



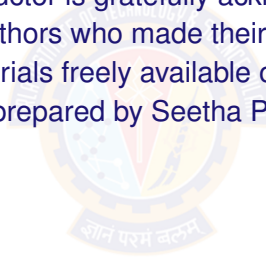
**BITS Pilani**  
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# DEEP NEURAL NETWORK MODULE # 4 : LINEAR NEURAL NETWORKS FOR CLASSIFICATION

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The instructor is gratefully acknowledging  
the authors who made their course  
materials freely available online.  
This deck is prepared by Seetha Parameswaran.



# TABLE OF CONTENTS

## 1 CLASSIFICATION

### 2 BINARY CLASSIFICATION

- Logistic Regression
- The Model: Single Neuron for Binary Classification
- Binary Classification: Worked Example
- Binary Classification: Evaluation Metrics

### 3 MULTI-CLASS CLASSIFICATION

- Multi-class Classification Model
- Mini-batch Stochastic Gradient Descent
- Multiclass Classification: Worked Example
- Making Predictions (Inference)
- Multiclass Classification: Evaluation Metrics

### 4 IMPLEMENTATION TIPS AND DEBUGGING

### 5 SUMMARY

# WHAT IS CLASSIFICATION?

## DEFINITION

Classification is a supervised learning task that predicts a discrete category or class label based on input features.

### Key Characteristics:

- Input: Feature vector  $\mathbf{x} \in \mathbb{R}^d$
- Output: Class label  $y \in \{1, 2, \dots, K\}$  (discrete)
- Goal: Learn a function  $f : \mathbb{R}^d \rightarrow \{1, 2, \dots, K\}$  that assigns inputs to classes

### Difference from Regression:

- Regression: Predicts **continuous** values (e.g., price, temperature)
- Classification: Predicts **discrete** categories (e.g., spam/not spam, cat/dog)

# EXAMPLES OF CLASSIFICATION PROBLEMS

## ① Email Spam Detection

- ▶ Input: Email text, sender information, attachments
- ▶ Output: Spam or Not Spam

## ② Medical Diagnosis

- ▶ Input: Patient symptoms, test results, medical history
- ▶ Output: Disease present or absent

## ③ Image Recognition

- ▶ Input: Pixel values of an image
- ▶ Output: Object category (cat, dog, car, etc.)

## ④ Sentiment Analysis

- ▶ Input: Customer review text
- ▶ Output: Positive, Negative, or Neutral

# TYPES OF CLASSIFICATION

## 1. Binary Classification

- Two classes:  $y \in \{0, 1\}$  or  $\{-1, +1\}$
- Examples: Spam detection, disease diagnosis, fraud detection

## 2. Multi-class Classification

- Multiple classes:  $y \in \{1, 2, \dots, K\}$  where  $K > 2$
- Examples: Digit recognition (0-9), animal classification
- Each example belongs to exactly one class

## 3. Multi-label Classification

- Each example can belong to multiple classes simultaneously
- Examples: Movie genres (action + comedy), document tagging

# TABLE OF CONTENTS

## 1 CLASSIFICATION

## 2 BINARY CLASSIFICATION

- Logistic Regression
- The Model: Single Neuron for Binary Classification
- Binary Classification: Worked Example
- Binary Classification: Evaluation Metrics

## 3 MULTI-CLASS CLASSIFICATION

- Multi-class Classification Model
- Mini-batch Stochastic Gradient Descent
- Multiclass Classification: Worked Example
- Making Predictions (Inference)
- Multiclass Classification: Evaluation Metrics

## 4 IMPLEMENTATION TIPS AND DEBUGGING

## 5 SUMMARY

# BINARY CLASSIFICATION PROBLEM

## DEFINITION

Binary classification assigns each input to one of two classes.

