INF721

2024/2

UFV

Deep Learning

L7: Evaluting Neural Networks

Logistics

Announcements

- PA2: Multilayer Perceptorn is out!

Last Lecture

- Backpropagation
  - Computational Graph
  - Demo
  - Logistic Regression
  - Multilayer Perceptron

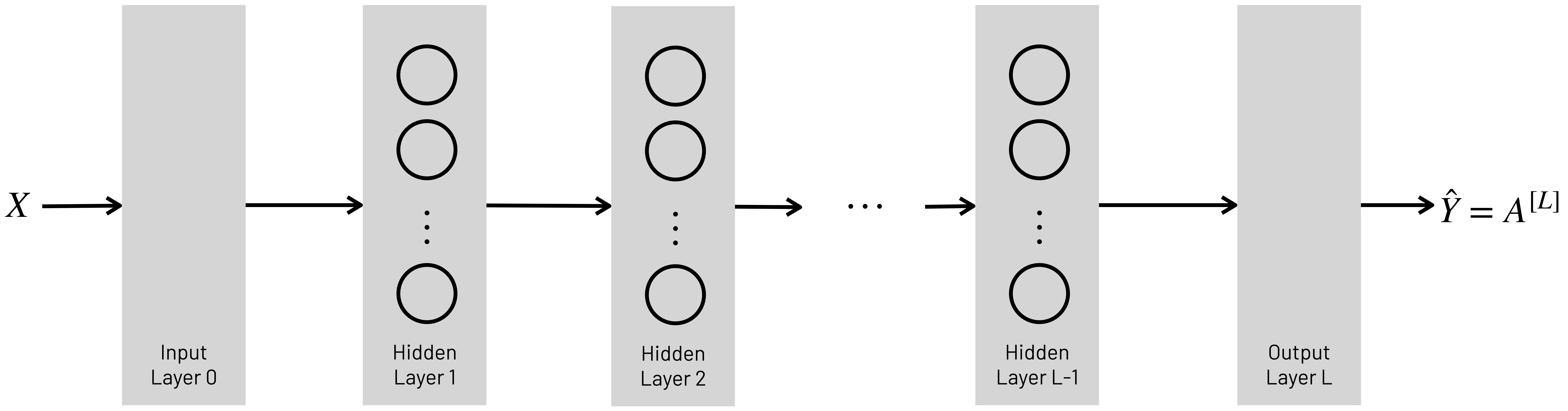
Lecture Outline

- Dataset Split
- Regression
  - Evalutation Metrics
- Classification
  - Confusion Matrix
  - Evalutation Metrics
    - Accuracy, Precision, Recall, F1-Score

Fully-Connected Neural Networks

Multilayer Perceptrons are more generally called Fully-Connected Neural Networks, since they can be adjusted to support different: (a) nº of layers L, (b) nº of hidden units, and (c) activation functions g

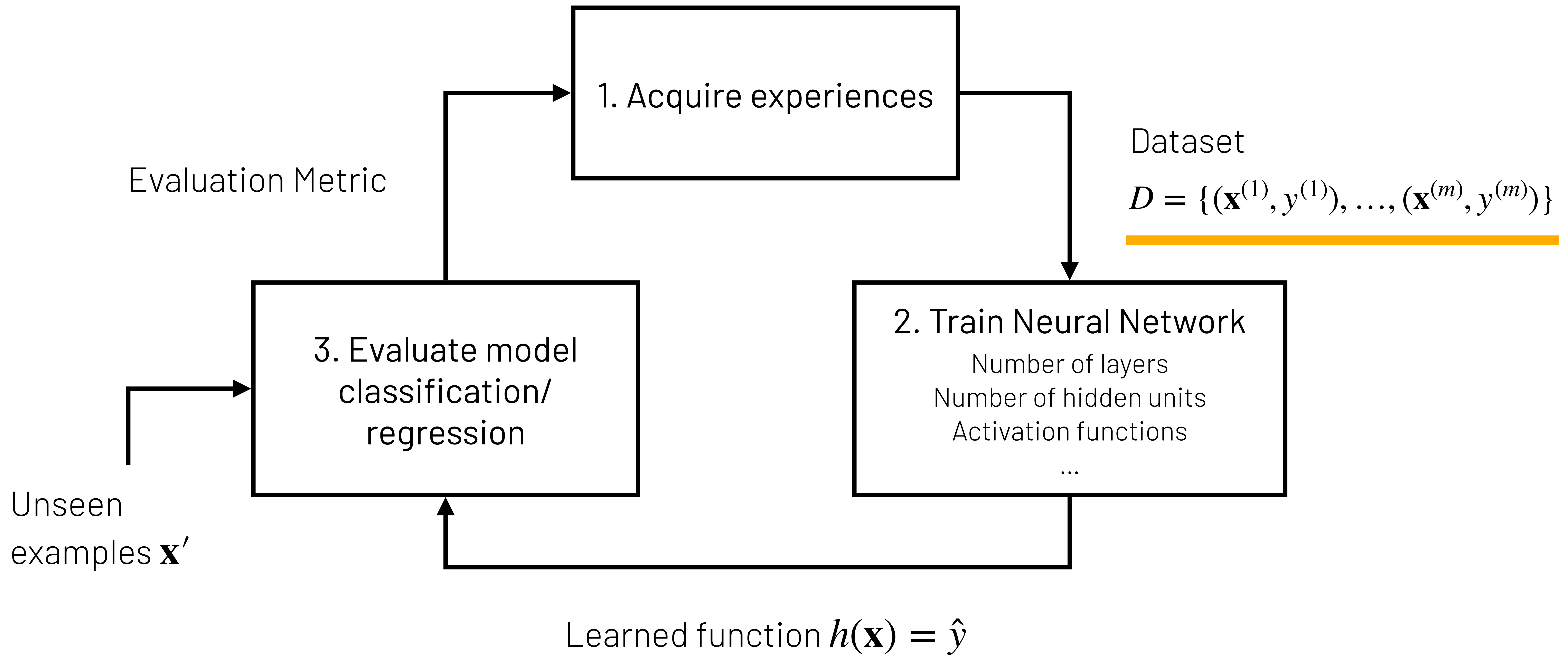
$$A^{[0]} = X \qquad A^{[1]} = g^{[1]}(A^{[0]}) \qquad A^{[2]} = g^{[2]}(A^{[1]}) \qquad A^{[L-1]} = g^{[L-1]}(A^{[L-2]}) \qquad A^{[L]} = g^{[L]}(A^{[L-1]})$$



How de we choose these hyperparameters (a), (b) and (c)?

