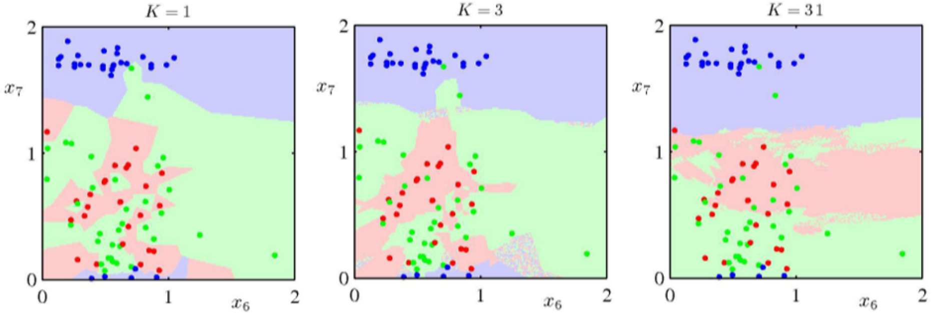


Figure adapted from R. Zhu, “Stat 542: Statistical learning - k-nearest neighbor and the bias-variancetrade-off.” Lecture notes.

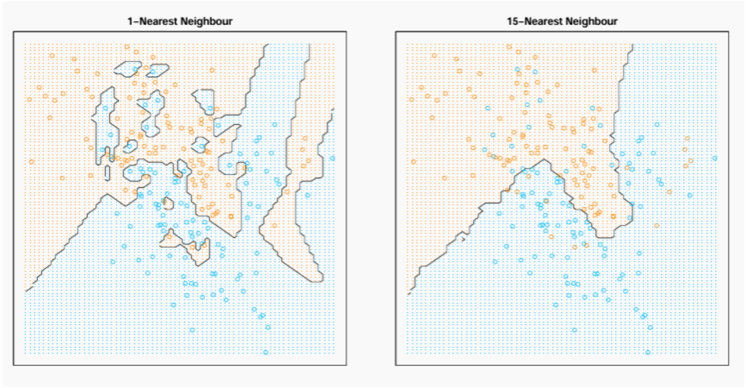
Effect of k



[Bishop]

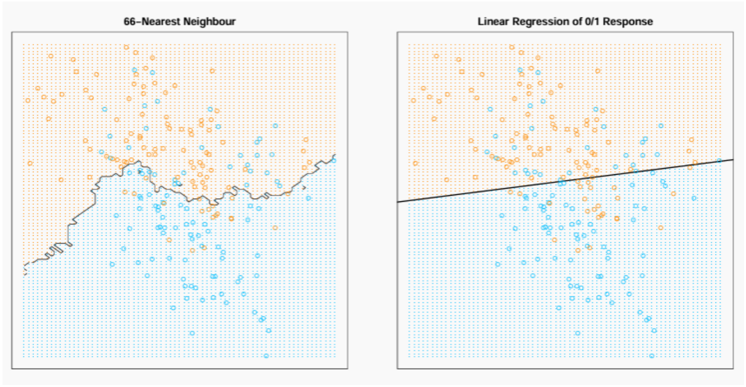
Effect of k cont.

- compare $k = 1$ with $k = 15$



Model complexity

- As we further increase k, the model tends to be less complex.
- Compare $66NN$ with a linear model that uses only 3 parameters:



Figures were adapted from R. Zhu, “Stat 542: Statistical learning - k-nearest neighbor and the bias-variance trade-off.” Lecture notes.

Instance-based learner

- Main things to construct an instance-based learner:
  - A distance metric
  - Number of nearest neighbors of the test data that we look at
  - A weighting function (optional)
  - How to find the output based on neighbors?