### Standard Notation:

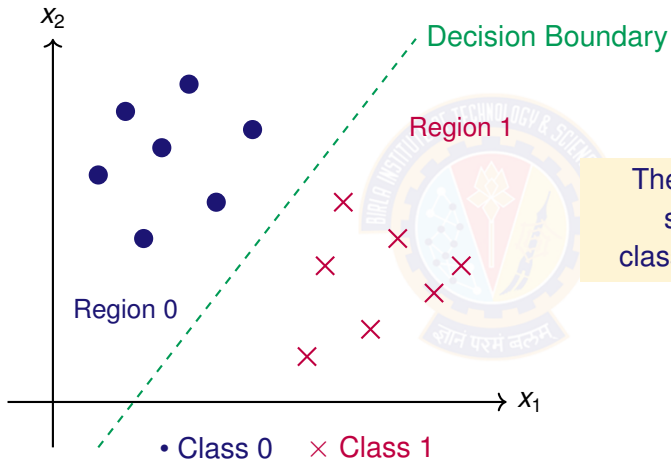
- Classes:  $y \in \{0, 1\}$ 
  - ▶  $y = 1$ : Positive class (e.g., spam, disease present)
  - ▶  $y = 0$ : Negative class (e.g., not spam, disease absent)
- Dataset:  $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$
- Goal: Learn  $f(\mathbf{x})$  that outputs probability of class 1

### Decision Boundary:

- Predict  $\hat{y} = 1$  if  $f(\mathbf{x}) \geq 0.5$
- Predict  $\hat{y} = 0$  if  $f(\mathbf{x}) < 0.5$



# BINARY CLASSIFICATION: VISUAL EXAMPLE

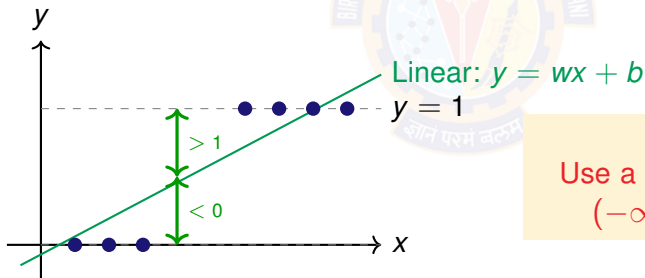


The decision boundary separates the two classes in feature space.

# WHY NOT USE LINEAR REGRESSION?

Problem with Linear Regression for Classification:

- Linear regression outputs:  $\hat{y} \in (-\infty, \infty)$
- We need probabilities:  $\hat{y} \in [0, 1]$
- Linear model can predict values  $< 0$  or  $> 1$



**Solution:**  
Use a function that maps  
 $(-\infty, \infty) \rightarrow [0, 1]$

# TABLE OF CONTENTS

## 1 CLASSIFICATION

## 2 BINARY CLASSIFICATION

- **Logistic Regression**

- The Model: Single Neuron for Binary Classification
- Binary Classification: Worked Example
- Binary Classification: Evaluation Metrics

## 3 MULTI-CLASS CLASSIFICATION

- Multi-class Classification Model
- Mini-batch Stochastic Gradient Descent
- Multiclass Classification: Worked Example
- Making Predictions (Inference)
- Multiclass Classification: Evaluation Metrics

## 4 IMPLEMENTATION TIPS AND DEBUGGING

## 5 SUMMARY

# WHAT IS LOGISTIC REGRESSION?

## DEFINITION

Logistic regression is a linear model for binary classification that uses the **sigmoid function** to output probabilities.

Key Idea:

- Compute linear combination:  $z = \mathbf{w}^T \mathbf{x} + w_0$
- Apply sigmoid function:  $\hat{y} = \sigma(z)$
- Interpret output as probability:  $\hat{y} = P(y = 1 | \mathbf{x}) \in [0, 1]$

Mathematical Form:

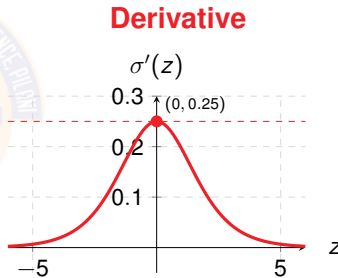
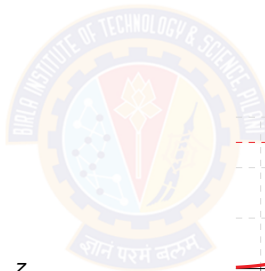
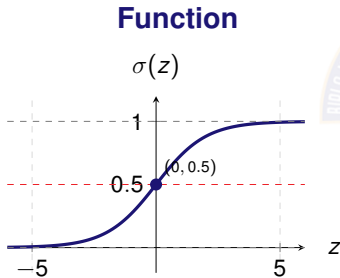
$$\hat{y} = \sigma(\mathbf{w}^T \mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w}^T \mathbf{x}}} \quad (1)$$

where  $\sigma(\cdot)$  is the sigmoid (logistic) function.

