Systematic Trading Strategies with Machine Learning Algorithms

Supervised Learning Algorithms

May 15, 2025

Outline

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Outline

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Decision Tree Algorithm for Classification

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Algorithm Decision Tree Learning Algorithm

Require: Training data $\{(F_i, y_i)\}_{i=1}^{n}$, stopping criteria

Ensure: Decision tree T

Initialize tree with single root node containing all data
while nodes can be split and stopping criteria not met **do**
    for each leaf node with region $\mathcal{R}$ **do**
        Find (j^*, τ^*) that maximizes:
        $IG(j, \tau) = I(\mathcal{R}) - \frac{|\mathcal{R}_L|}{|\mathcal{R}|} I(\mathcal{R}_L) - \frac{|\mathcal{R}_R|}{|\mathcal{R}|} I(\mathcal{R}_R)$
        Where $\mathcal{R}_L = \{F \in \mathcal{R} : F_j \leq \tau\}$ and $\mathcal{R}_R = \{F \in \mathcal{R} : F_j > \tau\}$
        Split node using rule $F_{j^*} > \tau^*$
    end for
end while
Assign prediction to each leaf node (majority class)
return T

Information Gain for Classification

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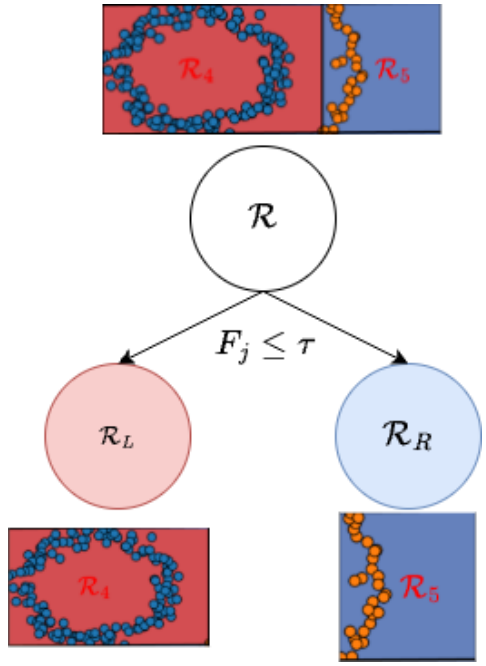
- **Information Gain** for feature j and threshold τ:

$$IG(j,\tau) = I(\mathcal{R}) - \frac{|\mathcal{R}_L|}{|\mathcal{R}|} I(\mathcal{R}_L) - \frac{|\mathcal{R}_R|}{|\mathcal{R}|} I(\mathcal{R}_R)$$

Where:

  - $\mathcal{R}_L = \{F \in \mathcal{R} : F_j \leq \tau\}$
  - $\mathcal{R}_R = \{F \in \mathcal{R} : F_j > \tau\}$



- The DT algorithm:
  1. For each feature j and possible threshold τ, compute $IG(j,\tau)$
  2. Select feature j^* and threshold τ^* that maximize IG
  3. Split node and create child regions $\mathcal{R}_L$ and $\mathcal{R}_R$
  4. Recursively apply to each child node until stopping criteria met

Finding the Optimal Split in Regression Trees

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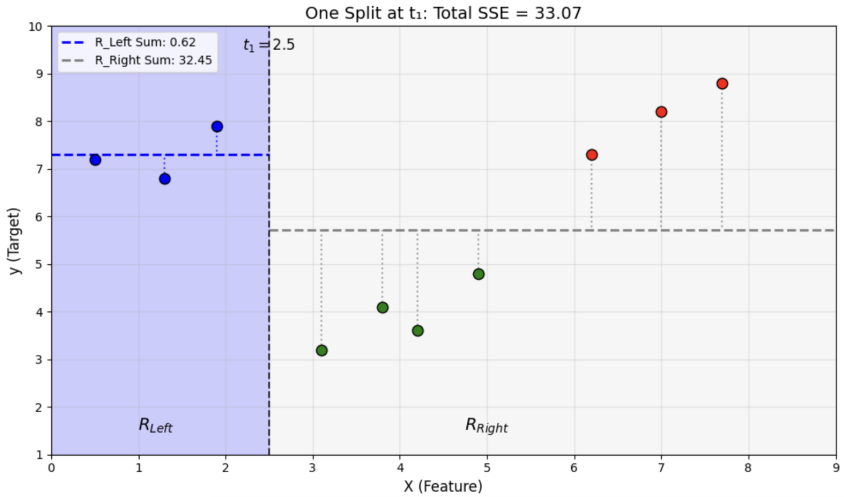
- For a split at value t_1 on feature X:
  - Left region: $R_{Left} = \{x_i | x_i \leq t_1\}$
  - Right region: $R_{Right} = \{x_i | x_i > t_1\}$



- For each region, we compute:
  - Prediction value: average of y_i in the region
  - SSE: sum of squared errors in the region

- **Optimization objective**: Choose feature j and threshold t that minimizes:

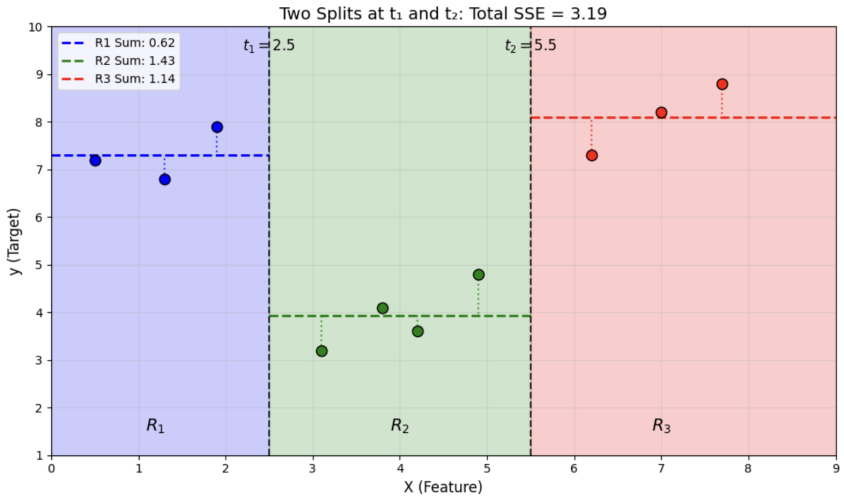
$$SSE_{total} = SSE_{Left} + SSE_{Right}$$

Growing a Regression Tree

- The prediction function for M regions $(R_m)_{1 \leq m \leq M}$ is:

$$f(x) = \sum_{m=1}^{M} c_m \mathbb{1}\{x \in R_m\}$$

- Where c_m is the average of all y_i for which $x_i \in R_m$



- After recursive splitting, we end up with multiple regions (leaves).
- Increasing the number of regions leads to lower training error
- To avoid overfitting, we need **stopping criteria**: Maximum depth, minimum samples per leaf, minimum error improvement.

Algorithm Regression Tree Learning Algorithm

Require: Training data $\{(F_i, y_i)\}_{i=1}^{n}$, stopping criteria

Ensure: Regression tree T

Initialize tree with single root node containing all data
while nodes can be split and stopping criteria not met **do**
    for each leaf node with region $\mathcal{R}$ **do**
        Find (j^*, τ^*) that minimizes:
        $SSE(j, \tau) = \sum_{i:F_i \in \mathcal{R}_L} (y_i - \bar{y}_{\mathcal{R}_L})^2 + \sum_{i:F_i \in \mathcal{R}_R} (y_i - \bar{y}_{\mathcal{R}_R})^2$
        Where $\mathcal{R}_L = \{F \in \mathcal{R} : F_j \leq \tau\}$ and $\mathcal{R}_R = \{F \in \mathcal{R} : F_j > \tau\}$
        Split node using rule $F_{j^*} > \tau^*$
    end for
end while
Assign prediction $\bar{y}_{\mathcal{R}_m}$ to each leaf node (average of y_i in the region)
return T

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Ensemble Learning: Bagging

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- **Motivation of Ensemble Models**: Aggregate weak learners to build a strong learner
- **Bagging Methodology** (Bagging: Bootstrap Aggregation):
  1. **Generate bootstrap samples** $\mathcal{B}_1, \ldots, \mathcal{B}_B$:
     - Create $\mathcal{B}_b$ by picking points from $\{x_1, \ldots, x_n\}$ randomly n times
     - A particular x_i can appear in $\mathcal{B}_b$ many times.
  2. **Train a model per bootstrap**:
     - Each bootstrap sample trains an independent model
  3. **Aggregate the predictions**:
     - **Classification**: Majority vote across all models
     - **Regression**: Average of individual model predictions

Random Forest: Intuition and Overview

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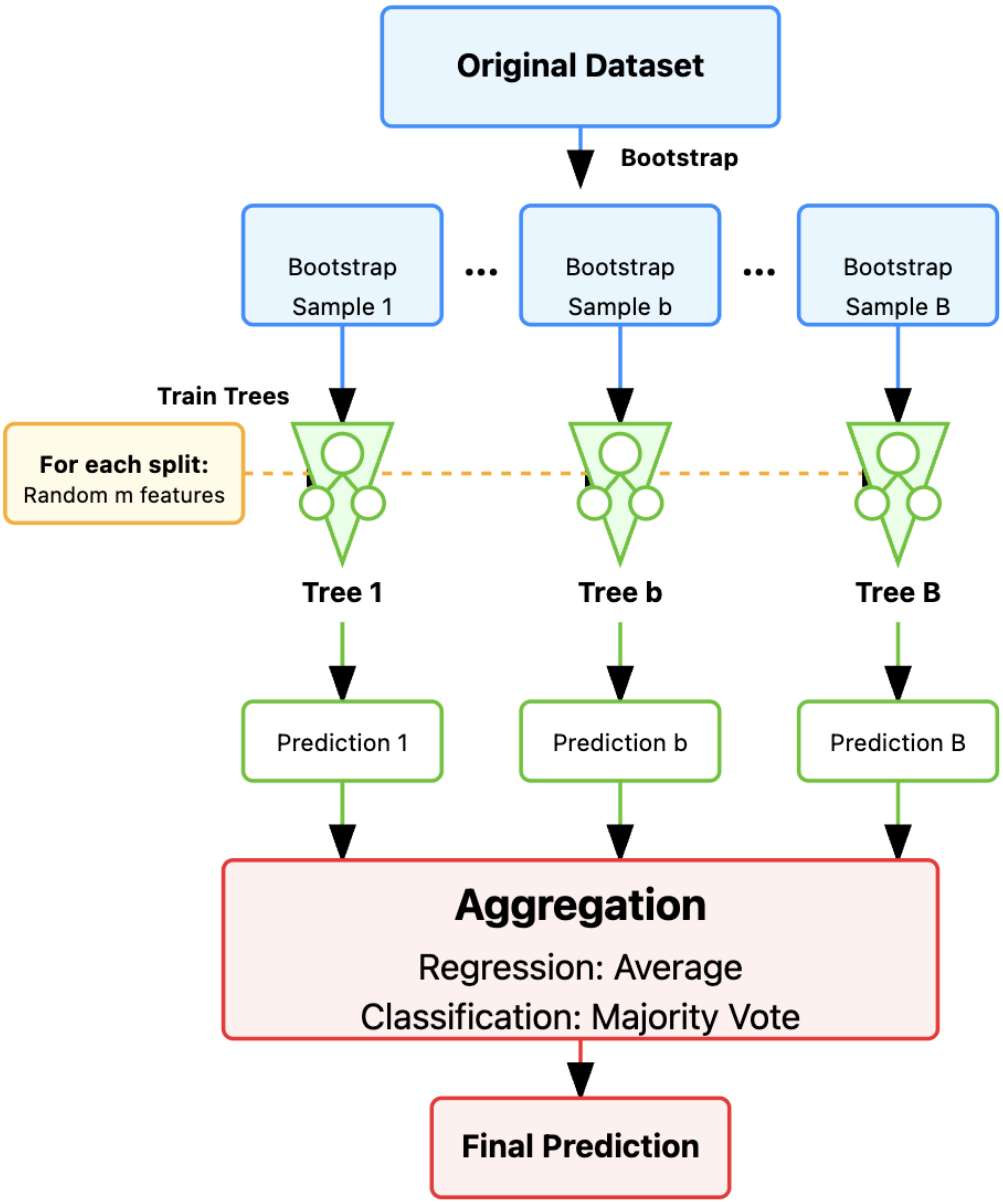
- **Random Forest** is an ensemble method that improves upon bagging decision trees by introducing additional randomness at each split for each decision tree:
  - During training, at each node, only consider a subset of features
  - Result: Less correlated trees