Distance measures

- Euclidean distance

$$d(x,x') = \sqrt[2]{\|x-x'\|_2^2} = \sqrt[2]{(x_1-x_1')^2+\cdots+(x_d-x_d')^2}$$

- Distance learning methods for this purpose
  - Weighted Euclidean distance

$$d_w(x,x') = \sqrt[2]{w_1(x_1-x_1')^2+\cdots+w_d(x_d-x_d')^2}$$

Distance measures cont.

- Minkowski distance

$$d(x,x') = (\sum_{i=1}^{n} |x_i - x'_i|^p)^{\frac{1}{p}}$$

  - for $p \geq 1$ is a distance metric
  - As you can see Minkowski distance with $p = 2$ is the same as Euclidean distance
  - Minkowski distance is the same as L^p norm of $(x - x')$
- Remember L^p norm from linear algebra:

$$\|x\|_p = \sqrt[p]{(|x_1|^p + \cdots + |x_n|^p)}$$

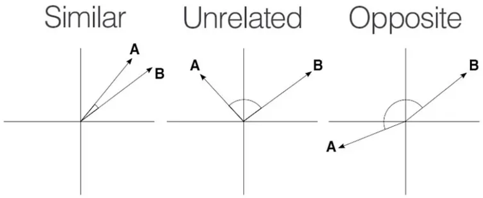
$$\text{Some famous } L^p \text{ norms} \begin{cases} \|x\|_1 & = \sum_{i=1}^{n} |x_i| \\ \|x\|_2 & = \sqrt{x_1^2 + \cdots + x_n^2} \\ \|x\|_\infty & = \max\{|x_1|, |x_2|, \ldots, |x_n|\} \end{cases}$$

Distance measures cont.

- Cosine distance (angle)

$$d(x, x') = 1 - \text{cosine similarity}(x, x')$$

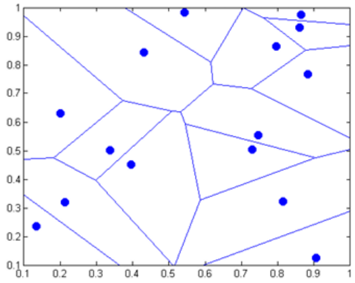
$$\text{Where,}\quad \text{cosine similarity}(x, x') = \frac{x.x'}{\|x\|_2\|x'\|_2} = \frac{\sum_{i=1}^{d} x_i x'_i}{\sqrt{\sum_{i=1}^{d} x_i^2}\sqrt{\sum_{i=1}^{d} x_i'^2}}$$



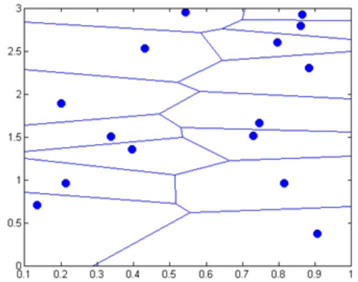
Example of angle difference for cosine similarity

Figure adapted from https://medium.com/@milana.shxanukova15/cosine-distance-and-cosine-similarity-a5da0e4d9ded