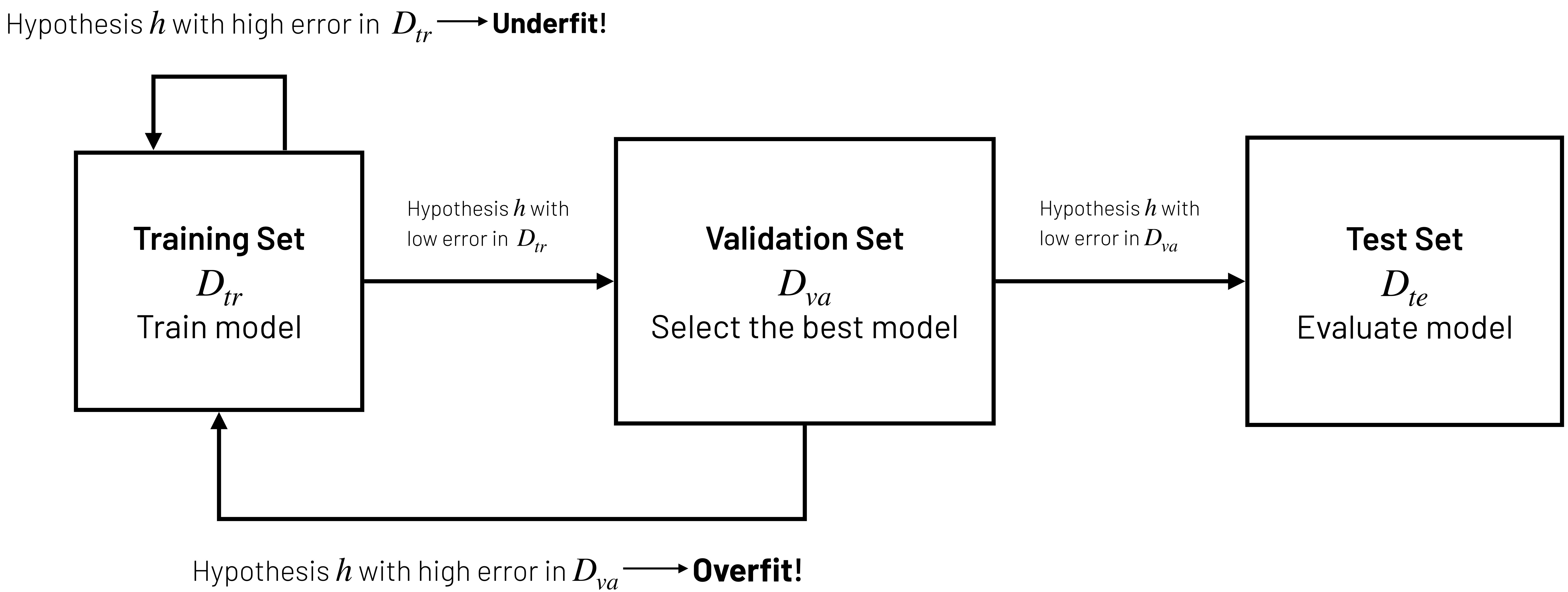
Supervised Deep Learning

Train a neural network $h(\mathbf{x}) = \hat{y}$ from a dataset $D = \{(\mathbf{x}^{(1)}, y^{(1)}), \ldots, (\mathbf{x}^{(m)}, y^{(m)})\}$ to predict the labels $y^{(i)}$ from the feature vectors $\mathbf{x}^{(i)}$, minimizing prediction error on unseen examples $\mathbf{x}'$



Evaluating Model's Performance

To evaluate a model on unseen examples, we typically divide the dataset D in 3 disjoint subsets: D_{tr}, D_{va} e D_{te}



Proportion of Dataset Splits

Dataset:

Training	Validation	Test

Traditional Machine Learning

- Low data regime: 1K examples
- Train/Test: 70/30%
- Train/Valid/Test: 60/20/20%

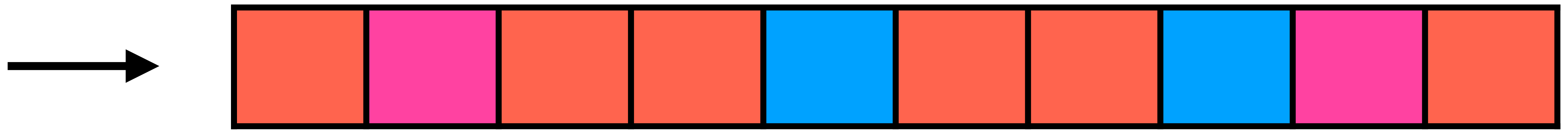
Modern Deep Learning

- Big data regime: 1M examples
- Train/Test: 95/5%
- Train/Valid/Test: 98/1/1%

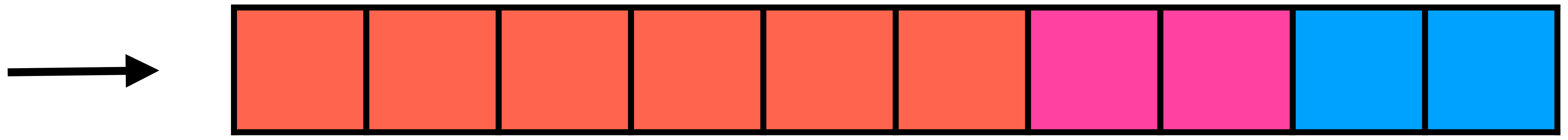
- It's common practice to **not have a validation set**, especially in low data regimes.
  - In this case your test set is your validation set!
- **The subsets are disjoint!**
  - Their can't be examples in the training set in the validation or test set!