Random Forest Training Algorithm

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Algorithm Random Forest Algorithm

Require: Training data $\{(F_i, y_i)\}_{i=1}^{n}$, number of trees B, features per split $m < p$

Ensure: Random Forest model RF

for $b = 1$ to B **do**
  Draw a bootstrap sample $\mathcal{B}_b$ of size n from the training data
  Initialize tree T_b with root node containing data from $\mathcal{B}_b$
  while nodes in T_b can be split **do**
    for each leaf node with region $\mathcal{R}$ **do**
      Randomly select m features from the available p
      Find best split (j^*, τ^*) among these m features
      Split node using rule $F_{j^*} > \tau^*$
    end for
  end while
end for
return $RF = \{T_1, T_2, \ldots, T_B\}$

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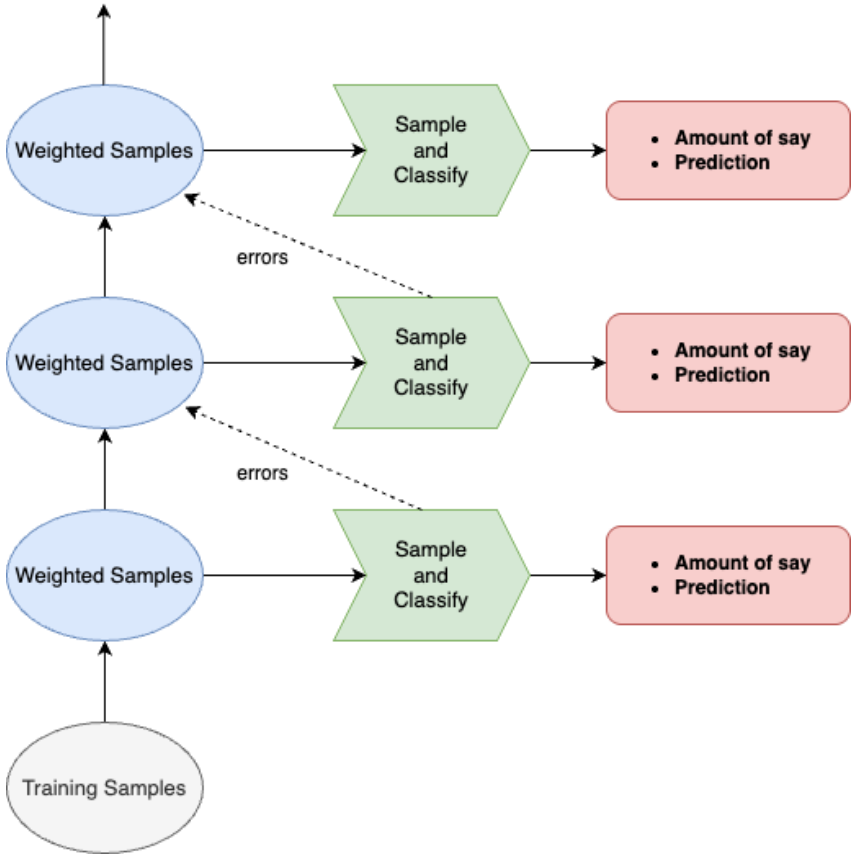
Adaptive Sample Weighting

- Unlike bagging, AdaBoost [2] does not use uniform sampling
- Samples are weighted based on classification difficulty
- Misclassified examples receive higher weights in subsequent iterations
- The algorithm creates models sequentially, each one focusing on correcting previous errors
- This adaptive weighting is the core mechanism behind boosting's effectiveness



AdaBoost: Key Idea 2

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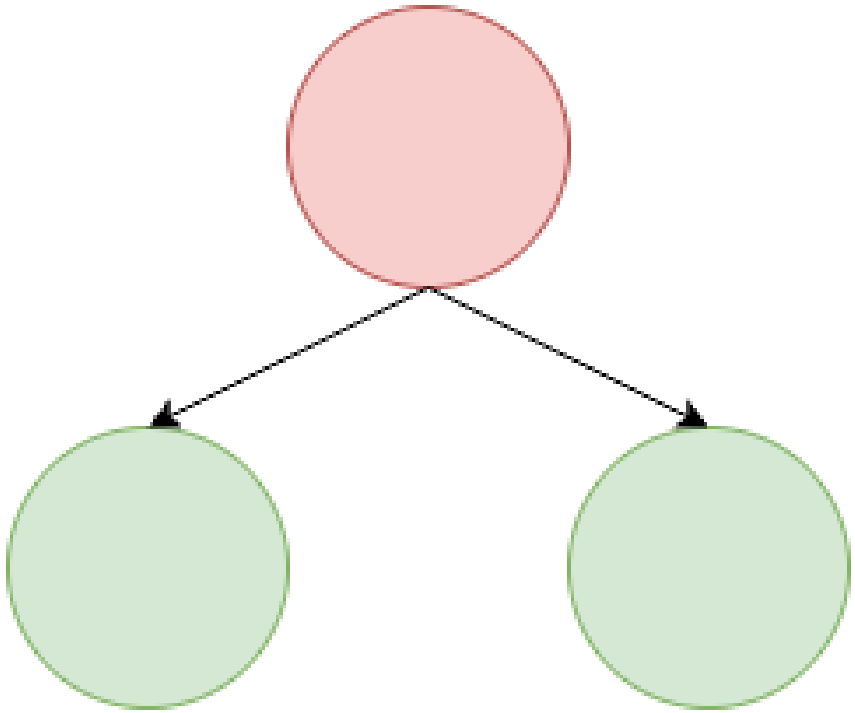
Leveraging Weak Learners (Decision Stumps)

- AdaBoost builds its power from simple decision trees (typically depth=1) called **stumps**
- Individually, each model performs only slightly better than random guessing
- However, they are computationally efficient and resistant to overfitting
- The algorithm's strength comes from combining many weak models into a strong ensemble



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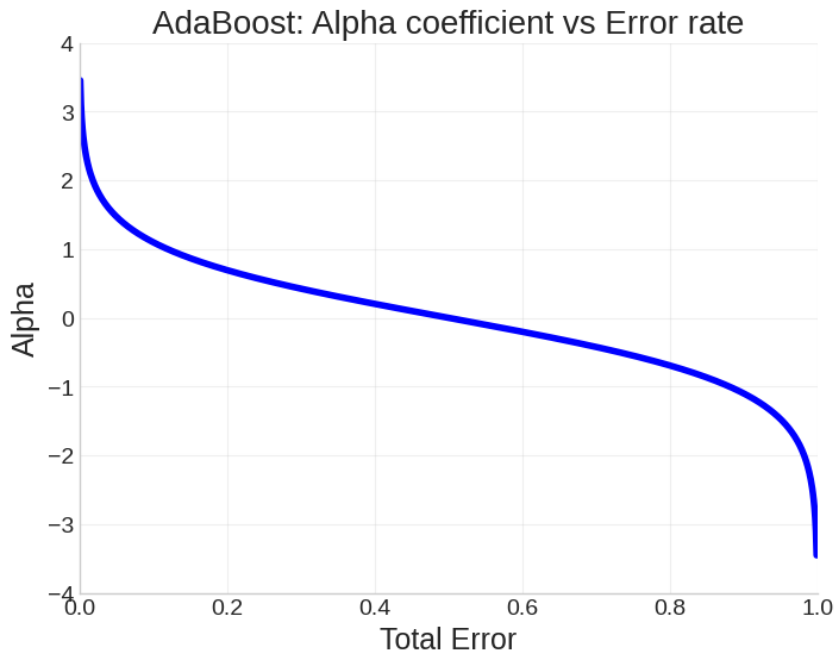
Performance-Based Model Weighting

- Unlike random forests where all trees contribute equally, AdaBoost assigns varying importance to each model
- The algorithm calculates an "amount of say" (α_t) for each classifier based on its accuracy
- Highly accurate classifiers receive strong positive weights
- Random-level performers (error rate $= 0.5$) receive zero weight
- Poor performers can contribute negatively by having their predictions reversed



AdaBoost: Key Algorithm Components

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1. How do we determine each model's contribution?
   - Model influence (α_t) is based on weighted error $\epsilon_t = \sum_{i=1}^{n} w_t(i)\mathbb{1}\{y_i \neq f_t(x_i)\}$
   - $\alpha_t = \frac{1}{2}\ln(\frac{1-\epsilon_t}{\epsilon_t})$ where ϵ_t is the proportion of weighted misclassifications

2. How do we adaptively weight training examples?
   - Weights are updated after each iteration: $w_{t+1}(i) \propto w_t(i) \cdot e^{\alpha_t(1-2\mathbb{1}\{y_i=f_t(x_i)\})}$
   - For binary classification where $y_i \in \{0,1\}$ and $f_t(x_i) \in \{0,1\}$
   - This means weights increase for misclassified examples and decrease for correctly classified ones
   - Weights are normalized to form a probability distribution

AdaBoost: Ensemble Prediction

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How do we make predictions with the ensemble?