Effect of distance measure



$$d(\boldsymbol{x}, \boldsymbol{x}') = \sqrt{(x_1 - x_1')^2 + (x_2 - x_2')^2}$$



$$d(\boldsymbol{x}, \boldsymbol{x}') = \sqrt{(x_1 - x_1')^2 + 3(x_2 - x_2')^2}$$

Figures adapted from M.Soleymani ML slides, Sharif University of Technology

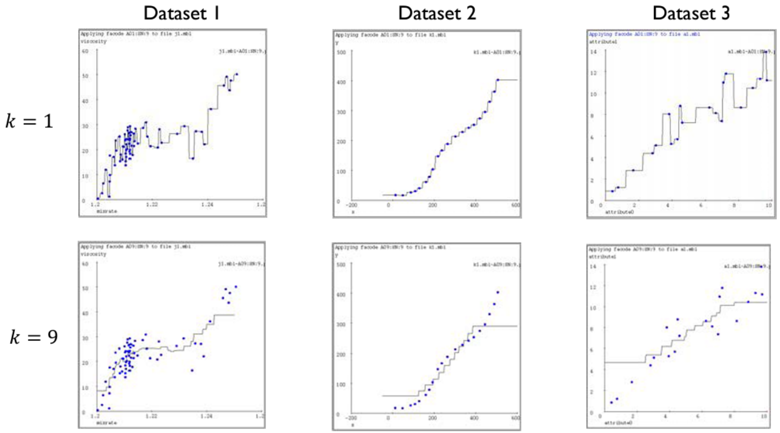
kNN regression

- Let $x'^{(1)}, \ldots, x'^{(k)}$ be the k nearest neighbors of x and $y'^{(1)}, \ldots, y'^{(k)}$ be their labels.

$$\hat{y} = \frac{1}{k} \sum_{j=1}^{k} y'^{(j)}$$

- Some problems of kNN regression for fitting functions:
    - Discontinuities in the estimated function
    - 1NN: noise-fitting problem
    - kNN ($k > 1$) smoothes away noise, but there could be other issues (e.g, flats the ends)

kNN regression cont.



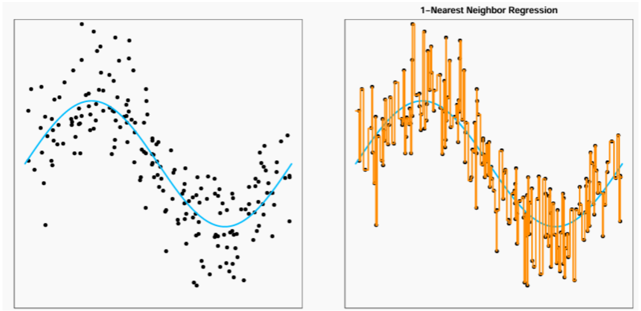
[Figs. have been adopted from Andrew Moore's tutorial on "Instance-based learning"]

kNN regression: example

- Suppose we have a dataset with only 1 feature from uniform $[0, 2\pi]$. The true model is:

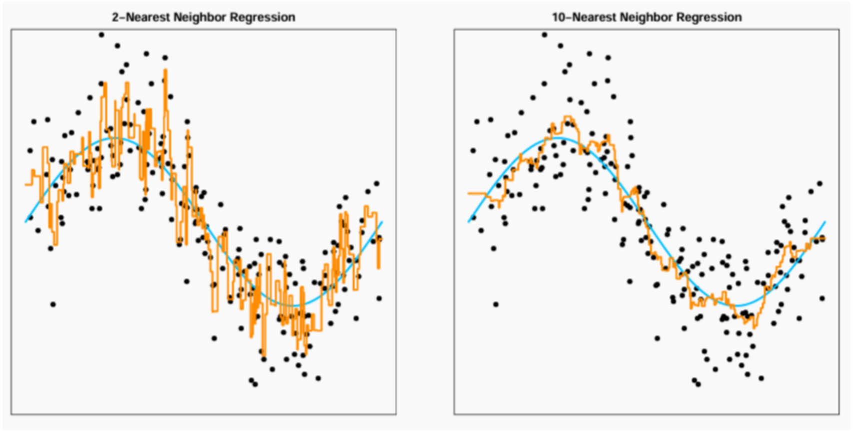
$$Y = 2sin(X) + \epsilon$$

- Where ϵ is the standard normal error.
- First we simulate 200 observations, and see the model for $k = 1$