How to Split the Dataset

- You have to be very careful when you split the data in **Train**, **Validation**, **Test**.
- The test set must simulate a real test scenario, i.e. you want to simulate the setting that you will encounter in real life.
- Common techniques to split the dataset:
  - **Uniformely at random**, if the data is i.i.d
    Example: image classification



  - **By time**, if the data has a temporal component
    Example: spam filtering



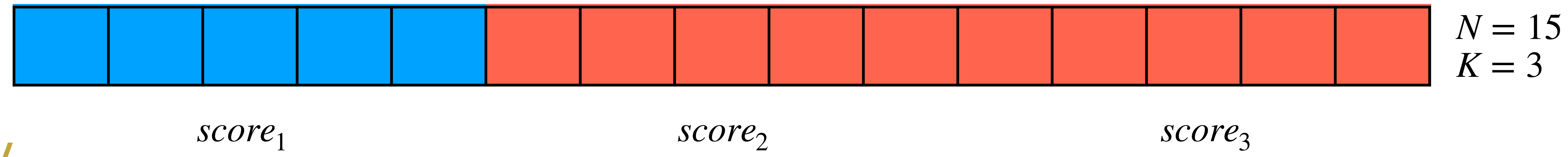
- **Definitely never split alphabetically, or by feature values.**

Cross-validation

When you are in a low data regime, using a single train-test split can lead to highly variable performance estimates. This problem can be solved by cross-validation:

k-fold Cross Validation

1. Split the dataset into k equal parts (folds)
2. For each fold i from 1 to k:
   - Use fold i as the **test set**
   - Use the remaining $k-1$ folds as the **training set**
   - Train the model and evaluate on the test set
3. Average the k evaluation scores (e.g., $score = \dfrac{score_1 + score_2 + score_3}{3}$)

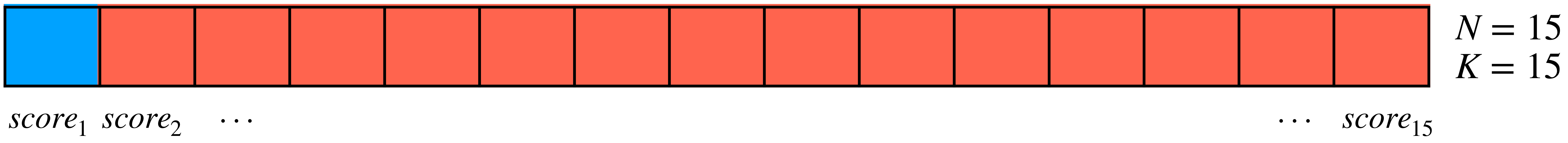


Cross-validation

When you are in a low data regime, using a single train-test split can lead to highly variable performance estimates. This problem can be solved by cross-validation:

Leave-One-Out Cross Validation

1. Split the dataset into $k = N$ equal parts (folds)
2. For each fold i from 1 to N:
   - Use fold i as the **test set**
   - Use the remaining $N - 1$ folds as the **training set**
   - Train the model and evaluate on the test set
3. Average the N evaluation scores (e.g., $score = \dfrac{score_1 + score_2 + \ldots + score_{15}}{15}$)



UFV

Examples of Datasets Splits

Here is the splits of popular deep learning datasets:

ImageNet (images)

- 1.4 million images of 1000 classes
- Train/Valid/Test: 90/3/7%

Penn Treebank (sentences)

- 46K sentences from Wall Street Journal
- Train/Valid/Test: 85/7.5/7.5%

MAESTRO Dataset (audio/MIDI)

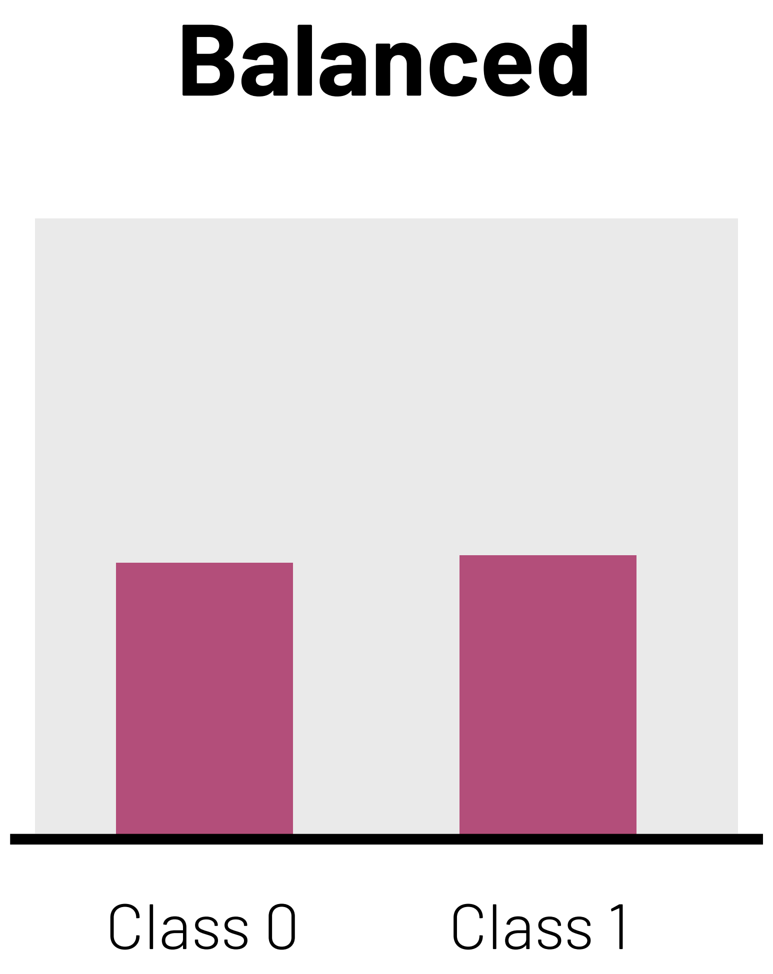
- 1276 classical music pieces
- Train/Valid/Test: 75/10/15%