- Final prediction uses a weighted majority vote:

$$f_{boost}(x) = \mathbb{1}\left\{\sum_{t=1}^{T} \alpha_t f_t(x) \geq \frac{1}{2}\sum_{t=1}^{T} \alpha_t\right\}$$

- Each weak learner's vote ($f_t(x) \in \{0, 1\}$) is weighted by its performance (α_t)
- Models with lower error rates have larger influence on the final prediction
- The threshold is half the sum of all model weights
- When the weighted sum favors class 1, we predict 1; otherwise, we predict 0

Algorithm AdaBoost Algorithm

Require: Training data $\{(x_i, y_i)\}_{i=1}^n$, $x \in \mathcal{X}$, $y \in \{0, 1\}$, number of iterations T

Ensure: AdaBoost model

1: Initialize weights $w_1(i) = \frac{1}{n}$ for $i = 1 : n$
2: **for** $t = 1$ to T **do**
3: Train classifier f_t on weighted training data with weights w_t
4: Calculate weighted error: $\epsilon_t = \sum_{i=1}^n w_t(i) \mathbb{1}\{y_i \neq f_t(x_i)\}$
5: Calculate model weight: $\alpha_t = \frac{1}{2} \ln \left(\frac{1-\epsilon_t}{\epsilon_t} \right)$
6: Scale weights: $\hat{w}_{t+1}(i) = w_t(i) \cdot e^{\alpha_t (1 - 2\mathbb{1}\{y_i = f_t(x_i)\})}$
7: Normalize: $w_{t+1}(i) = \frac{\hat{w}_{t+1}(i)}{\sum_j \hat{w}_{t+1}(j)}$
8: **end for**
9: **return** Classification rule: $f_{boost}(x_0) = \mathbb{1}\{\sum_{t=1}^T \alpha_t f_t(x_0) \geq \frac{1}{2} \sum_{t=1}^T \alpha_t\}$

AdaBoost Example: First Decision Tree

Key calculations for Tree 1:

- Initial weights:

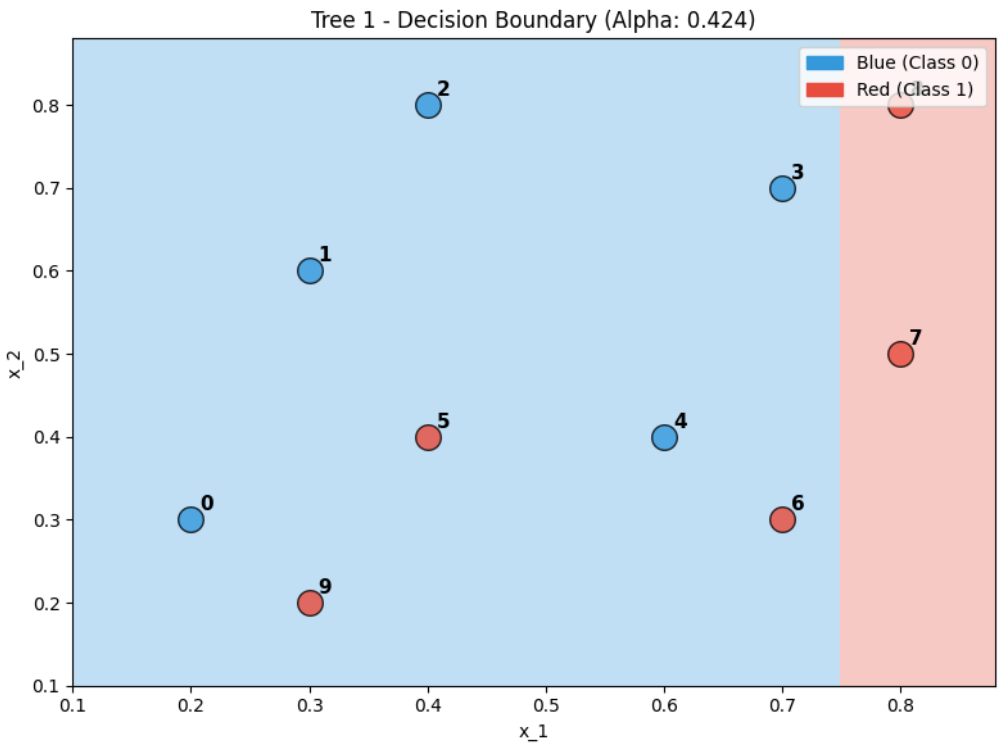
  $w_1(i) = 0.1$ for all samples

- Weighted Error:

$$\epsilon_1 = 0.300$$

- Model Contribution:

$$\begin{aligned}\alpha_1 &= \frac{1}{2}\ln\left(\frac{1-\epsilon_1}{\epsilon_1}\right) \\ &= \frac{1}{2}\ln\left(\frac{0.7}{0.3}\right) \\ &= 0.424\end{aligned}$$



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Weight Update Process:

- For misclassified:

$$w_2(i) \propto w_1(i) \cdot e^{+\alpha_1}$$
$$= 0.1 \cdot e^{0.424}$$

- For correctly classified:

$$w_2(i) \propto w_1(i) \cdot e^{-\alpha_1}$$
$$= 0.1 \cdot e^{-0.424}$$

- Weights are then normalized.

Sample	x_1	x_2	y	w_1	$f_1(x)$	w_2
0	0.2	0.3	0	0.1	0	0.071
1	0.3	0.6	0	0.1	0	0.071
2	0.4	0.8	0	0.1	0	0.071
3	0.7	0.7	0	0.1	0	0.071
4	0.6	0.4	0	0.1	0	0.071
5	**0.4**	**0.4**	**1**	**0.1**	**0**	**0.167**
6	**0.7**	**0.3**	**1**	**0.1**	**0**	**0.167**
7	0.8	0.5	1	0.1	1	0.071
8	0.8	0.8	1	0.1	1	0.071
9	**0.3**	**0.2**	**1**	**0.1**	**0**	**0.167**

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Key calculations for Tree 2:

- Initial weights:

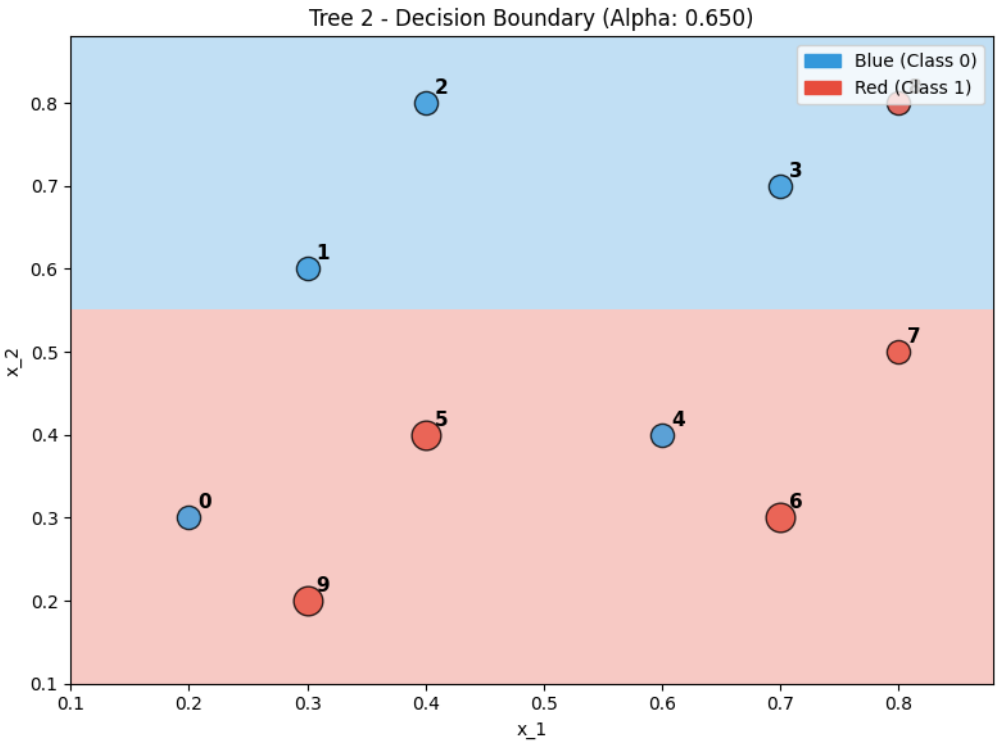
  $w_2(i)$ from previous iteration

- Weighted Error:

$$\epsilon_2 = 0.214$$

- Model Contribution:

$$\begin{aligned}\alpha_2 &= \frac{1}{2}\ln\left(\frac{1-\epsilon_2}{\epsilon_2}\right) \\ &= \frac{1}{2}\ln\left(\frac{0.786}{0.214}\right) \\ &= 0.650\end{aligned}$$



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Weight Update Process:

- For misclassified:

$$w_3(i) \propto w_2(i) \cdot e^{+\alpha_2}$$
$$= w_2(i) \cdot e^{0.650}$$

- For correctly classified:

$$w_3(i) \propto w_2(i) \cdot e^{-\alpha_2}$$
$$= w_2(i) \cdot e^{-0.650}$$

- Weights are then normalized.

Sample	x_1	x_2	y	w_2	$f_2(x)$	w_3
0	**0.2**	**0.3**	**0**	**0.071**	**1**	**0.166**
1	0.3	0.6	0	0.071	0	0.045
2	0.4	0.8	0	0.071	0	0.045
3	0.7	0.7	0	0.071	0	0.045
4	**0.6**	**0.4**	**0**	**0.071**	**1**	**0.166**
5	0.4	0.4	1	0.166	1	0.106
6	0.7	0.3	1	0.166	1	0.106
7	0.8	0.5	1	0.071	1	0.045
8	**0.8**	**0.8**	**1**	**0.071**	**0**	**0.166**
9	0.3	0.2	1	0.166	1	0.106

AdaBoost Example: Third Decision Tree

Key calculations for Tree 3:

- Initial weights:

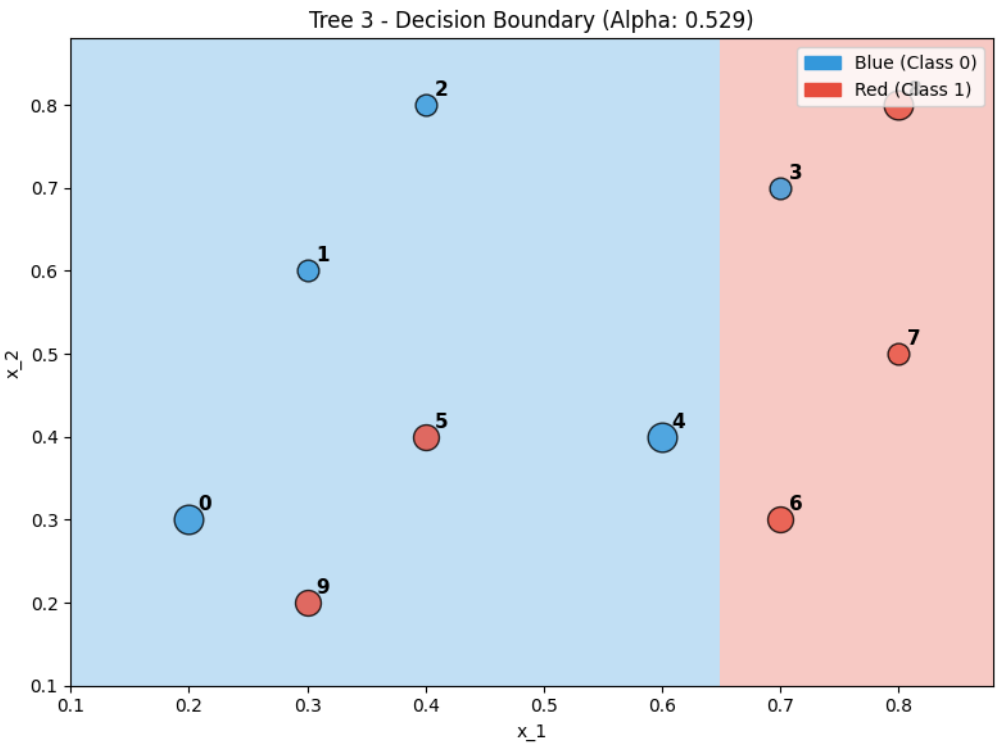
  $w_3(i)$ from previous iteration

- Weighted Error:

$$\epsilon_3 = 0.258$$

- Model Contribution:

$$\begin{aligned}\alpha_3 &= \frac{1}{2}\ln\left(\frac{1-\epsilon_3}{\epsilon_3}\right) \\ &= \frac{1}{2}\ln\left(\frac{0.742}{0.258}\right) \\ &= 0.529\end{aligned}$$



