# EE2211 Pre-Tutorial 10

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# Agenda

- Recap
- Self-learning
- Tutorial 10

# Recap

- Dataset Partition:
  - Training/Validation/Testing
- Cross Validation
- Evaluation Metrics
  - Evaluating the quality of a trained machine learning system
  - Mean Square Error
  - Mean Absolute Error
  - Confusion Matrix
  - Cost Matrix

# Training, Validation, Test

| Training set | Validation set | Test set |
|---|---|---|
| For training the ML models | For validation: choosing the parameter or model | For testing the “real” performance and generalization |

Example of hyper-parameters, which are set before the training process begins:

- Order of polynomial
- Regularization parameters ($\lambda$)
- Tree depth (decision trees, random forests)
- Number of trees (random forests)
- ...

# K-fold Cross Validation

- In practice, we do the **k-fold cross validation**

4-fold cross validation

Test

Step 1: take out *test set* from the dataset

# K-fold Cross Validation

- In practice, we do the **k-fold cross validation**

Test

4-fold cross validation

Step 2: We partition the ***remaining part of the dataset*** (after taking out the test set), into ***k*** equal parts (equal in terms of number of samples).

# K-fold Cross Validation

- In practice, we do the **k-fold cross validation**

Test

4-fold cross validation

| | | | | |
|---|---|---|---|---|
| Fold 1 | Train | Train | Train | Validation |
| Fold 2 | Train | Train | Validation | Train |
| Fold 3 | Train | Validation | Train | Train |
| Fold 4 | Validation | Train | Train | Train |

Order of the samples are kept the same across all folds.

Step 3: We run ***k folds*** (i.e., k times) of experiments.
Within each fold, we use ***one part*** as ***validation set***, and the ***k-1 remaining parts*** as ***training set***. We use different validation sets for different folds.

# K-fold Cross Validation

- In practice, we do the **k-fold cross validation**

Test

4-fold cross validation

| | | | | | Classifiers Trained |
|---|---|---|---|---|---|
| Fold 1 | Train | Train | Train | Validation | $C_1^1$ $C_2^1$ |
| Fold 2 | Train | Train | Validation | Train | $C_1^2$ $C_2^2$ |
| Fold 3 | Train | Validation | Train | Train | $C_1^3$ $C_2^3$ |
| Fold 4 | Validation | Train | Train | Train | $C_1^4$ $C_2^4$ |

**1) $C_1$: Random Forest with 100 trees**
**2) $C_2$: Random Forest with 200 trees**

Step 3.1: Within each fold, if we have $n$ parameter/model candidates, we will train $n$ models, and we check their validation performance.

# K-fold Cross Validation

- In practice, we do the **k-fold cross validation**

Test

4-fold cross validation

| | | | | | Classifiers Trained |
|---|---|---|---|---|---|
| Fold 1 | Train | Train | Train | Validation | $C_1^1$ $C_2^1$ |
| Fold 2 | Train | Train | Validation | Train | $C_1^2$ $C_2^2$ |
| Fold 3 | Train | Validation | Train | Train | $C_1^3$ $C_2^3$ |
| Fold 4 | Validation | Train | Train | Train | $C_1^4$ $C_2^4$ |

Example: which one to select for test?

| | Fold 1 Accuracy on Validation Set 1 | Fold 2 Accuracy on Validation Set 2 | Fold 3 Accuracy on Validation Set 3 | Fold 4 Accuracy on Validation Set 4 | Average Accuracy on All Validation Sets |
|---|---|---|---|---|---|
| Classifier with Param1 (e.g. 100 trees) | 88% $C_1^1$ | 89% $C_1^2$ | 93% $C_1^3$ | 92% $C_1^4$ | 90.5% |
| Classifier with Param2 (e.g. 200 trees) | 90% $C_2^1$ | 88% $C_2^2$ | 91% $C_2^3$ | 91% $C_2^4$ | 90% |

Step 4: We select the parameter/model with best average validation performance over k folds.