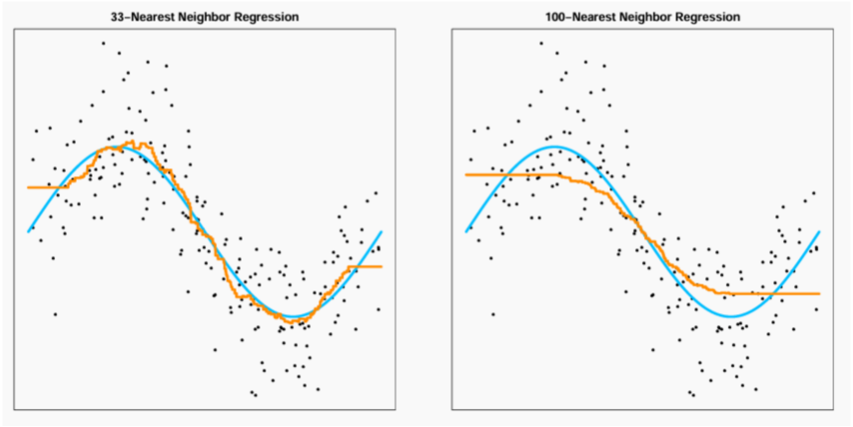
kNN regression: example

- Now for $k = 2$ and $k = 10$



kNN regression: example

- As you can see the model becomes smoother as k increases. However, this eventually deviates from the truth if k is too large



Figures were adapted from R. Zhu, “Stat 542: Statistical learning - k-nearest neighbor and the bias-variance trade-off.” Lecture notes.

Accuracy in classification problems

- **Accuracy** is one of the simplest and most commonly used performance metrics.
- It is defined as the ratio of correctly predicted instances to the total instances:

$$\text{Accuracy} = \frac{\text{True Positives} + \text{True Negatives}}{\text{Total Samples}}$$

- However, accuracy alone can be misleading, especially with imbalanced datasets.

Example: cancer detection problem

- Imagine a dataset with 1000 patients:
  - Only 10 have cancer (**positive class**).
  - 990 do not have cancer (**negative class**).
- A classifier predicts that no one has cancer (predicts all as negative).
- What will be the accuracy of this model?

Example: cancer detection problem cont.

Look at this table for our model which predict negative all the time:

	Predicted Negative	**Predicted Positive**
Actual Negative	990 (TN)	0 (FP)
Actual Positive	10 (FN)	0 (TP)

$$\text{Accuracy} = \frac{990 + 0}{1000} = 99\%$$

High accuracy, but the model fails to detect any actual cases of cancer!

Why accuracy can be misleading

- In highly imbalanced datasets (e.g., cancer detection), the **minority class** (positive cases) is often underrepresented.
- A model that always predicts the majority class can still have high accuracy, but poor real-world performance.
- In the cancer detection example, 99% accuracy sounds good, but the model doesn't detect any actual cancer cases.
- We need better metrics to evaluate model performance.

Performance metrics

- **Scenario:**
  - An alarm system can either ring or not ring when a thief is present.
  - Let's define the outcomes:
    - **True Positive (TP)**: Alarm rings (correctly) when a thief is present.
    - **True Negative (TN)**: Alarm does not ring (correctly) when no thief is present.
    - **False Positive (FP)**: Alarm rings (incorrectly) when no thief is present (a false alarm).
    - **False Negative (FN)**: Alarm does not ring (incorrectly) when a thief is present (a missed alarm).

	Thief Present	**No Thief Present**
Alarm Rings	TP	FP
Alarm Does Not Ring	FN	TN

Photo adapted from https://stock.adobe.com/search?k=thief+cartoon

Performance metrics cont.

- **Metrics:**
  - **Sensitivity (Recall)**:

$$\text{Sensitivity} = \frac{TP}{TP + FN}$$

Indicates the ability of the alarm system to correctly identify a thief. It is the proportion of actual positives (thief present) that are correctly identified.