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Weight Update Process:

- For misclassified:

$$w_4(i) \propto w_3(i) \cdot e^{+\alpha_3}$$
$$= w_3(i) \cdot e^{0.529}$$

- For correctly classified:

$$w_4(i) \propto w_3(i) \cdot e^{-\alpha_3}$$
$$= w_3(i) \cdot e^{-0.529}$$

- Weights are then normalized.

Sample	x_1	x_2	y	w_3	$f_3(x)$	w_4
0	0.2	0.3	0	0.166	0	0.112
1	0.3	0.6	0	0.045	0	0.031
2	0.4	0.8	0	0.045	0	0.031
3	**0.7**	**0.7**	**0**	**0.045**	**1**	**0.088**
4	0.6	0.4	0	0.166	0	0.112
5	**0.4**	**0.4**	**1**	**0.106**	**0**	**0.206**
6	0.7	0.3	1	0.106	1	0.071
7	0.8	0.5	1	0.045	1	0.031
8	0.8	0.8	1	0.166	1	0.112
9	**0.3**	**0.2**	**1**	**0.106**	**0**	**0.206**

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Key calculations for Tree 4:

- Initial weights:

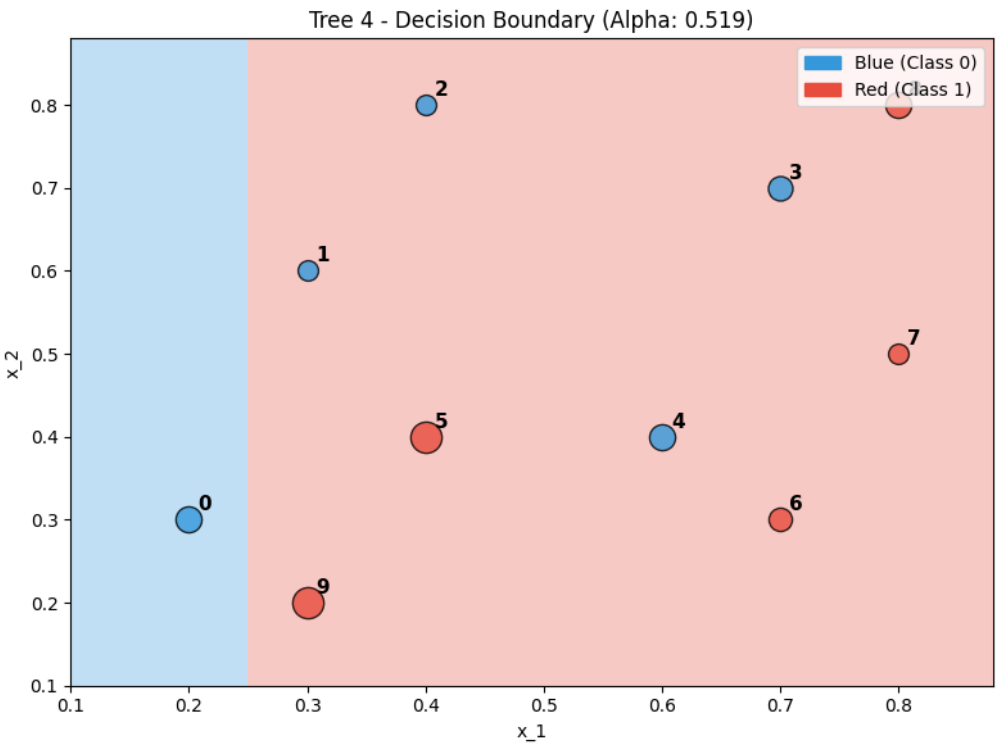
  $w_4(i)$ from previous iteration

- Weighted Error:

$$\epsilon_4 = 0.262$$

- Model Contribution:

$$\begin{aligned}\alpha_4 &= \frac{1}{2}\ln\left(\frac{1-\epsilon_4}{\epsilon_4}\right) \\ &= \frac{1}{2}\ln\left(\frac{0.738}{0.262}\right) \\ &= 0.519\end{aligned}$$



Weight Update Process:

- For misclassified:

$$w_5(i) \propto w_4(i) \cdot e^{+\alpha_4}$$
$$= w_4(i) \cdot e^{0.519}$$

- For correctly classified:

$$w_5(i) \propto w_4(i) \cdot e^{-\alpha_4}$$
$$= w_4(i) \cdot e^{-0.519}$$

- Weights are then normalized.

Sample	x_1	x_2	y	w_4	$f_4(x)$	w_5
0	0.2	0.3	0	0.112	0	0.076
1	**0.3**	**0.6**	**0**	**0.031**	**1**	**0.058**
2	**0.4**	**0.8**	**0**	**0.031**	**1**	**0.058**
3	**0.7**	**0.7**	**0**	**0.088**	**1**	**0.169**
4	**0.6**	**0.4**	**0**	**0.112**	**1**	**0.214**
5	0.4	0.4	1	0.206	1	0.139
6	0.7	0.3	1	0.071	1	0.048
7	0.8	0.5	1	0.031	1	0.021
8	0.8	0.8	1	0.112	1	0.076
9	0.3	0.2	1	0.206	1	0.139

AdaBoost: Final Ensemble Predictions

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Sample	y	f_1	α_1	f_2	α_2	f_3	α_3	f_4	α_4	f_{boost}
0	0	0	0.424	1	0.650	0	0.529	0	0.519	0
1	0	0	0.424	0	0.650	0	0.529	1	0.519	0
2	0	0	0.424	0	0.650	0	0.529	1	0.519	0
3	0	0	0.424	0	0.650	1	0.529	1	0.519	0
4	0	0	0.424	1	0.650	0	0.529	1	0.519	1
5	1	0	0.424	1	0.650	0	0.529	1	0.519	1
6	1	0	0.424	1	0.650	1	0.529	1	0.519	1
7	1	1	0.424	1	0.650	1	0.529	1	0.519	1
8	1	1	0.424	0	0.650	1	0.529	1	0.519	1
9	1	0	0.424	1	0.650	0	0.529	1	0.519	1

AdaBoost: Final Decision Boundary

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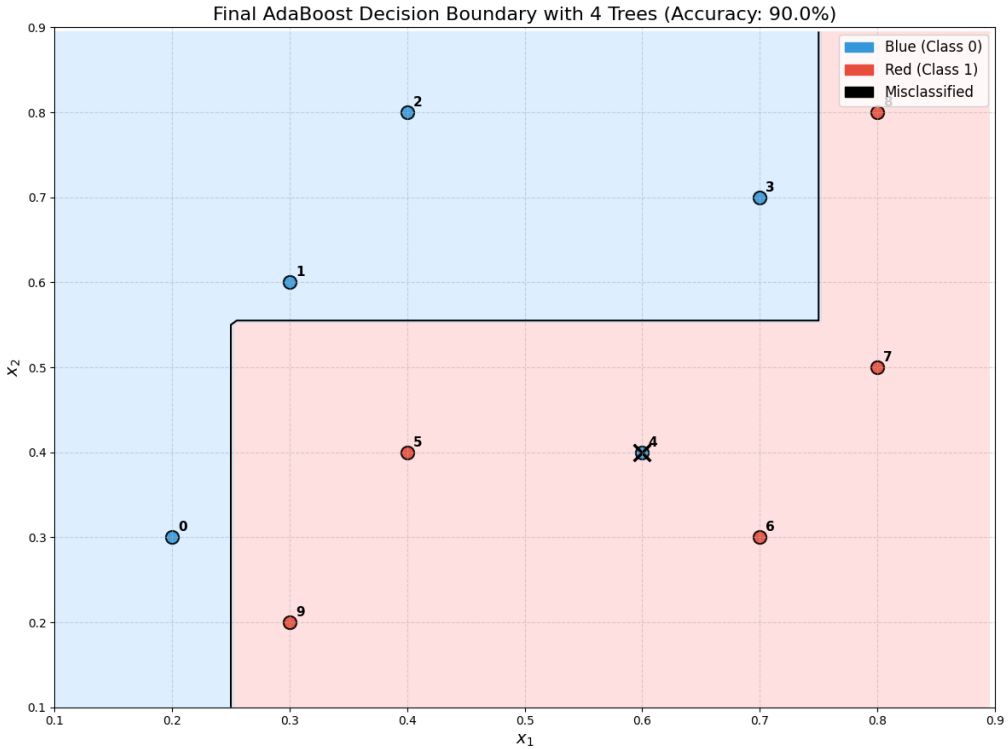
The Power of Ensemble Learning

- The final decision boundary combines all four weak classifiers
- This demonstrates how AdaBoost transforms simple models into sophisticated classifiers
- Accuracy improves from 70% (individual trees) to 90% (ensemble)



Outline

Algorithm Gradient Boosting Algorithm

Require: Training data $\{(x_i, y_i)\}_{i=1}^n$, loss function L, number of trees M, learning rate η

Ensure: Gradient Boosted model

1: Initialize model with a constant: $F_0(x) = \arg\min_{\hat{y}} \sum_{i=1}^n L(y_i, \hat{y})$

2: **for** $m = 1$ to M **do**

3: Compute pseudo-residuals:

$$r_{im} = -\left[\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)}\right]_{F(x)=F_{m-1}(x)} \quad \text{for } i = 1 : n$$

4: Fit a new regression tree to the pseudo-residuals r_{im}

5: Compute optimal value for each leaf region R_{jm}:

$$\gamma_{jm} = \arg\min_{\gamma} \sum_{x_i \in R_{jm}} L(y_i, F_{m-1}(x_i) + \gamma)$$