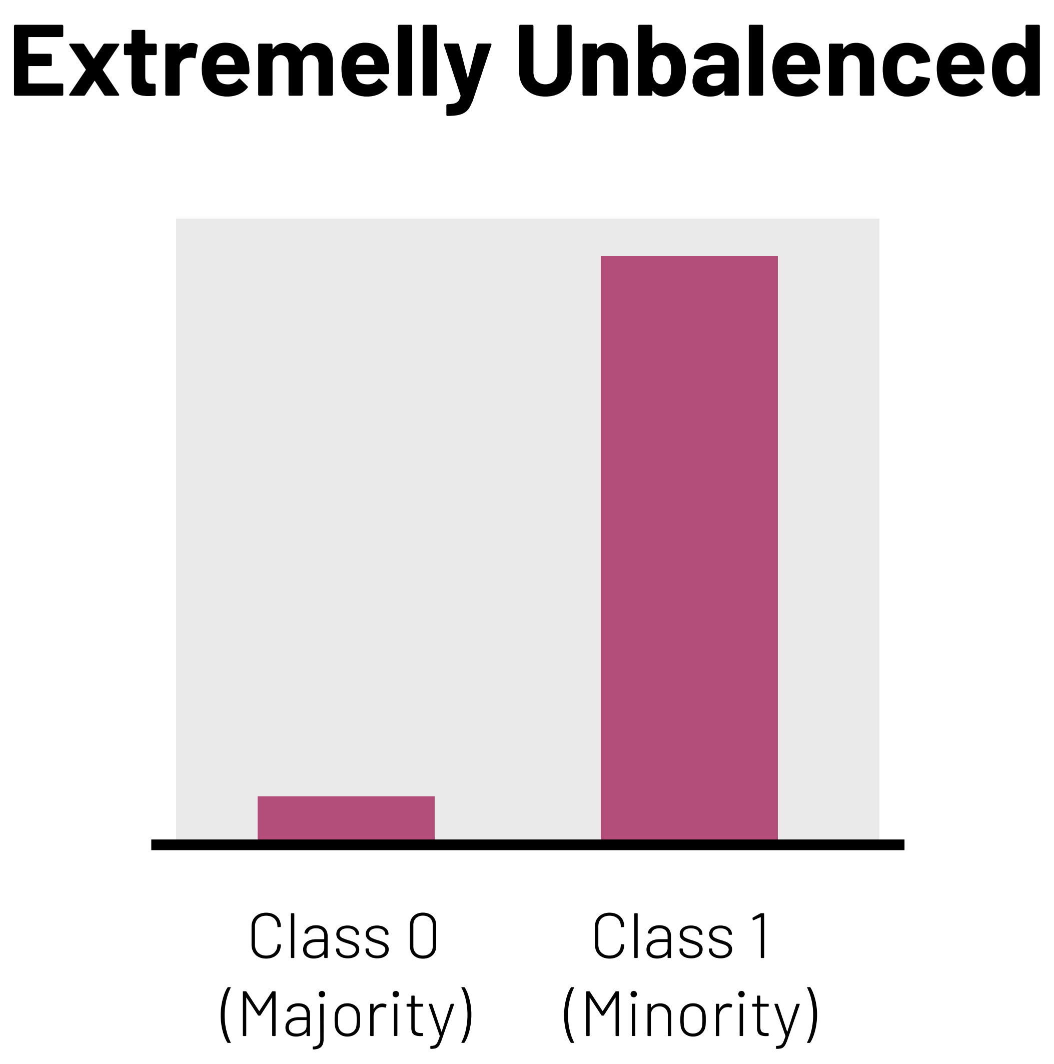
MNIST (images)

- 70K images of handwritten digits (10 classes)
- Train/Test: 85/15%

Imbalanced Datasets

Ideally, when training classification models, your distribution of classes should be balanced:



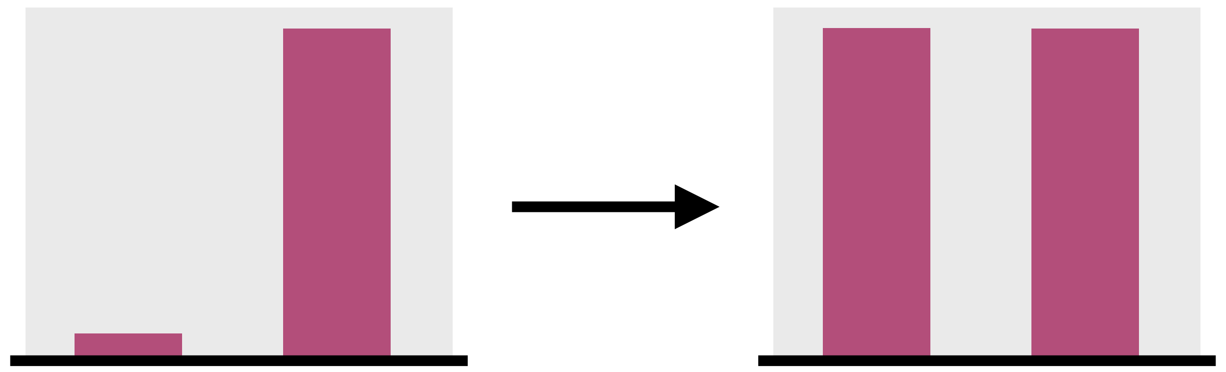


With (especially extremelly) unbalanced datasets:

- Splitting the data randomly can **produce splits with different distribution of classes**
- Your model migh **overfitt to the majority class**!