  - **Specificity**:

$$\text{Specificity} = \frac{TN}{TN + FP}$$

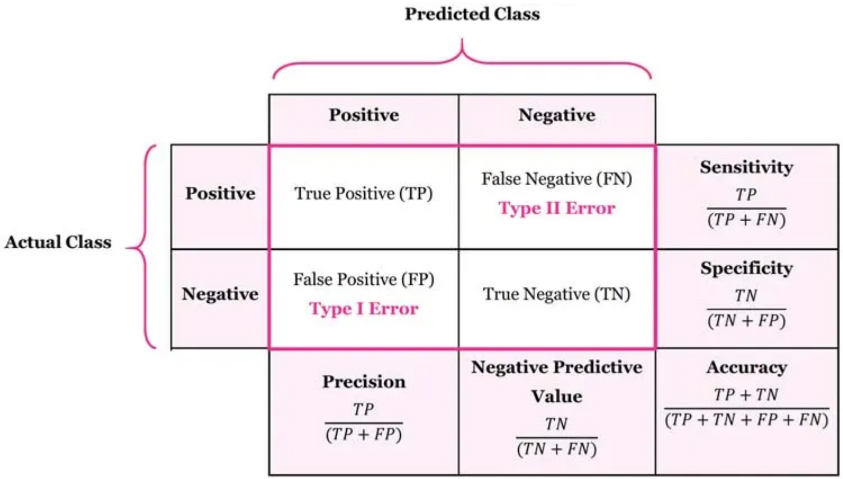
Measures the ability of the alarm system to correctly identify when no thief is present. It is the proportion of actual negatives that are correctly identified.

  - **Precision**:

$$\text{Precision} = \frac{TP}{TP + FP}$$

Indicates the accuracy of the alarm when it rings. It is the proportion of times the alarm rang and a thief was indeed present out of all the times the alarm was activated.

Performance metrics cont.



Predicted Class; Actual Class

Actual Class	Predicted: Positive	Predicted: Negative	
Positive	True Positive (TP)	False Negative (FN) **Type II Error**	**Sensitivity** $\frac{TP}{(TP+FN)}$
Negative	False Positive (FP) **Type I Error**	True Negative (TN)	**Specificity** $\frac{TN}{(TN+FP)}$
	Precision $\frac{TP}{(TP+FP)}$	**Negative Predictive Value** $\frac{TN}{(TN+FN)}$	**Accuracy** $\frac{TP+TN}{(TP+TN+FP+FN)}$

Figure adapted from https://medium.com

A combined measure: F1

- Combined measure: **F1 measure**
  - allows us to trade off precision and recall
  - harmonic mean of P and R

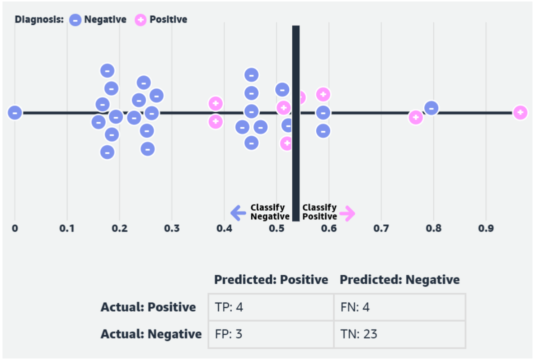
$$F = \frac{1}{\frac{1}{2P} + \frac{1}{2R}} = \frac{2PR}{P+R}$$

- Harmonic mean of P and R:

$$\frac{1}{F} = \frac{1}{2}(\frac{1}{P} + \frac{1}{R})$$

Precision/recall/F1

- This website could give you a perfect intuition about precision recall trade-off



	Predicted: Positive	Predicted: Negative
Actual: Positive	TP: 4	FN: 4
Actual: Negative	FP: 3	TN: 23

- Link: https://mlu-explain.github.io/precision-recall/

Why harmonic mean?

- Why don’t we use a different mean of P and R as a measure?
  - e.g., the arithmetic mean
- The simple (arithmetic) mean is 50% for "return true for every thing", which is too high.
- Desideratum: Punch really bad performance either on precision or recall
  - Taking the minimum achieves this.
  - F (harmonic mean) is a kind of **smooth minimum**.