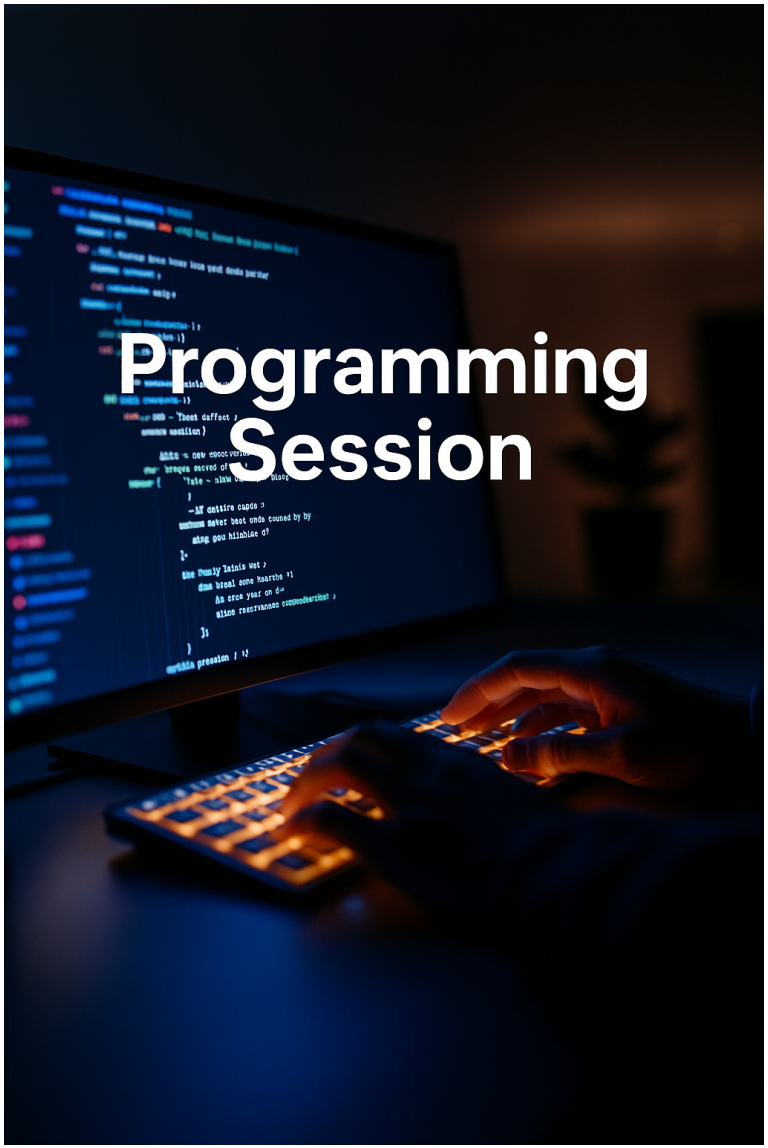
6: Update equation: $F_m(x) = F_{m-1}(x) + \eta \cdot \gamma_m$

7: **end for**

8: **return** Final model $F_M(x)$

Feedback Poll

Click here to participate in the poll



Programming Session 4: Introducing Supervised Learning Algorithms for Time Series Forecasting

- Section 1: Preprocessing the Dataset.
- Section 2: Tree based Models for Time Series Forecasting.
- *Click here to access the programming session*

Solution will be posted tonight on the GitHub page.

- *Click here to access ccess the GitHub Page*

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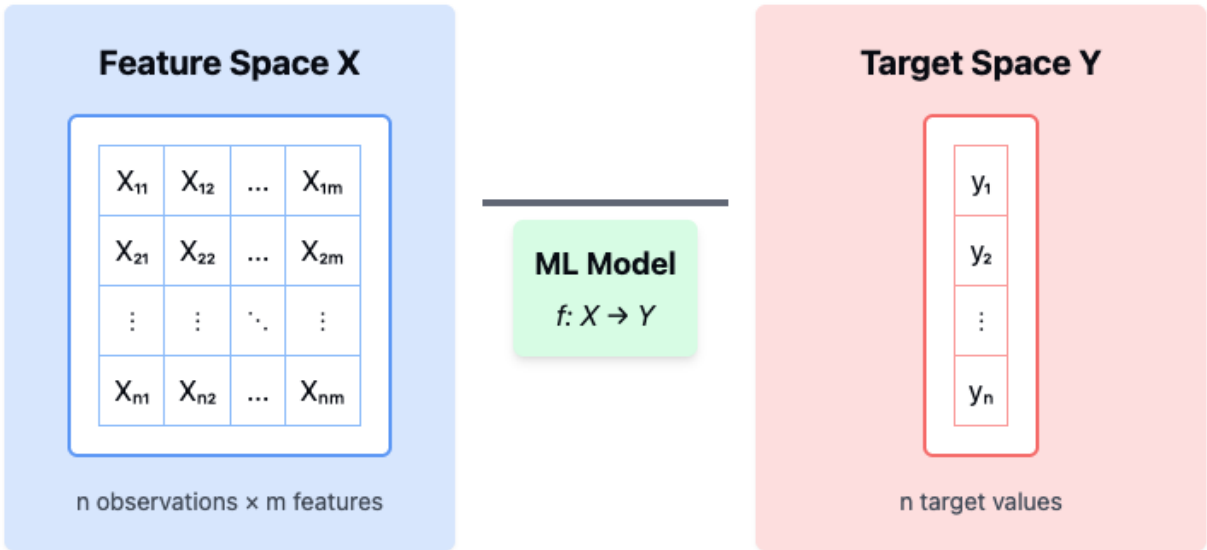
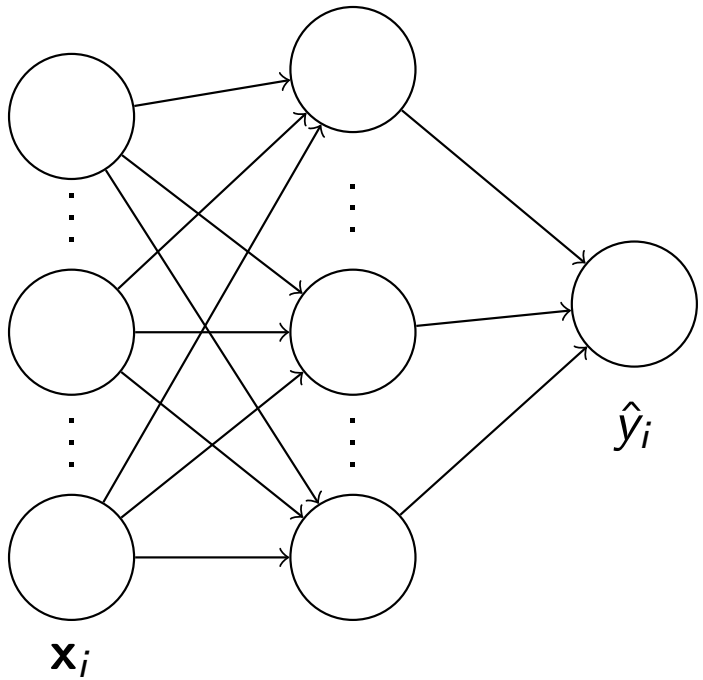
Supervised Learning:

- Learn a function $f : X \to Y$ from labeled data.
- **Feature space** X: matrix of features, n observations $\times$ m features.
- **Target space** Y: vector of n labels (or target values).



Shallow Neural Network

- **Feature vector**:
  $\mathbf{x}_i = (x_{i1}, \ldots, x_{im}) \in \mathbb{R}^m$
- **Parameters**:
  $\theta = \{(\mathbf{W}^{(1)}, \mathbf{b}^{(1)}), (\mathbf{W}^{(2)}, \mathbf{b}^{(2)})\}$
  - $\mathbf{W}^{(1)} \in \mathbb{R}^{m \times L}$: weights connecting input to hidden layer
  - $\mathbf{b}^{(1)} \in \mathbb{R}^{L}$: biases for hidden layer
  - $\mathbf{W}^{(2)} \in \mathbb{R}^{L \times 1}$: weights connecting hidden to output
  - $\mathbf{b}^{(2)} \in \mathbb{R}$: bias for output layer
- **Model**: $f_\theta : \mathbb{R}^m \to \mathbb{R}$ mapping features to predictions
- **Output**: $\hat{y}_i$ (category for classification or continuous value for regression)



Forward Propagation

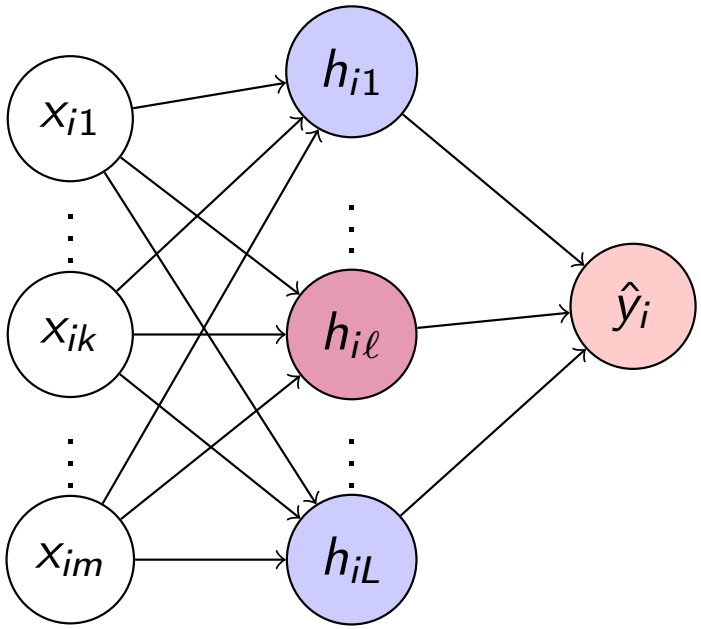
- For all $\ell \in \{1, 2, \ldots, L\}$:

$$h_{i\ell} = \sigma_1 \left(\sum_{k=1}^{m} W_{k\ell}^{(1)} \cdot x_{ik} + b_{\ell}^{(1)} \right)$$

- Then the output:

$$\hat{y}_i = \sigma_2 \left(\sum_{\ell=1}^{L} W_{\ell}^{(2)} \cdot h_{i\ell} + b^{(2)} \right)$$