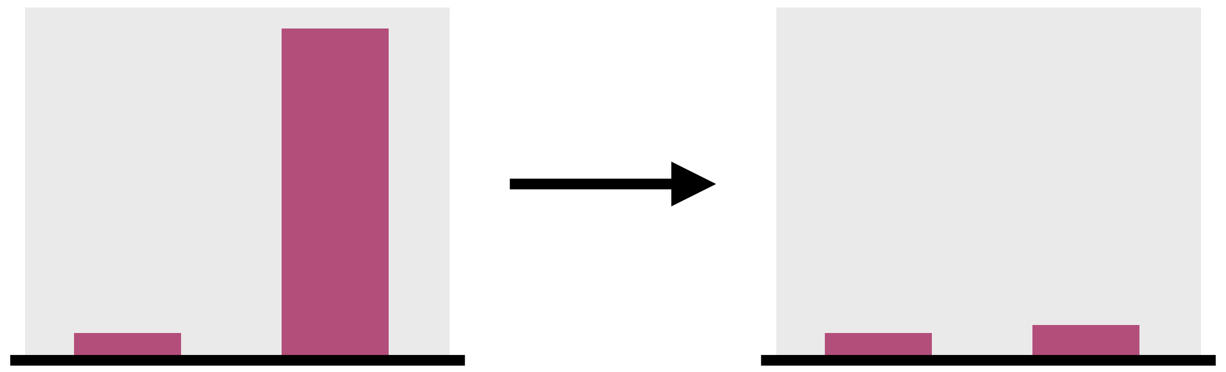
UFV

Balancing Datasets



Oversampling – Increase the nº of minority class samples.

- Duplicate existing samples or generating synthetic samples



Downsample – Decrease the nº of majority class samples.

- Randomly select majority class examples to remove

$$L(h) = -\frac{1}{m}\sum_{i=1}^{m}\left[w_1 y_i \log(\hat{y}^{(i)}) + w_0(1-y^{(i)})\log(1-\hat{y}^{(i)})\right]$$

Weights – Assign weights to classes in the loss function.

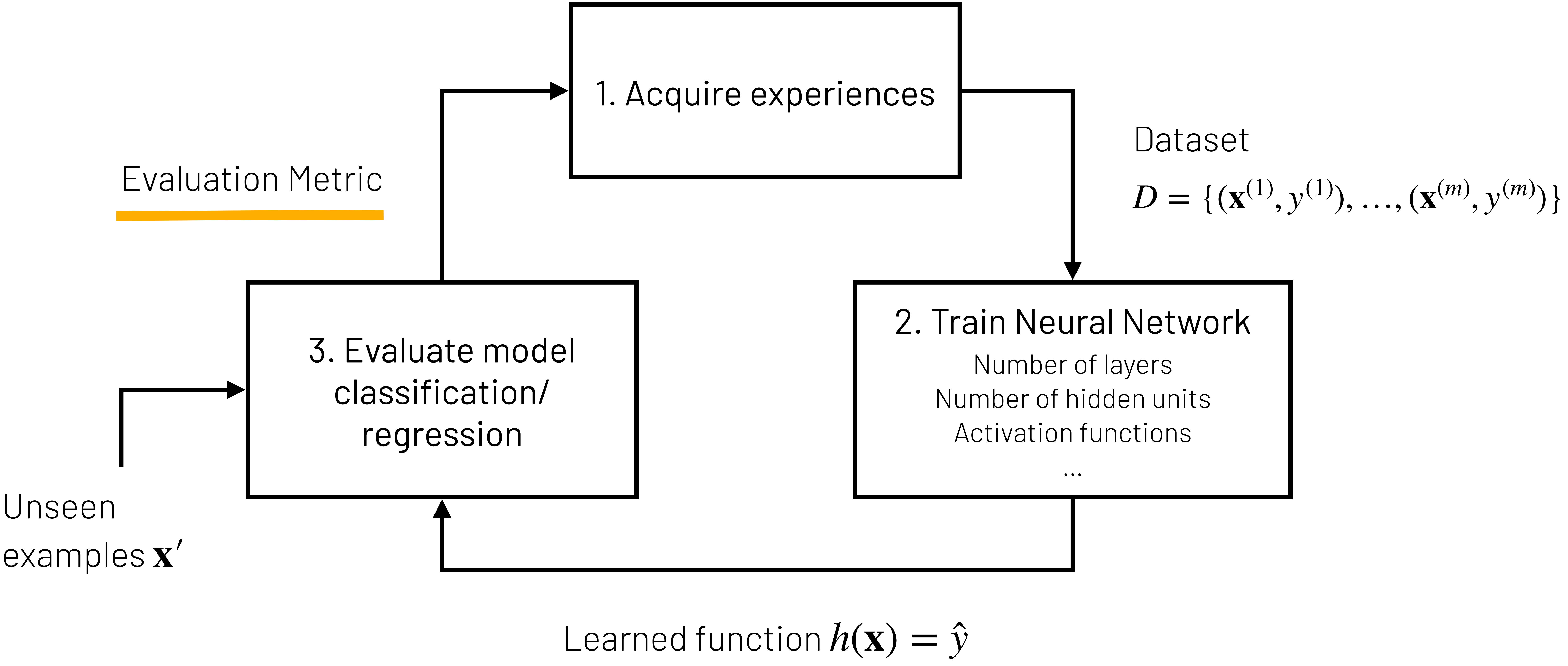
We want $w_0 n_0 = w_1 n_1 = \dfrac{n_0 + n_1}{2}$