# Evaluation Metrics

## Regression

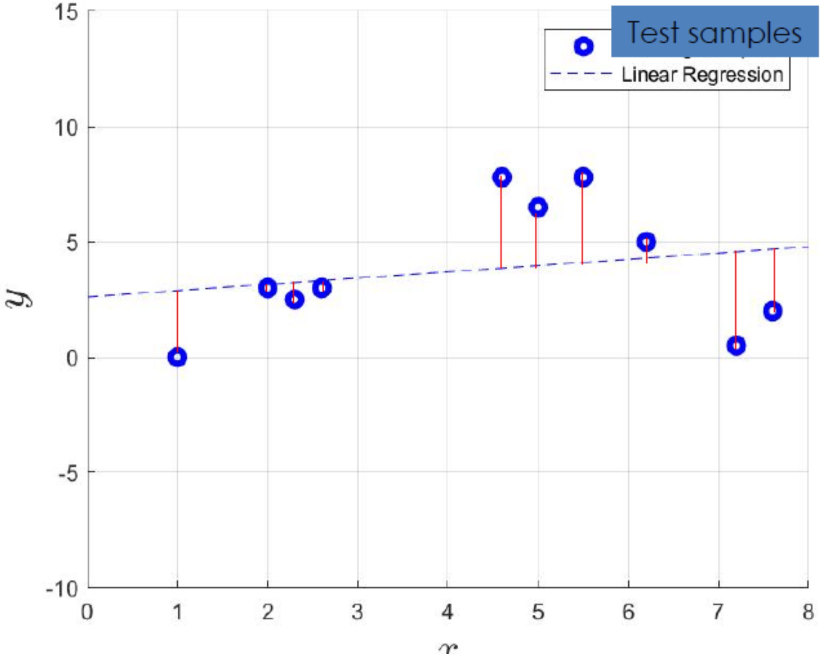
Mean Square Error

$$(\text{MSE} = \frac{\Sigma_{i=1}^{n}(y_i - \hat{y}_i)^2}{n})$$

Mean Absolute Error

$$(\text{MAE} = \frac{\Sigma_{i=1}^{n}|y_i - \hat{y}_i|}{n})$$

where $y_i$ denotes the target output and $\hat{y}_i$ denotes the predicted output for sample $i$.



# Evaluation Metrics

## Classification

(True Positive Rate) TPR = TP/(TP+FN) Recall
(False Negative Rate) FNR = FN/(TP+FN)

(True Negative Rate) TNR = TN/(FP+TN)
(False Positive Rate) FPR = FP/(FP+TN)

TPR + FNR = 1 (100% of positive-class data)
TNR + FPR = 1 (100% of negative-class data)

Confusion Matrix for Binary Classification

| | $\hat{P}$ (predicted) | $\hat{N}$ (predicted) | |
|---|---|---|---|
| P (actual) | TP | FN | Recall TP/(TP+FN) |
| N (actual) | FP | TN | |
| | Precision TP/(TP+FP) | | Accuracy (TP+TN)/(TP+TN+FP+FN) |

# Evaluation Metrics

## Classification

### Cost Matrix for Binary Classification

| | $\hat{\mathrm{P}}$ (predicted) | $\hat{\mathrm{N}}$ (predicted) |
|---|---|---|
| **P** (actual) | $C_{p,p}$ * TP | $C_{p,n}$ * FN |
| **N** (actual) | $C_{n,p}$ * FP | $C_{n,n}$ * TN |

**Total cost:**
$C_{p,p}$ * TP +
$C_{p,n}$ * FN +
$C_{n,p}$ * FP +
$C_{n,n}$ * TN

Main Idea: To assign different ***penalties*** for different entries. Higher penalties for more severe results. Smaller costs are preferred.

Usually, $C_{p,p}$ and $C_{n,n}$ are set to 0; $C_{n,p}$ and $C_{p,n}$ may and may not equal

# Evaluation Metrics

- Example of cost matrix
  - Assume we would like to develop a self-driving car system
  - We have an ML system that detects the pedestrians using camera, by conducing a binary classification
    - When it detects a person (positive class), the car should stop
    - When no person is detected (negative class), the car keeps going

Credit: automotiveworld.com

**True Positive (cost $C_{p,p}$)**
There is person, ML detects person and car stops

**True Negative (cost $C_{n,n}$)**
There is no person, car keeps going

**False Positive (cost $C_{n,p}$)**
There is no person, ML detects person and car stops

**False Negative (cost $C_{p,n}$)**
There is person, ML fails to detect person and car keeps going

$$C_{n,p} \; ? \; C_{p,n} \; (>, <, \text{or} =)$$

# Evaluation Metrics

- For unbalanced data…
  - Assume we have 1000 samples, of which 10 are ***positive*** and 990 are ***negative***
  - Accuracy = 990/1000=0.99!
    Very high number!
  - Yet, half of the Class-1 are Classified to Class-2!

| | Class-1 (predicted) | Class-2 (predicted) |
|---|---|---|
| Class-1 (actual) | 5 (TP) | 5 (FN) |
| Class-2 (actual) | 5 (FP) | 985 (TN) |