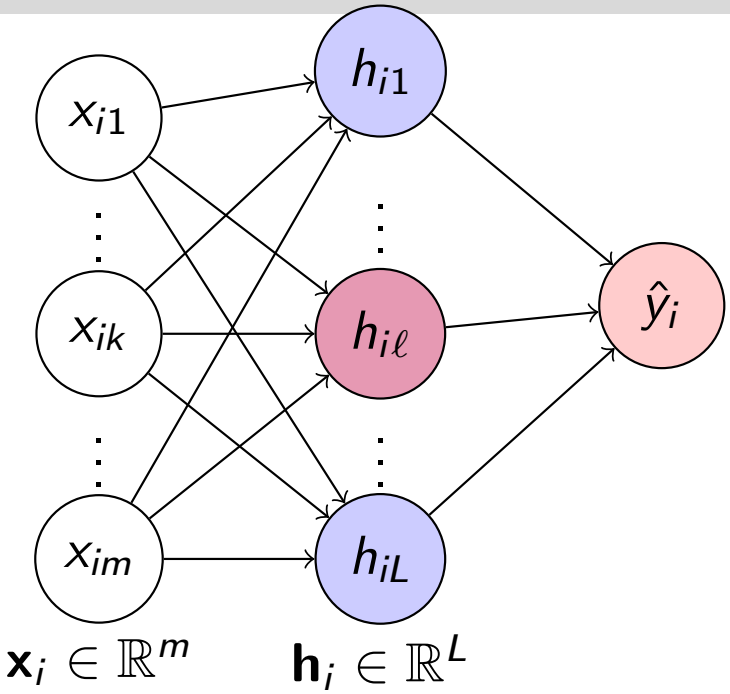
- σ_1, σ_2 are activation functions.
- Parameters:
  $\theta = \{(\mathbf{W}^{(1)}, \mathbf{b}^{(1)}), (\mathbf{W}^{(2)}, \mathbf{b}^{(2)})\}$



Forward Propagation - Matrix Notation

- $\mathbf{x}_i \in \mathbb{R}^m$ is the input feature vector
- $\mathbf{h}_i \in \mathbb{R}^L$ is the hidden layer vector
- The model output $\hat{y}_i \in \mathbb{R}$ is calculated as follows:

$$\mathbf{h}_i = \sigma_1(\mathbf{W}^{(1)T}\mathbf{x}_i + \mathbf{b}^{(1)})$$
$$\hat{y}_i = \sigma_2((\mathbf{W}^{(2)})^T\mathbf{h}_i + b^{(2)})$$



- The final output is:

$$\boxed{\hat{y}_i = f_\theta(x_i) = \sigma_2\left((\mathbf{W}^{(2)})^T\sigma_1\left(\mathbf{W}^{(1)T}\mathbf{x}_i + \mathbf{b}^{(1)}\right) + b^{(2)}\right)}$$

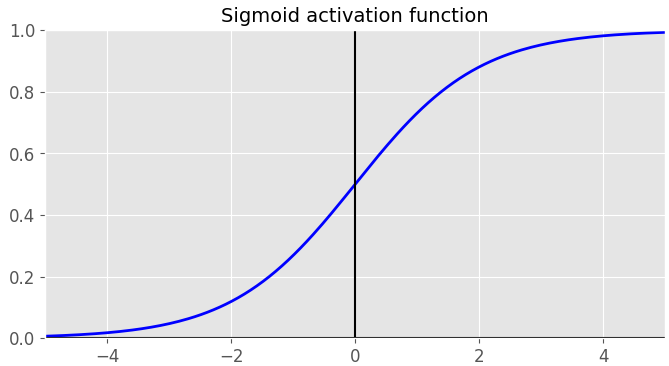
- **Next step:** Learning the parameters $\theta = \{(\mathbf{W}^{(1)}, \mathbf{b}^{(1)}), (\mathbf{W}^{(2)}, \mathbf{b}^{(2)})\}$ from training data using a loss function

Outline

Activation Functions

Sigmoid:

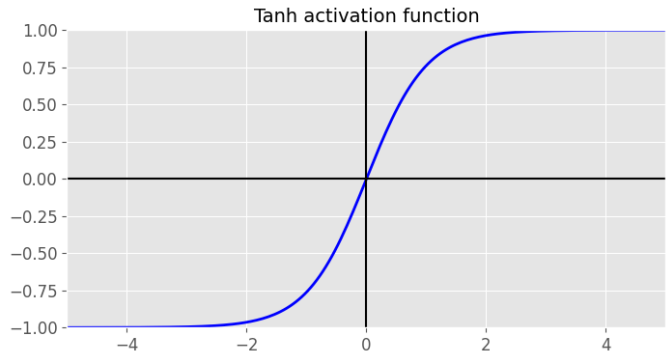
$$\sigma(z) = \frac{1}{1 + e^{-z}} \in [0, 1]$$



- Used as final activation for binary classification
- Output interpreted as probability: $\hat{y}_i = P(Y = 1|\mathbf{x}_i)$

Tanh:

$$\tanh(z) = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}} \in [-1, 1]$$

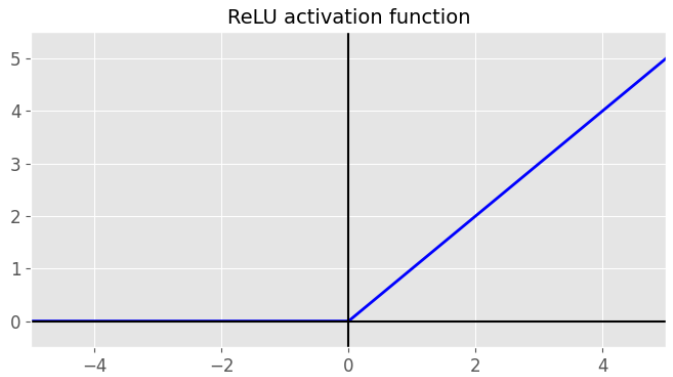


- Zero-centered, helps with convergence
- Often used in hidden layers

ReLU Activation Function

ReLU (Rectified Linear Unit):

$$\text{ReLU}(z) = \max(0, z)$$

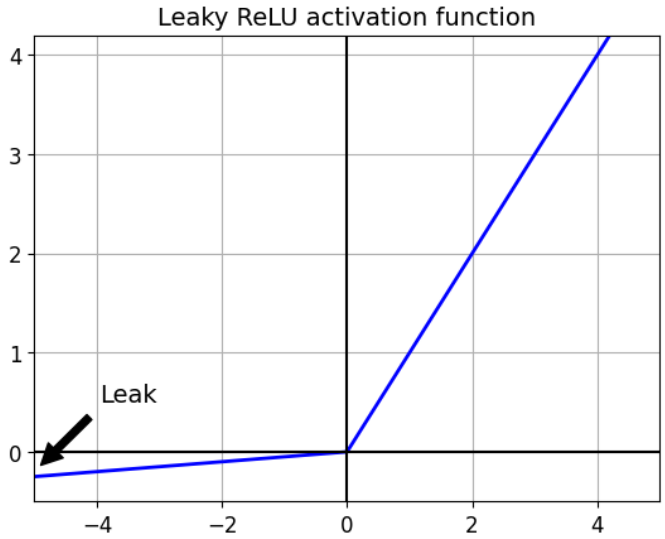


- Faster to compute, computational efficiency
- No saturation for positive values, helps with gradient flow
- Problem: "dying ReLU" (neurons can get stuck at 0)
- Most widely used in hidden layers
- Sparse activation: typically 50% of neurons inactive
- No vanishing gradient for positive inputs

Leaky ReLU Activation Function

Leaky ReLU:

$$\text{LeakyReLU}(z) = \begin{cases} z & \text{if } z > 0 \\ \alpha z & \text{if } z \leq 0 \end{cases}$$

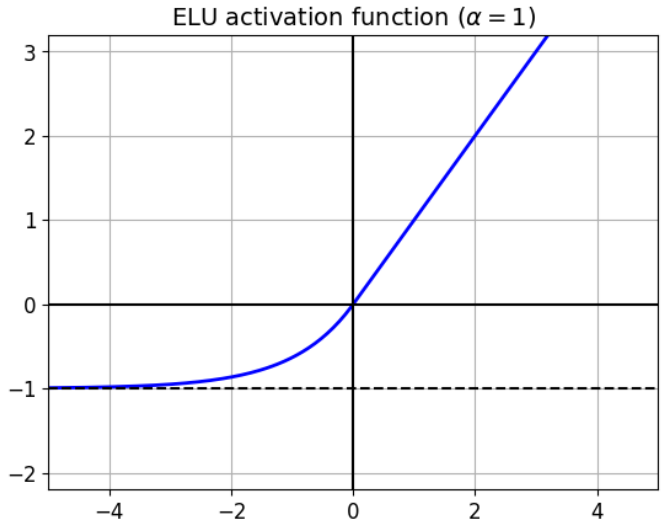


- Introduced in [4].
- Prevents "dying ReLU" problem with small slope α
- Typical values for α range from 0.01 to 0.2
- Allows small gradient flow for negative inputs
- Maintains most of the computational efficiency of ReLU
- Not always superior to ReLU in practice

ELU Activation Function

ELU (Exponential Linear Unit):

$$\text{ELU}(z) = \begin{cases} z & \text{if } z > 0 \\ \alpha(e^z - 1) & \text{if } z \leq 0 \end{cases}$$

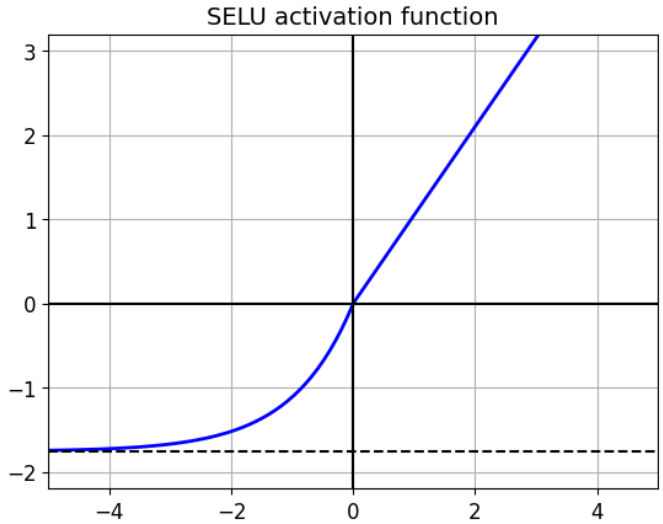


- Introduced in [1].
- Smooth curve for negative values, reducing noise
- Approaches $-\alpha$ as z becomes very negative
- Self-regularizing: can help with internal covariate shift
- More computationally expensive than ReLU
- Often produces faster convergence in training

SELU Activation Function

SELU (Scaled ELU):

$$\text{SELU}(z) = \lambda \begin{cases} z & \text{if } z > 0 \\ \alpha(e^z - 1) & \text{if } z \leq 0 \end{cases}$$



- Introduced in [3].
- Fixed parameters: $\alpha \approx 1.67$ and $\lambda \approx 1.05$
- Scaling factor λ enables self-normalization
- Automatically preserves mean and variance of inputs
- Helps training deep networks without batch normalization
- Requires "SELU initialization" (LeCun Normal)

Outline

- **Why do we need loss functions?**
  - Quantify how well our model f_θ performs on data
  - Provide a differentiable objective to optimize
  - Guide the learning of parameters θ
- **From predictions to learning:**
  - Forward propagation gives us: $\hat{y}_i = f_\theta(\mathbf{x}_i)$
  - Loss function measures: $\mathcal{L}(\hat{y}_i, y_i)$ - the discrepancy between predictions and true values
- **Overall objective:**

$$\min_\theta \frac{1}{n} \sum_{i=1}^{n} \mathcal{L}(f_\theta(\mathbf{x}_i), y_i)$$