# THE SIGMOID ACTIVATION FUNCTION

Sigmoid (Logistic) Function:  $\sigma(z) = \frac{1}{1+e^{-z}}$

Derivative formula:  $\sigma'(z) = \sigma(z)(1 - \sigma(z))$



At  $z = 0$ :  $\sigma(0) = 0.5$     $\sigma'(0) = 0.25$

# PROPERTIES OF SIGMOID FUNCTION

## Key Properties:

- **Range:**  $\sigma(z) \in (0, 1) \rightarrow$  perfect for probabilities!
- **Monotonic:** Always increasing
- **Smooth:** Differentiable everywhere
- **Symmetry:**  $\sigma(-z) = 1 - \sigma(z)$
- **Derivative:**  $\sigma'(z) = \sigma(z)(1 - \sigma(z))$

## Behavior:

- When  $z \rightarrow +\infty$ :  $\sigma(z) \rightarrow 1$  (confident class 1)
- When  $z \rightarrow -\infty$ :  $\sigma(z) \rightarrow 0$  (confident class 0)
- When  $z = 0$ :  $\sigma(z) = 0.5$  (uncertain)

The derivative property makes sigmoid ideal for gradient-based learning!

# TABLE OF CONTENTS

## 1 CLASSIFICATION

## 2 BINARY CLASSIFICATION

- Logistic Regression
- The Model: Single Neuron for Binary Classification
- Binary Classification: Worked Example
- Binary Classification: Evaluation Metrics

## 3 MULTI-CLASS CLASSIFICATION

- Multi-class Classification Model
- Mini-batch Stochastic Gradient Descent
- Multiclass Classification: Worked Example
- Making Predictions (Inference)
- Multiclass Classification: Evaluation Metrics

## 4 IMPLEMENTATION TIPS AND DEBUGGING

## 5 SUMMARY

# THE FOUR COMPONENTS

A complete deep learning system for classification consists of:

- ① **Data:**  $d$ -dimensional input vectors and binary labels
- ② **Model:** Single neuron with sigmoid activation
- ③ **Objective Function:** Binary cross-entropy loss
- ④ **Learning Algorithm:** Stochastic gradient descent (SGD)

Note: We use **stochastic** gradient descent instead of batch gradient descent for efficiency. (This is for learning purposes only.)



# MATRIX FORM OF DATA

For efficient computation, we organize data into matrices:

Input Data =  $\mathbf{x}^{(i)} = [1, x_1^{(i)}, \dots, x_d^{(i)}]^T$

Design Matrix:  $\mathbf{X} \in \mathbb{R}^{N \times (d+1)}$   $\mathbf{X} = \begin{bmatrix} 1 & x_1^{(1)} & \dots & x_d^{(1)} \\ 1 & x_1^{(2)} & \dots & x_d^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(N)} & \dots & x_d^{(N)} \end{bmatrix}$

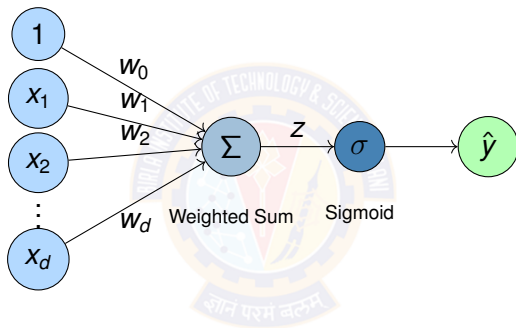
Label Vector:  $\mathbf{y} \in \{0, 1\}^N$   $\mathbf{y} = [y^{(1)} \ y^{(2)} \ \dots \ y^{(N)}]^T$

Weight Vector:  $\mathbf{w} \in \mathbb{R}^{d+1}$   $\mathbf{w} = [w_0 \ w_1 \ w_2 \ \dots \ w_d]^T$

Key difference from regression:  $y^{(i)} \in \{0, 1\}$  (discrete), not continuous!