**The goal is to highlight the problems of the results!**

In this case, we shall

1) Use cost matrix, assign different costs for each entry
2) Use Precision and Recall! Precision = 0.5 and Recall = 0.5

# Evaluation Metrics

## Classification

Prediction function y = f(x)

| sample | N1 | N2 | P1 | N3 | P2 | P3 |
|---|---|---|---|---|---|---|
| input x | -4 | -3 | -2.5 | -2 | -1.5 | -0.5 |
| Prediction y | -1.1 | -0.5 | -0.1 | 0.2 | 0.6 | 0.9 |
| Actual Label | -1 | -1 | 1 | -1 | 1 | 1 |

If threshold set to be y=0,
N3, P2, P3 will be taken as +1
P1, N2, N1 will be taken as -1

| | $\hat{P}$ (predicted) | $\hat{N}$ (predicted) |
|---|---|---|
| P (actual) | $TP = 2$ | $FN = 1$ |
| N (actual) | $FP = 1$ | $TN = 2$ |

# Evaluation Metrics

## Classification

Prediction function y = f(x)

We can change the threshold!

| sample | N1 | N2 | P1 | N3 | P2 | P3 |
|---|---|---|---|---|---|---|
| input x | -4 | -3 | -2.5 | -2 | -1.5 | -0.5 |
| Prediction y | -1.1 | -0.5 | -0.1 | 0.2 | 0.6 | 0.9 |
| Actual Label | -1 | -1 | 1 | -1 | 1 | 1 |

If threshold set to be y=0.4,
P2, P3 will be taken as +1
N3, P1, N2, N1 will be taken as -1

| | $\hat{P}$ (predicted) | $\hat{N}$ (predicted) |
|---|---|---|
| P (actual) | $TP = 2$ | $FN = 1$ |
| N (actual) | $FP = 0$ | $TN = 3$ |

# Evaluation Metrics

## Classification

Prediction function y = f(x)

We can change the threshold!

| sample | N1 | N2 | P1 | N3 | P2 | P3 |
|---|---|---|---|---|---|---|
| input x | -4 | -3 | -2.5 | -2 | -1.5 | -0.5 |
| Prediction y | -1.1 | -0.5 | -0.1 | 0.2 | 0.6 | 0.9 |
| Actual Label | -1 | -1 | 1 | -1 | 1 | 1 |

If threshold set to be y=-0.2
P1, N3, P2, P3 will be taken as +1
N1, N2 will be taken as -1

| | $\hat{P}$ (predicted) | $\hat{N}$ (predicted) |
|---|---|---|
| P (actual) | $TP = 3$ | $FN = 0$ |
| N (actual) | $FP = 1$ | $TN = 2$ |

# Evaluation Metrics

**Classification:**

TP, FP, FN, TN will change wrt thresholds!

If threshold set to be y=0,
N3, P2, P3 will be taken as +1
P1, N2, N1 will be taken as -1

| | $\hat{P}$ (predicted) | $\hat{N}$ (predicted) |
|---|---|---|
| P (actual) | $TP = 2$ | $FN = 1$ |
| N (actual) | $FP = 1$ | $TN = 2$ |

If threshold set to be y=0.4,
P2, P3 will be taken as +1
N3, P1, N2, N1 will be taken as -1

| | $\hat{P}$ (predicted) | $\hat{N}$ (predicted) |
|---|---|---|
| P (actual) | $TP = 2$ | $FN = 1$ |
| N (actual) | $FP = 0$ | $TN = 3$ |

# Evaluation Metrics

## Classification

### Confusion Matrix for Multicategory Classification

| | $P_{\hat{1}}$ (predicted) | $P_{\hat{2}}$ (predicted) | | $P_{\hat{C}}$ (predicted) |
|---|---|---|---|---|
| $P_1$ (actual) | $P_{1,\hat{1}}$ | $P_{1,\hat{2}}$ | $\cdots$ | $P_{1,\hat{C}}$ |
| $P_2$ (actual) | $P_{2,\hat{1}}$ | $P_{2,\hat{2}}$ | $\cdots$ | $P_{2,\hat{C}}$ |
| $\vdots$ | $\vdots$ | $\vdots$ | $\ddots$ | $\vdots$ |
| $P_C$ (actual) | $P_{C,\hat{1}}$ | $P_{C,\hat{2}}$ | | $P_{C,\hat{C}}$ |

# THANK YOU