Binary Cross Entropy Loss Function - MLE

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- **Dataset**: $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$ where $y_i \in \{0, 1\}$
- **Probabilistic view**: Neural network outputs represent probabilities
- **For binary classification:**
  $\forall i \in \{1, \ldots, n\} \quad \hat{y}_i = f_\theta(\mathbf{x}_i) = p_\theta(Y = 1|\mathbf{x}_i)$
- **Log-likelihood for all data:**

$$\begin{aligned}\log \mathcal{L}(\theta) &= \sum_{i=1}^{n} \log p_\theta(Y = y_i|\mathbf{x}_i) \\ &= \sum_{i=1}^{n} [y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i)]\end{aligned}$$

- **The loss function is the normalized negative Log-Likelihood:**

$$\min_\theta -\frac{1}{n} \log \mathcal{L}(\theta) \iff \min_\theta -\frac{1}{n} \sum_{i=1}^{n} [y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i)]$$

Categorical Cross Entropy Loss Function - MLE

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- **Dataset**: $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$ where $y_i \in \{1, 2, \ldots, K\}$
- **Probabilistic view**: Neural network outputs represent probability distribution over K classes
- **For multi-class classification:**
  $\forall i \in \{1, \ldots, n\} \quad \hat{\mathbf{y}}_i = f_\theta(\mathbf{x}_i) = (p_\theta(Y = 1|\mathbf{x}_i), \ldots, p_\theta(Y = K|\mathbf{x}_i))$
- **One-hot encoding of target:** $\mathbf{y}_i = (y_{i1}, y_{i2}, \ldots, y_{iK})$ where $y_{ik} = \mathbb{1}_{[y_i = k]}$
- **Log-likelihood for all data:**

$$\log \mathcal{L}(\theta) = \sum_{i=1}^{n} \log p_\theta(Y = y_i|\mathbf{x}_i) = \sum_{i=1}^{n} \sum_{k=1}^{K} y_{ik} \log \hat{y}_{ik}$$

- **The loss function is the normalized negative Log-Likelihood:**

$$\min_\theta -\frac{1}{n} \log \mathcal{L}(\theta) \iff \min_\theta -\frac{1}{n} \sum_{i=1}^{n} \sum_{k=1}^{K} y_{ik} \log \hat{y}_{ik}$$

Regression Loss Functions Overview

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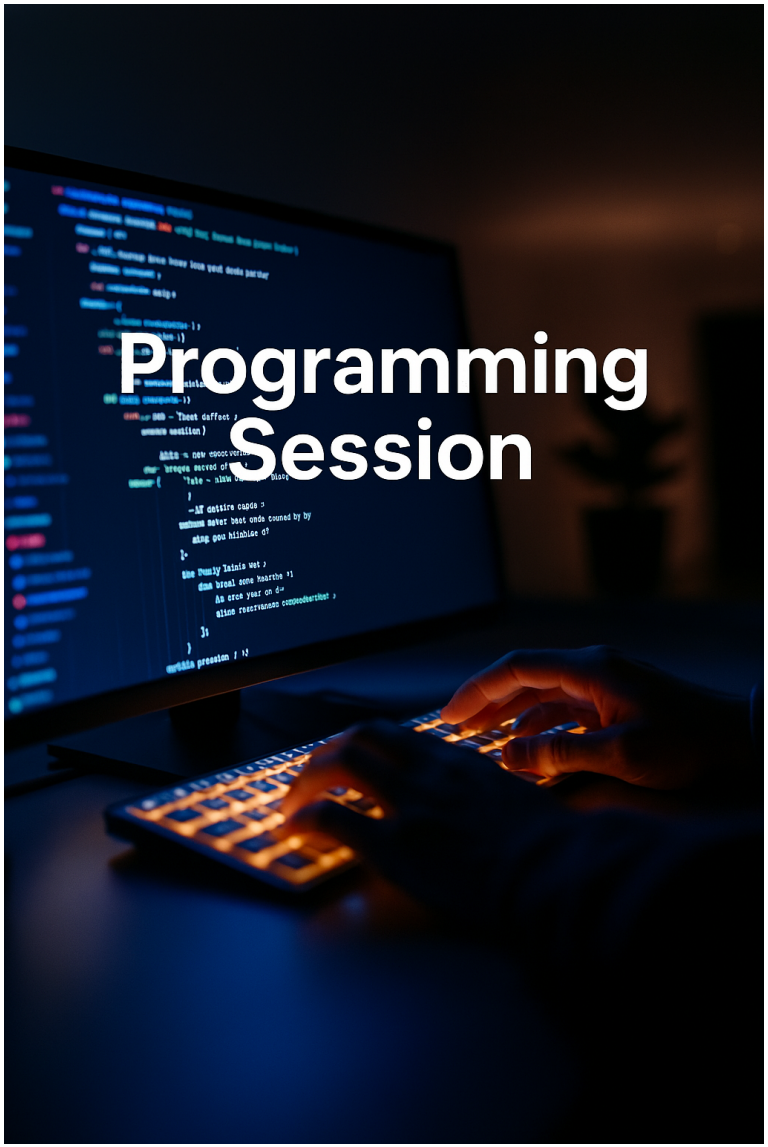
Loss	Formula	Key Properties
MSE	$\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$	▶ Differentiable everywhere ▶ Sensitive to outliers
MAE	$\frac{1}{n}\sum_{i=1}^{n}\lvert y_i - \hat{y}_i\rvert$	▶ Less sensitive to outliers ▶ Non-differentiable at zero
MAPE	$\frac{1}{n}\sum_{i=1}^{n}\frac{\lvert y_i - \hat{y}_i\rvert}{\lvert y_i\rvert}$	▶ Scale-independent



Optional Programming Session: The Custom Huber Loss function

- *Click here to access the programming session*

Content:

- Tensors and operations in TensorFlow.
- Computing Gradients with Autodiff.
- Custom Loss Function: The Huber Loss.

- **For classification:**
  - **Binary classification**: Binary Cross-Entropy with sigmoid

$$\mathcal{L}_{BCE} = -\frac{1}{n}\sum_{i=1}^{n}[y_i \log \hat{y}_i + (1-y_i)\log(1-\hat{y}_i)]$$

  - **Multi-class classification**: Categorical Cross-Entropy with softmax

$$\mathcal{L}_{CCE} = -\frac{1}{n}\sum_{i=1}^{n}\sum_{k=1}^{K} y_{ik} \log \hat{y}_{ik}$$

  - **Multi-label classification**: Binary Cross-Entropy per label

$$\mathcal{L}_{ML} = -\frac{1}{n}\sum_{i=1}^{n}\sum_{k=1}^{K}[y_{ik} \log \hat{y}_{ik} + (1-y_{ik})\log(1-\hat{y}_{ik})]$$

Loss Function Guidelines - Regression

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- **For regression:**
  - **Clean data, normal distribution**: MSE

$$\mathcal{L}_{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

  - **Data with outliers**: MAE

$$\mathcal{L}_{MAE} = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|$$

  - **Data with outliers (alternative)**: Huber Loss

$$\mathcal{L}_{\delta} = \frac{1}{n}\sum_{i=1}^{n}\begin{cases}\frac{1}{2}(y_i - \hat{y}_i)^2 & \text{if } |y_i - \hat{y}_i| \leq \delta \\ \delta|y_i - \hat{y}_i| - \frac{1}{2}\delta^2 & \text{otherwise}\end{cases}$$

  - **Relative error important**: MAPE

$$\mathcal{L}_{MAPE} = \frac{1}{n}\sum_{i=1}^{n}\frac{|y_i - \hat{y}_i|}{|y_i|} \times 100\%$$

Outline

Algorithm Gradient Descent Algorithm

Require: Training data $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$, loss function $\mathcal{L}$, learning rate α, iterations T

Ensure: Optimized parameters θ

1: Initialize parameters $\theta^{(0)}$ randomly
2: **for** $t = 1$ to T **do**
$$\theta^{(t)} = \theta^{(t-1)} - \alpha \cdot \nabla_\theta \mathcal{L}(\theta^{(t-1)})$$
3: **if** Convergence criteria met **then**
4: **break**
5: **end if**
6: **end for**
7: **return** Final parameters $\theta^{(T)}$

Visualizing Gradient Descent

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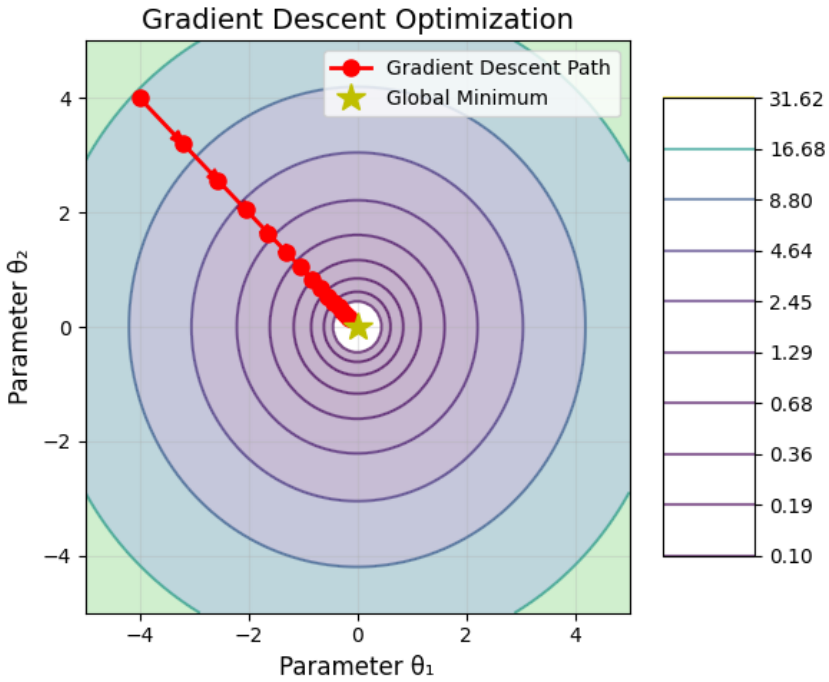
Key aspects of Gradient Descent:

- **Intuition**: Move downhill in the direction of steepest descent
- **Learning rate** α controls step size:
  - Too small: slow convergence
  - Too large: overshooting or divergence
- For neural networks, loss landscapes are typically **non-convex**, so we often converge to a **local minimum**