- w_1 weight for the positive class $w_1 = \dfrac{n_0 + n_1}{2n_1}$
- w_0 weight for the negative class $w_0 = \dfrac{n_0 + n_1}{2n_0}$

UFV

Supervised Deep Learning

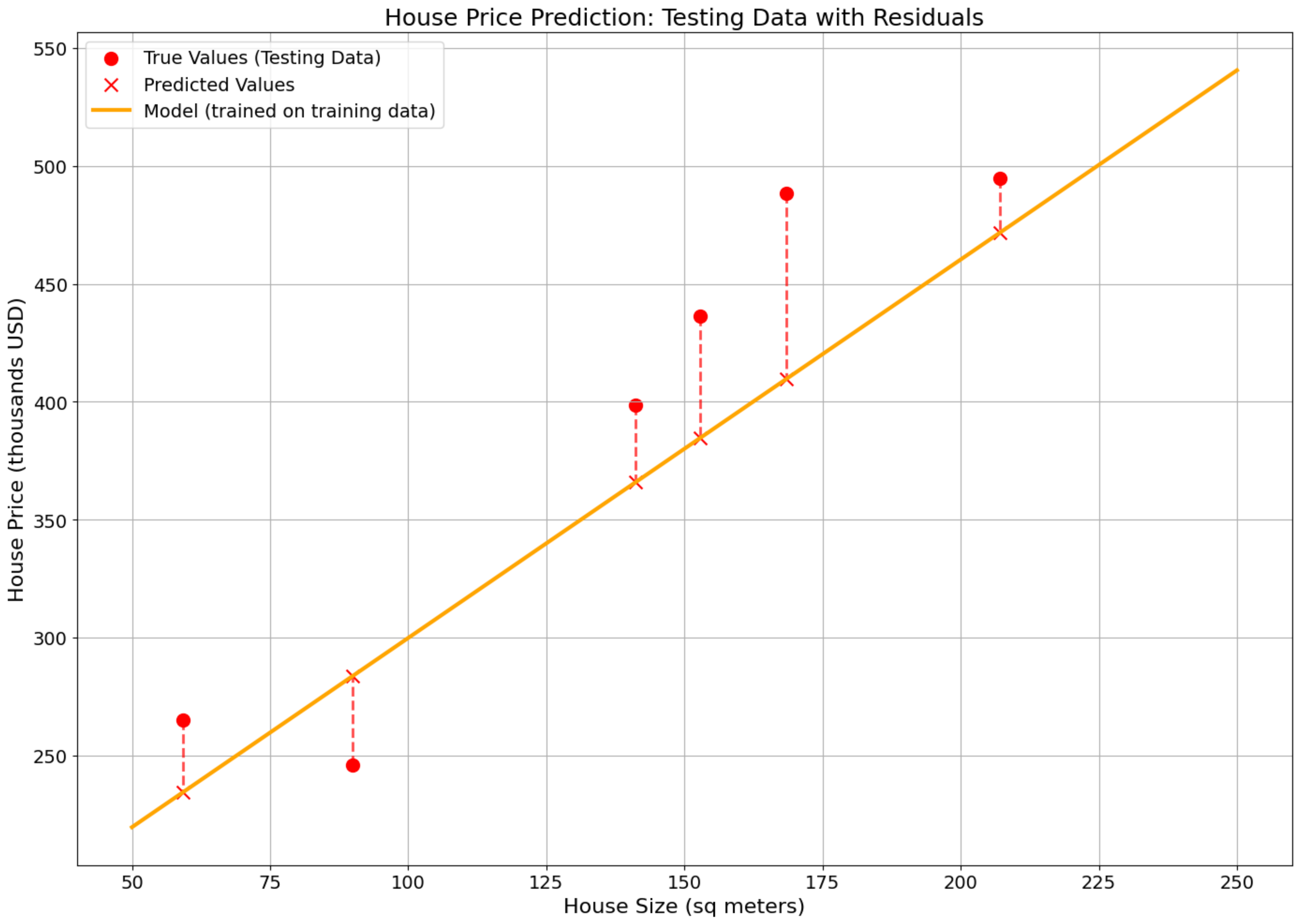
Train a neural network $h(\mathbf{x}) = \hat{y}$ from a dataset $D = \{(\mathbf{x}^{(1)}, y^{(1)}), \ldots, (\mathbf{x}^{(m)}, y^{(m)})\}$ to predict the labels $y^{(i)}$ from the feature vectors $\mathbf{x}^{(i)}$, minimizing prediction error on unseen examples $\mathbf{x}'$



UFV

Regression Evaluation Metrics

Most metrics to evaluate the performance of regression models are based on the residuals $y - \hat{y}$, i.e., a difference between the true value y and the predicted value $\hat{y}$.



- Residual: $y - \hat{y}$
- Popular evaluation metrics for regression models:

Mean Squared Error: $MSE = \frac{1}{m} \sum_{i=1}^{n} (y^{(i)} - \hat{y}^{(i)})^2$

Mean Absolute Error: $MAE = \frac{1}{m} \sum_{i=1}^{n} | y^{(i)} - \hat{y}^{(i)} |$

Root Mean Squared Error: $RMSE = \sqrt{\frac{1}{m} \sum_{i=1}^{n} (y^{(i)} - \hat{y}^{(i)})^2}$

R-squared: $R^2 = 1 - \frac{\sum_{i=1}^{m} (y^{(i)} - \hat{y}^{(i)})^2}{\sum_{i=1}^{m} (y^{(i)} - \bar{y}^{(i)})^2}$