# LOGISTIC REGRESSION AS A SINGLE NEURON

Model binary classification as a **single artificial neuron with sigmoid activation**:



- **Input:**  $\mathbf{x} \in \mathbb{R}^d$
- **Linear combination:**  $z = \mathbf{w}^T \mathbf{x}$
- **Activation:** Sigmoid  $\hat{y} = \sigma(z)$
- **Output:** Predicted probability  $\hat{y} = P(y = 1|\mathbf{x}) \in [0, 1]$

# MODEL PREDICTION

**Model:** A single neuron computes weighted sum and applies sigmoid activation.

**Prediction for input  $\mathbf{x}$ :**

$$z = \mathbf{w}^T \mathbf{x} = w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_d x_d \quad (2)$$

$$\hat{y} = \sigma(z) = \frac{1}{1 + e^{-z}} \quad (3)$$

$$\hat{y} = P(y = 1 | \mathbf{x}) \in [0, 1] \quad (4)$$

where:

- $z$  is the **logit** (pre-activation).
- $\hat{y}$  is the predicted probability.

# MAKING PREDICTIONS

## Decision Rule:

Given predicted probability  $\hat{y} = P(y = 1|\mathbf{x})$ :

$$\text{Predicted class} = \begin{cases} 1 & \text{if } \hat{y} \geq 0.5 \\ 0 & \text{if } \hat{y} < 0.5 \end{cases} \quad (5)$$

Equivalently, since  $\sigma(z) = 0.5$  when  $z = 0$ :

$$\text{Predicted class} = \begin{cases} 1 & \text{if } \mathbf{w}^T \mathbf{x} \geq 0 \\ 0 & \text{if } \mathbf{w}^T \mathbf{x} < 0 \end{cases} \quad (6)$$

The decision boundary is:  $\mathbf{w}^T \mathbf{x} = 0$  (a hyperplane in feature space)

# BINARY CROSS-ENTROPY LOSS

We cannot use squared error for classification. Instead, we use **cross-entropy loss**.

**Cross-entropy Loss for a single example:**

$$\ell(\mathbf{w}; \mathbf{x}^{(i)}, y^{(i)}) = - [y^{(i)} \log(\hat{y}^{(i)}) + (1 - y^{(i)}) \log(1 - \hat{y}^{(i)})] \quad (7)$$

where  $\hat{y}^{(i)} = \sigma(\mathbf{w}^T \mathbf{x}^{(i)})$

**Interpretation:**

- If  $y^{(i)} = 1$ : Loss =  $-\log(\hat{y}^{(i)})$ 
  - ▶ Penalizes if  $\hat{y}^{(i)}$  is far from 1
- If  $y^{(i)} = 0$ : Loss =  $-\log(1 - \hat{y}^{(i)})$ 
  - ▶ Penalizes if  $\hat{y}^{(i)}$  is far from 0

# TOTAL LOSS FUNCTION

Average Binary Cross-Entropy Loss:

$$J(\mathbf{w}) = \frac{-1}{N} \sum_{i=1}^N [y^{(i)} \log(\hat{y}^{(i)}) + (1 - y^{(i)}) \log(1 - \hat{y}^{(i)})] \quad (8)$$

Goal:

Find  $\mathbf{w}^*$  that minimizes  $J(\mathbf{w})$

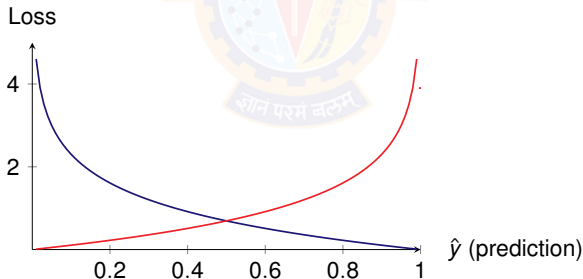
$$\mathbf{w}^* = \arg \min_{\mathbf{w}} J(\mathbf{w}) \quad (9)$$

# WHY CROSS-ENTROPY LOSS?

## Advantages:

- Probabilistic interpretation: Derived from maximum likelihood estimation
- Appropriate for probabilities: Heavily penalizes confident wrong predictions
- Convex: Has a single global minimum for logistic regression
- Well-behaved gradients: Works well with sigmoid activation

Loss behavior: Loss increases exponentially as prediction diverges from true label!