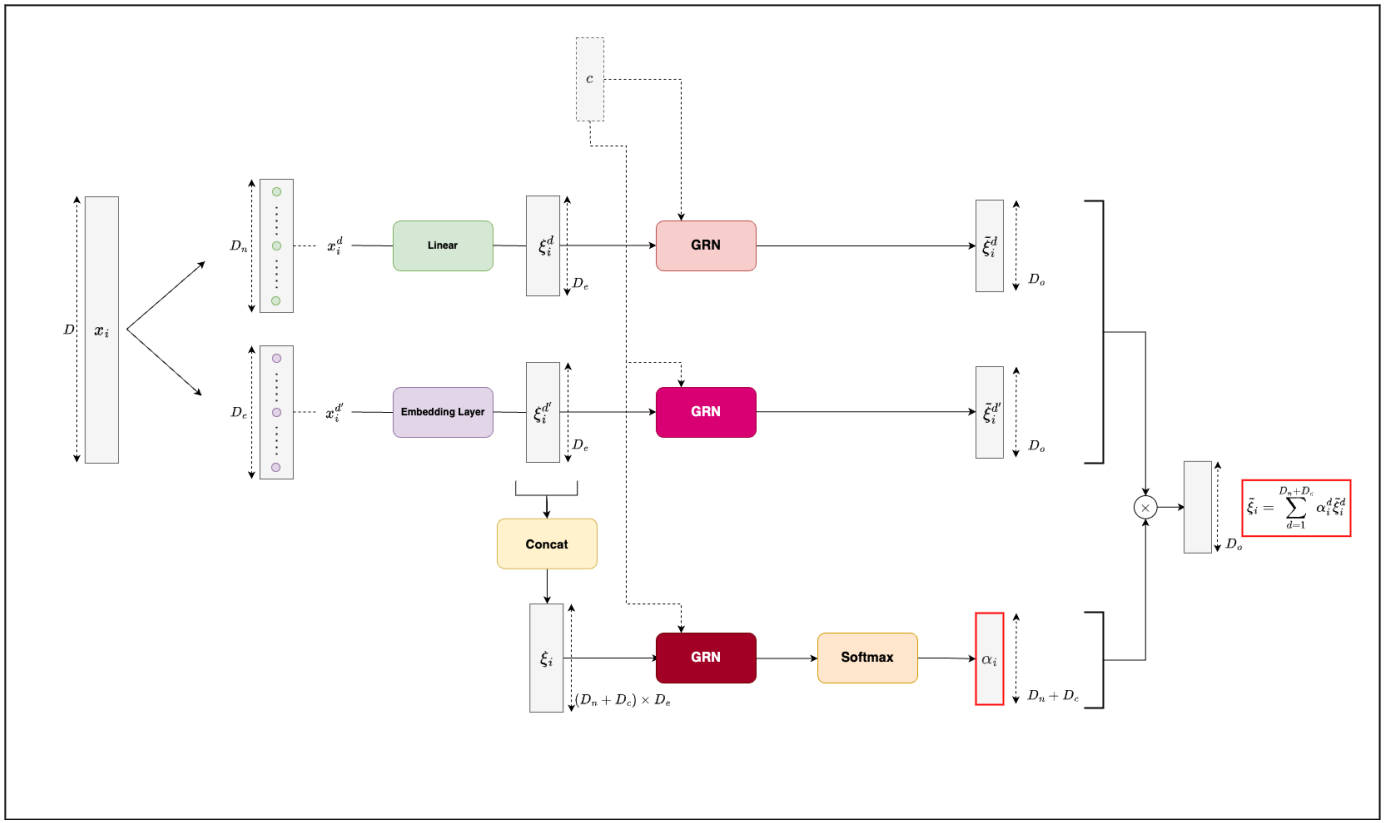


- In this figure, we reach the **global minimum** since the function is **convex**

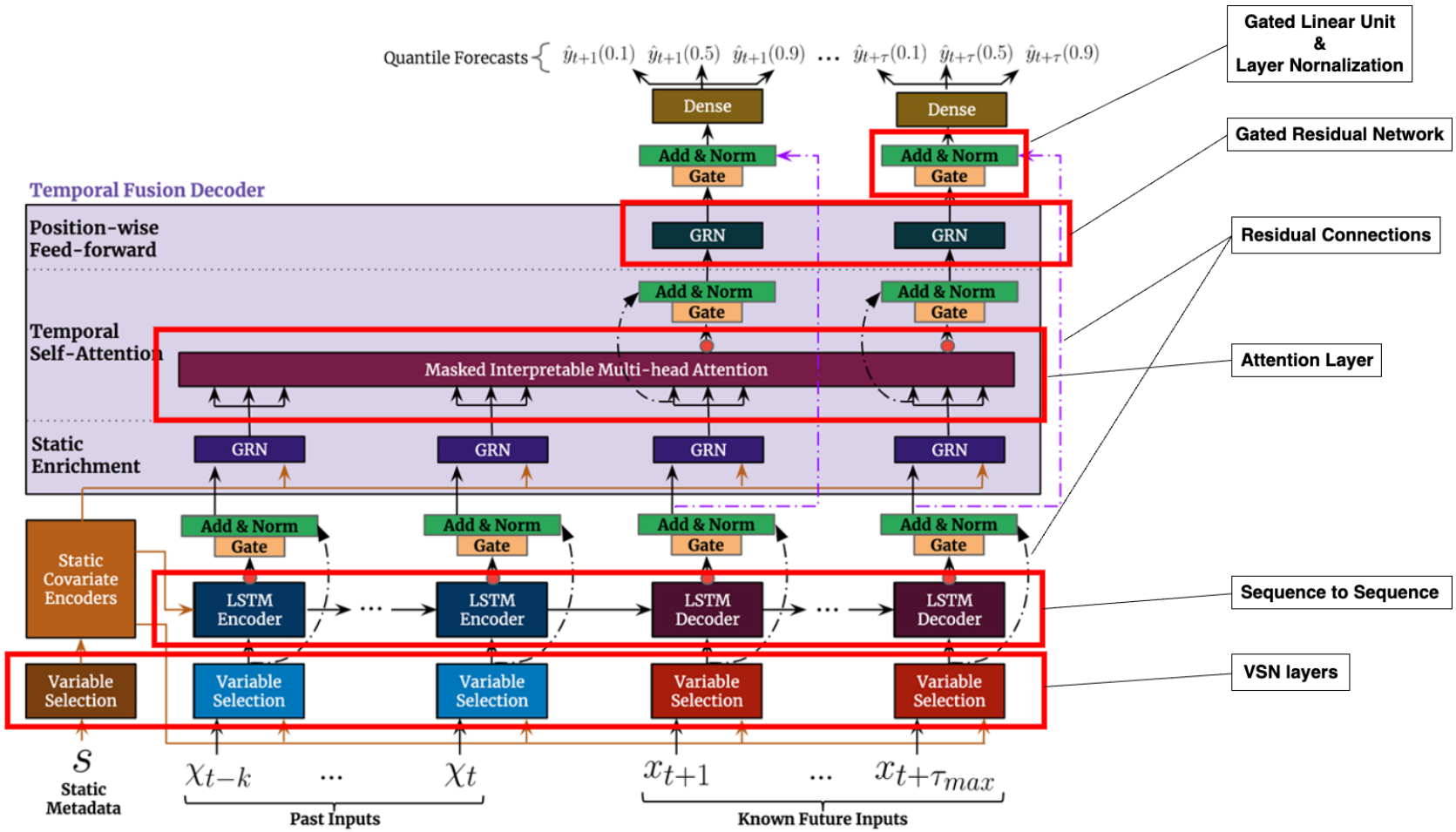
Outline

Variable Selection Network (VSN)

- We will explore the Variable Selection Network (VSN) in Lecture 7 as part of the Temporal Fusion Transformer Architecture.

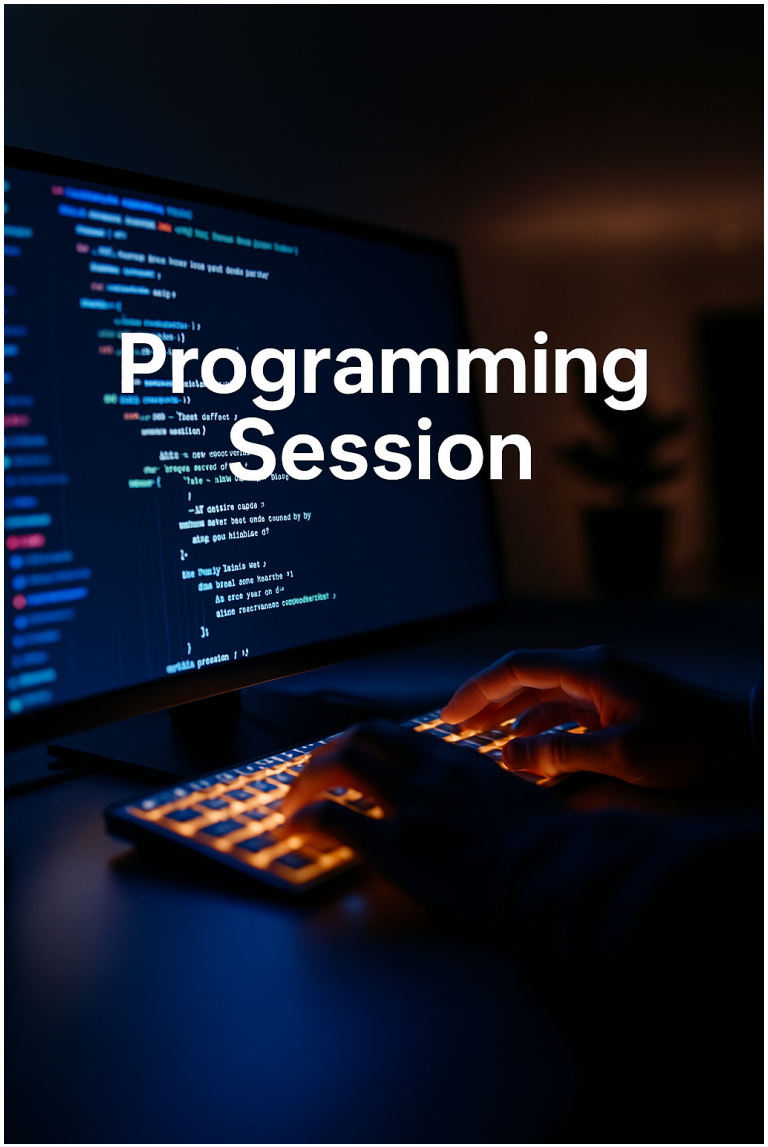


TFT Architecture: High-Level View



Feedback Poll

Click here to participate in the poll



Programming Session 4: Introducing Supervised Learning Algorithms for Time Series Forecasting

- Section 3: Neural Networks.
- Section 4: Performance Analysis.
- *Click here to access the programming session*

Solution will be posted tonight on the GitHub page.

- *Click here to access ccess the GitHub Page*

Quiz Time!

Click here to take the quiz

Thank you for your attention

References I

[1] Djork-Arné Clevert, Thomas Unterthiner, and Sepp Hochreiter. "Fast and accurate deep network learning by exponential linear units (elus)". In: *arXiv preprint arXiv:1511.07289* (2015).

[2] Yoav Freund, Robert E Schapire, et al. "Experiments with a new boosting algorithm". In: *icml*. Vol. 96. Citeseer. 1996, pp. 148–156.

[3] Günter Klambauer et al. "Self-normalizing neural networks". In: *Advances in neural information processing systems* 30 (2017).

[4] Bing Xu et al. "Empirical evaluation of rectified activations in convolutional network". In: *arXiv preprint arXiv:1505.00853* (2015).