F1 and other averages

- Harmonic mean is a conservative average. We can view the harmonic mean as a kind of soft minimum

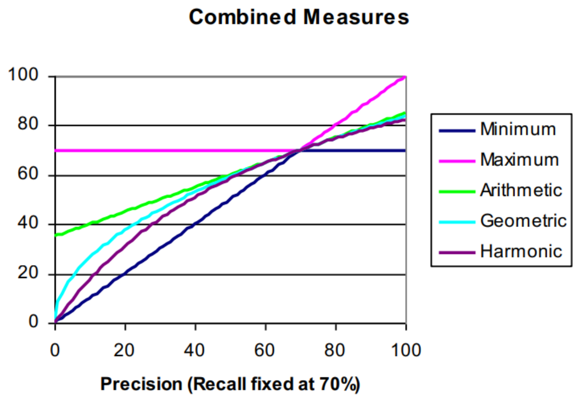


Figure adapted from M.Soleymani ML slides, Sharif University of Technology

Confusion matrix

- The **confusion matrix** is a **table** used to evaluate the performance of a classification model.
- It compares the **actual values (true labels)** with the **predicted values** from the model.
- Each **row** of the matrix represents the **actual class**, while each **column** represents the **predicted class**.
- It helps us understand not just how often the model is correct, but also **where it makes mistakes**.

Confusion matrix cont.

- Let's consider an image classification task where we classify images into three categories: **Cat**, **Dog**, and **Horse**.
- After training the model, we evaluate its predictions against the actual labels.

	Predicted Cat	**Predicted Dog**	**Predicted Horse**
Actual Cat	True Positive (TP)	False Negative (FN)	False Negative (FN)
Actual Dog	False Negative (FN)	True Positive (TP)	False Negative (FN)
Actual Horse	False Negative (FN)	False Negative (FN)	True Positive (TP)

Confusion matrix cont.

- Here is an example confusion matrix for a model that classifies images of cats, dogs, and horses:
- We can see that the model classified 8 images of cats correctly, but it classified 1 cat as a dog and 1 cat as a horse (False Negatives).
- Similarly, it made 2 mistakes when predicting dogs and horses.

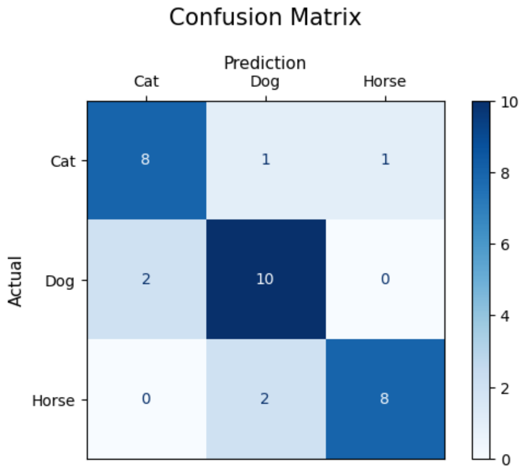


Figure adapted from https://www.geeksforgeek

Per class evaluation measures

- **Definition:** For our **confusion matrix C**, each **element $\mathbf{C_{ij}}$** denotes the number of samples actually in class i that were put in class j by our classifier.
  - Now we could rewrite our performance metrics with confusion matrix view

---

- Recall: Fraction of the samples in class i classified correctly:

$$\frac{C_{ii}}{\sum_j C_{ij}}$$

- Precision: Fraction of the samples assigned class i that are actually about class i:

$$\frac{C_{ii}}{\sum_j C_{ji}}$$

- Accuracy: Fraction of the samples classified correctly:

$$\frac{\sum_i C_{ii}}{\sum_j \sum_i C_{ij}}$$

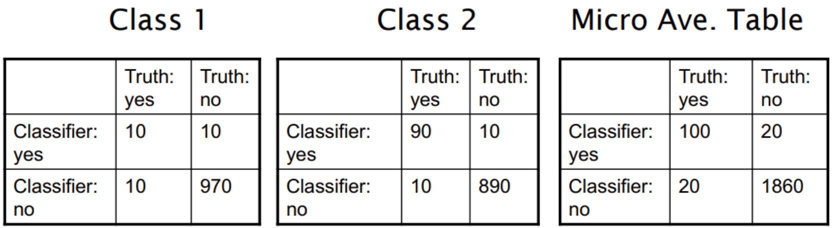
Averaging: macro vs. micro

- We now have an evaluation measure (F1) for one class.
- But we also want a single number that shows aggregate performance over all classes

Micro- vs. Macro-Averaging

- If we have more than one class, how do we combine multiple performance measures into one quantity?
- Macroaveraging: Compute performance for each class, then average
  - Compute F1 for each of the C classes
  - Average these C numbers
- Microaveraging: Collect decisions for all classes, aggregate them and then compute measure.
  - Compute TP, FP, FN for each of the C classes.
  - Sum these C numbers(e.g, all TP to get aggregate TP)
  - Compute F1 for aggregate TP, FP, FN

Micro- vs. Macro-Averaging: example



Class 1

	Truth: yes	Truth: no
Classifier: yes	10	10
Classifier: no	10	970

Class 2

	Truth: yes	Truth: no
Classifier: yes	90	10
Classifier: no	10	890

Micro Ave. Table

	Truth: yes	Truth: no
Classifier: yes	100	20
Classifier: no	20	1860

- Macroaveraged precision: $(0.5+0.9)/2 = 0.7$
- Microaveraged precision: $100/120 = 0.83$
- Microaveraged score is dominated by score on common classes

AUC-ROC

- Area Under the Receiver Operating Characteristic Curve
  - ROC (Receiver Operating Characteristic) is a graphical representation of the performance of a binary classification model.
  - It plots the true positive rate (TPR) against the false positive rate (FPR) at different classification thresholds.

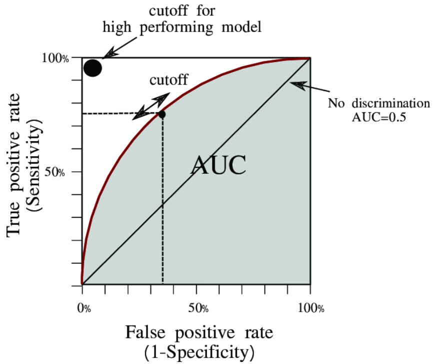


Figure adapted from https://www.researchgate.net/figure/ROC-curves-and-area-under-curve-AUC$_fig2_3$51506473

AUC-ROC cont.

- A high AUC score indicates that the model has good discrimination ability, i.e., it can effectively differentiate between positive and negative instances at different classification thresholds.
- Conversely, a lower AUC-ROC score suggests that the model struggles to differentiate between the two classes.
- AUC ranges from 0 to 1, with 0.5 indicating random guessing and 1 indicating a perfect classifier.

Model Selection via Cross Validation

- **Cross-Validation**
  - **Purpose**: Technique for evaluating how well a model generalizes to unseen data.
  - **How It Works**: Split data into k folds; train on $k-1$ folds and validate on the remaining fold.
  - **Repeat Process**: Repeat k times, rotating the test fold each time. Average of all scores is the final score of the model.
  - Cross-validation reduces overfitting and provides a more reliable estimation of model performance.
  - Note that the model must be **retrained** at each iteration to avoid reusing a model that has already seen the test data, ensuring unbiased evaluation.