# FROM BATCH TO STOCHASTIC GRADIENT DESCENT

## Batch Gradient Descent (from Module 3):

- Uses **all** training examples in each update
- Computes gradient:  $\nabla J(\mathbf{w}) = \frac{1}{N} \sum_{i=1}^N \nabla \ell(\mathbf{w}; \mathbf{x}^{(i)}, y^{(i)})$
- Update:  $\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla J(\mathbf{w})$

## Problems with Batch GD:

- Slow for large datasets (must process all  $N$  examples per update)
- High memory requirements
- Redundant computations when examples are similar

## Solution: Stochastic Gradient Descent (SGD)

- Update weights using **one random example** at a time
- Much faster iterations
- Lower memory requirements



# STOCHASTIC GRADIENT DESCENT (SGD)

## Key Idea:

Instead of computing gradient over entire dataset, use gradient from a **single random example**.

## SGD Update Rule:

At iteration  $t$ :

- 1 Randomly select one example  $(\mathbf{x}^{(i)}, y^{(i)})$
- 2 Compute gradient for this example:  $\nabla \ell(\mathbf{w}; \mathbf{x}^{(i)}, y^{(i)})$  (noisy gradient estimate)
- 3 Update weights:  $\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \nabla \ell(\mathbf{w}^{(t)}; \mathbf{x}^{(i)}, y^{(i)})$

The noise in SGD actually helps escape local minima and often leads to better generalization!

# COMPUTING THE GRADIENT FOR SGD

Gradient of cross-entropy loss for one example:

For example  $(\mathbf{x}^{(i)}, y^{(i)})$ :

$$\nabla_{\mathbf{w}} \ell(\mathbf{w}; \mathbf{x}^{(i)}, y^{(i)}) = \frac{\partial \ell}{\partial \mathbf{w}_j} = (\hat{y}^{(i)} - y^{(i)}) \mathbf{x}^{(i)} \quad (10)$$

where  $\hat{y}^{(i)} = \sigma(\mathbf{w}^T \mathbf{x}^{(i)})$  for  $j = 0, 1, \dots, d$  (where  $x_0^{(i)} = 1$  for bias)

Remarkably simple form!

- Error:  $(\hat{y}^{(i)} - y^{(i)})$
- Direction:  $\mathbf{x}^{(i)}$
- Same structure as linear regression gradient!

# STOCHASTIC GRADIENT DESCENT ALGORITHM

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**Algorithm 1:** Stochastic Gradient Descent for Logistic Regression

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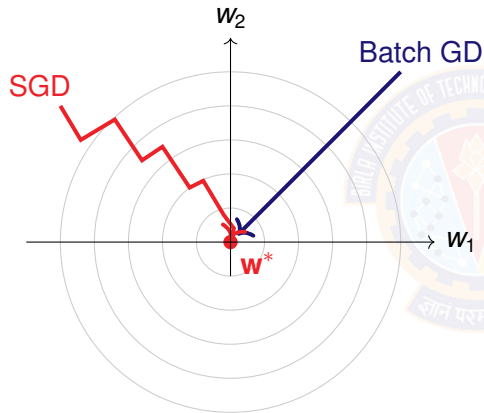
**Input:** Dataset  $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ , learning rate  $\eta$ , epochs  $T$