UFV

Mean Squared and Absolute Errors

Mean Squared Error: $MSE(h) = \frac{1}{m}\sum_{i=1}^{n}(y^{(i)} - \hat{y}^{(i)})^2$ – Average of squared differences between predicted and actual values

- Sensitive to outliers due to squaring
- Units: Squared units of the target variable
- Use when: Large errors are particularly undesirable (e.g., predicting stock prices)

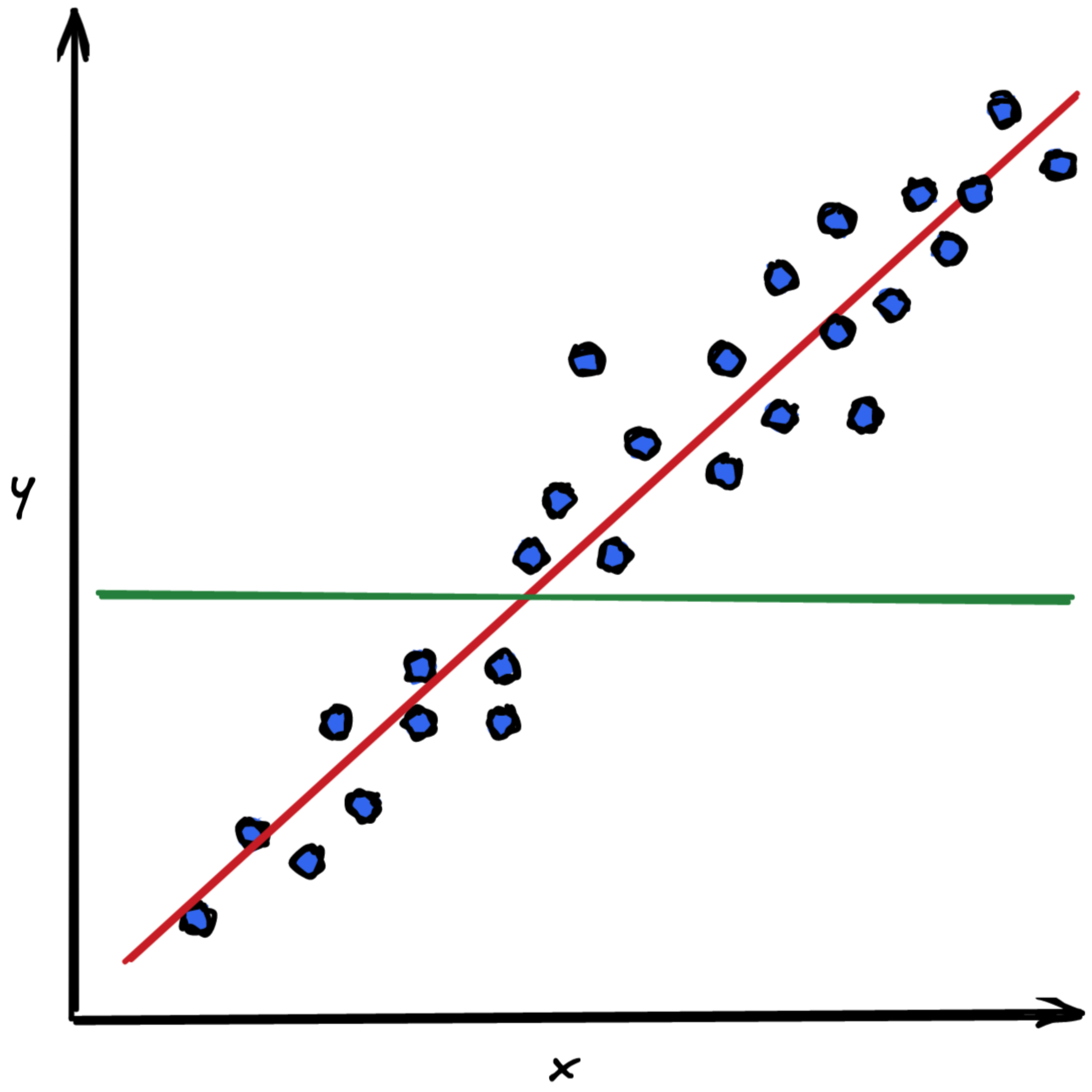
Mean Absolute Error: $MAE(h) = \frac{1}{m}\sum_{i=1}^{n}|y^{(i)} - \hat{y}^{(i)}|$ – Average of absolute differences between predicted and actual values

- Less sensitive to outliers than MSE
- Units: Same as the target variable (Easier to interpret than MSE)
- Use when: You want to treat all errors equally (e.g., forecasting daily temperature)

Root Mean Squared Error: $RMSE(h) = \sqrt{\frac{1}{m}\sum_{i=1}^{n}(y^{(i)} - \hat{y}^{(i)})^2}$ – Square root of MSE

- Sensitive to outliers
- Units: Same as the target variable (Easier to interpret than MSE)
- Use when: You want a balance between MSE and MAE properties (e.g., estimating house prices)

Coefficient of determination (R2)