K-Fold Cross Validation

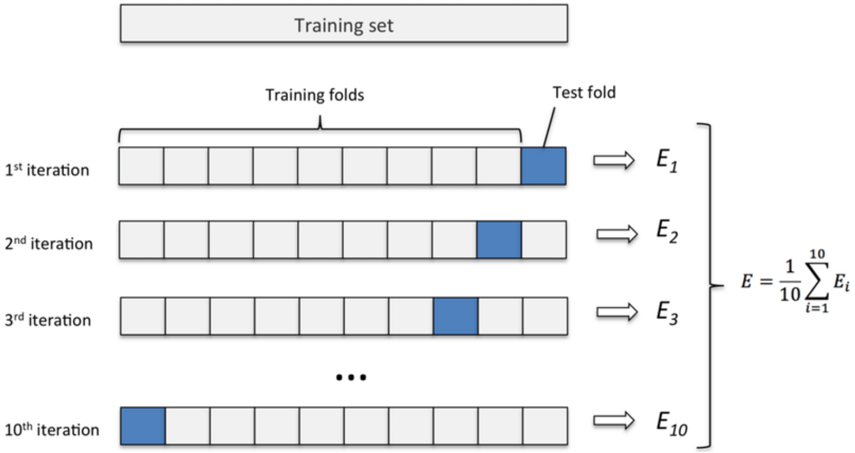


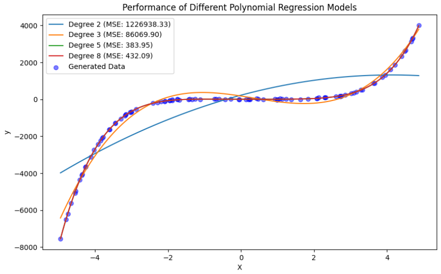
Figure adapted from Introduction to Support Vector Machines and Kernel Methods, J.M. Ashfaque.

Leave-One-Out Cross-Validation (LOOCV)

- **Leave-One-Out Cross-Validation (LOOCV)**
  - **How It Works**: Uses a single data point as the validation set ($k = 1$) and the rest as the training set. Repeat for all data points.
  - **Properties:**
    - **No Data Wastage**: Every data point is used for both training and validation.
    - **High Variance, Low Bias**.
    - **Computationally Expensive**: Requires training the model N times for N data points, making it slow for large datasets.
    - **Best for small datasets**.

Cross-Validation for Better Generalization

- Cross-validation is one of the methods used to find the optimal model degree and regularization parameter, ensuring better generalization by minimizing validation error and balancing model complexity.



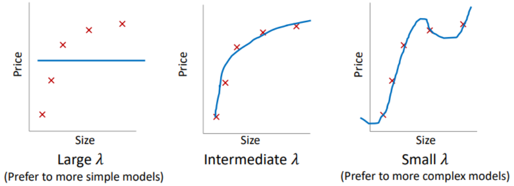


Figure on the right adapted from slides of F.Salehi, Machine Learning course, Sharif University of Technology.

Cross-Validation for Evaluating Model Performance

- Metrics like accuracy, precision, recall, and F1 score are assessed across different folds.
- Averaging these scores gives a reliable estimate of performance and stability.
- Ensures the model is effective before final testing and use on the test dataset.
- For example, high variance in cross-validation metrics means the model's performance is inconsistent, likely overfitting to specific data subsets.

Contributions

- **These slides are authored by:**
  - Danial Gharib
  - Mahan Bayhaghi
  - Erfan Jafari

[1] C. M., *Pattern Recognition and Machine Learning.*
Information Science and Statistics, New York, NY: Springer, 1 ed., Aug. 2006.

[2] M. Soleymani Baghshah, "Machine learning." Lecture slides.

[3] M. Soleymani Baghshah, "Modern information retrieval." Lecture slides.

[4] T. Mitchell, *Machine Learning.*
McGraw-Hill series in computer science, New York, NY: McGraw-Hill Professional, Mar. 1997.

[5] R. Zhu, "Stat 542: Statistical learning - k-nearest neighbor and the bias-variance trade-off." Lecture notes.

[6] E. Xing, "Theory of classification and nonparametric classifier." Lecture notes.