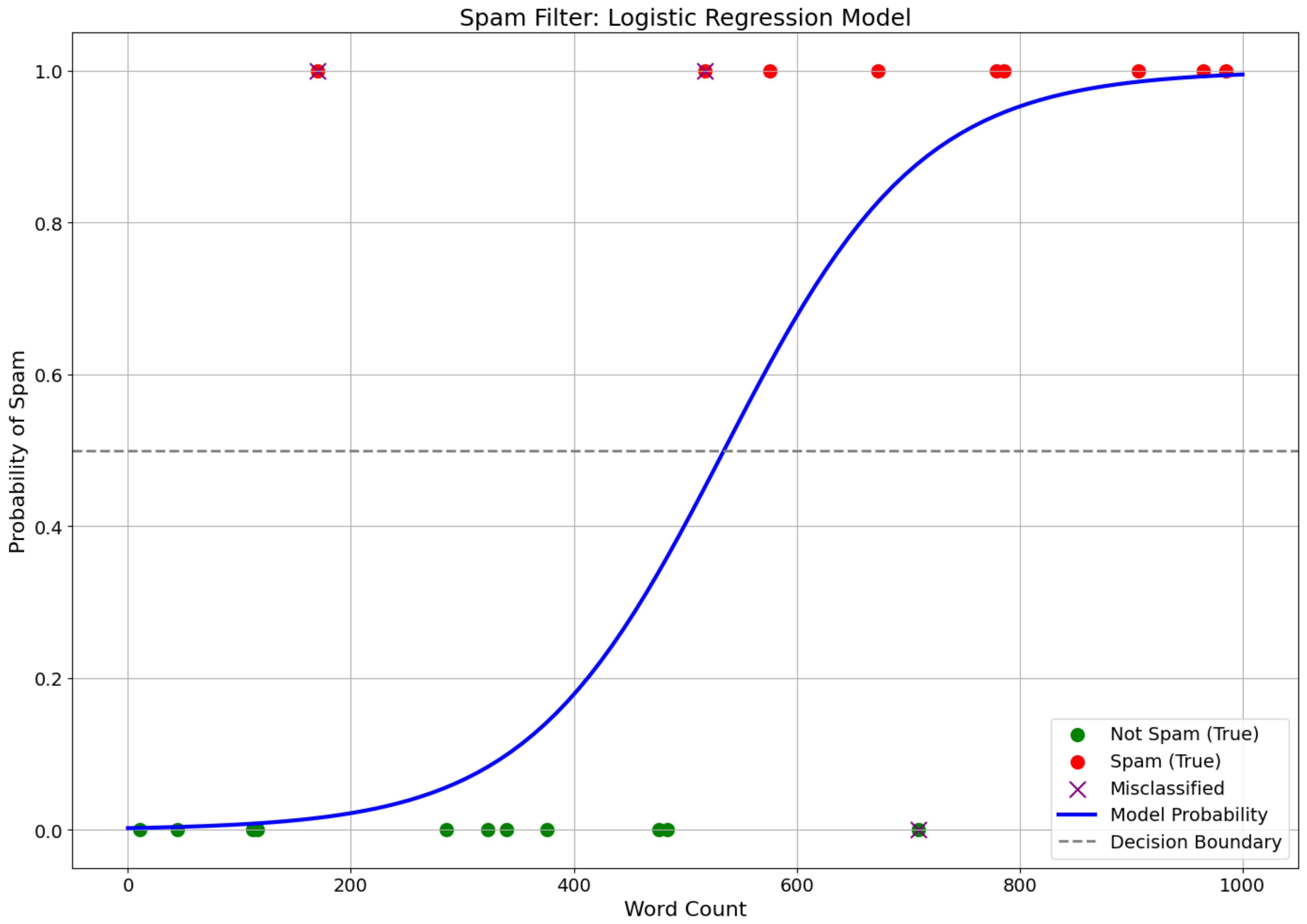
$$R^2 = 1 - \frac{\sum_{i=1}^{m} (y^{(i)} - \hat{y}^{(i)})^2}{\sum_{i=1}^{m} (y^{(i)} - \bar{y}^{(i)})^2}$$

Measures the proportion of variance that is explained by the model. In other words, it compares the fit of a model (red line) to that of a simple mean model (green line).

- Values range from 0 to 1
- The higher the R^2, the better the model
- Scale-independent, allowing comparisons across different datasets

Classification Evaluation Metrics

Most metrics to evaluate the performance of classification models are based on the **confusion matrix**, which shows the number of true and false negatives and positives:



Predicted

Ground Truth	**Spam** (Positive)	**!Spam** (Negative)
Spam (Positive)	7 **True Positive** Spam marked as spam	2 **False Nevative** Spam marked as !Spam
!Spam (Negative)	1 **False Positive** !Spam marked as Spam	10 **True Negative** !Spam marked as !Spam

Confusion Matrix

Classification Evaluation Metrics

Based on the confusion matrix, we can compute the following performance metrics:

Ground Truth \ Predicted	Spam	!Spam
Spam	7 **TP**	2 **FN**
!Spam	1 **FP**	10 **TN**

Metric	Formula	Computation	Result	Description
Accuracy	(TP + TN)/Total	(7 + 10) / 20	0.85 (85%)	Proportion of all emails correctly classified (both spam and non-spam)
Precision	TP/(TP + FP)	7 / (7 + 1)	0.875 (87.5%)	When the filter marks an email as spam, how often it is correct. **Use when FP is high cost**
Recall	TP/(TP + FN)	7 / (7 + 2)	0.778 (77.8%)	Proportion of actual spam emails that were correctly identified. **Use when FN is high cost**
F1 Score	2 * (Precision * Recall) / (Precision + Recall)	2 * (0.875 * 0.778) / (0.875 + 0.778)	0.824 (82.4%)	Harmonic mean of precision and recall, providing a balanced measure

Multiclass Classification Evaluation Metrics

Accuracy, Precision, Recall and F1-scores can also be used in multiclass problems:

Predicted

Ground Truth	Class 1	Class 2	Class 3
Class 1	50	10	5
Class 2	6	80	4
Class 3	4	6	35

- **Accuracy**: (TP1 + TP2 + TP3) / Total = (50 + 80 + 35) / 200 = 0.825 (82.5%)
- **Precision**: (P1 + P2 + P3) /3 = (50/60 + 80/96 + 35/44) / 3 = 0.845 (84.5%)
- **Recall**: (R1 + R2 + R3) / 3 = (50 + 80 + 35) / 200 = 0.822 (82.2%)
- **F1-scores**: 2 * (Macro-Precision * Macro-Recall) / (Macro-Precision + Macro-Recall)

Next Lecture

L8: Regularization & Normalization

Techniques to reduce overfitting and improve model's performance