**Output:** Learned weights  $\mathbf{w}$

```
1 Initialize  $\mathbf{w}^{(0)} = \mathbf{0}$  (or small random values);
2 for  $epoch = 1$  to  $T$  do
3     Shuffle dataset  $\mathcal{D}$ ;
4     for each example  $(\mathbf{x}^{(i)}, y^{(i)})$  in  $\mathcal{D}$  do
5         Compute prediction:  $\hat{y}^{(i)} = \sigma(\mathbf{w}^T \mathbf{x}^{(i)})$ ;
6         Compute gradient:  $\nabla \ell = (\hat{y}^{(i)} - y^{(i)}) \mathbf{x}^{(i)}$ ;
7         Update weights:  $\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla \ell$ ;
8         Optional: Compute total loss  $J(\mathbf{w})$  for monitoring;
9 return  $\mathbf{w}$ ;
```

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# SGD vs BATCH GD: VISUAL COMPARISON



**Batch GD:** Smooth, deterministic path

**SGD:** Noisy, stochastic path but faster iterations

# BENEFITS AND CHALLENGES OF SGD

## Benefits:

- **Speed:** Much faster per iteration (only one example)
- **Memory:** Can handle datasets that don't fit in memory
- **Online learning:** Can update model as new data arrives
- **Generalization:** Noise helps escape sharp minima
- **Scalability:** Works well with massive datasets

## Challenges:

- **Noisy updates:** Path to minimum is not smooth
- **Learning rate:** More sensitive to  $\eta$  choice
- **Convergence:** May oscillate near minimum
- **Hyperparameter tuning:** Requires careful tuning

Common compromise: Mini-batch SGD

# TABLE OF CONTENTS

## 1 CLASSIFICATION

## 2 BINARY CLASSIFICATION

- Logistic Regression
- The Model: Single Neuron for Binary Classification
- **Binary Classification: Worked Example**
- Binary Classification: Evaluation Metrics

## 3 MULTI-CLASS CLASSIFICATION

- Multi-class Classification Model
- Mini-batch Stochastic Gradient Descent
- Multiclass Classification: Worked Example
- Making Predictions (Inference)
- Multiclass Classification: Evaluation Metrics

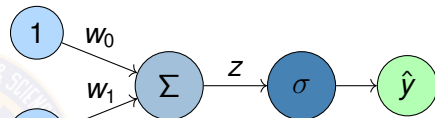
## 4 IMPLEMENTATION TIPS AND DEBUGGING

## 5 SUMMARY

# NUMERICAL EXAMPLE: SETUP

**Tiny Dataset:** Classify whether a student passes based on study hours

Hours ( $x_1$ )	Pass ( $y$ )
1	0
2	0
3	1
4	1



**Matrix Formulation:**

$$\mathbf{X} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}, \quad \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}$$

# NUMERICAL EXAMPLE: INITIALIZATION

Hyperparameters:  $\eta = 0.5$ ,  $N = 4$

Initialize weights:  $\mathbf{w}^{(0)} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$

Sigmoid function:  $\sigma(z) = \frac{1}{1 + e^{-z}}$

Loss function:  $\ell(\mathbf{w}; \mathbf{x}, y) = -[y \log(\hat{y}) + (1 - y) \log(1 - \hat{y})]$

Initial predictions with  $\mathbf{w}^{(0)} = \begin{bmatrix} 0 & 0 \end{bmatrix}^T$ : For all examples:  $z = 0 \Rightarrow \hat{y} = \sigma(0) = 0.5$

$$\hat{\mathbf{y}}^{(0)} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix}$$



# NUMERICAL EXAMPLE: FIRST SGD ITERATION

Randomly select first example:  $(\mathbf{x}^{(1)}, y^{(1)}) = ([1 \ 1], 0)$

Step 1 - Forward pass:  $z^{(1)} = \mathbf{x}^{(1)} \mathbf{w}^{(0)} = [1 \ 1] \begin{bmatrix} 0 \\ 0 \end{bmatrix} = 0$

$$\hat{y}^{(1)} = \sigma(0) = 0.5$$

Step 2 - Compute error:  $\text{error} = \hat{y}^{(1)} - y^{(1)} = 0.5 - 0 = 0.5$

Step 3 - Compute gradient:  $\nabla \ell = (\hat{y}^{(1)} - y^{(1)}) \mathbf{x}^{(1)} = 0.5 \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix}$

Step 4 - Update weights:  $\mathbf{w}^{(1)} = \mathbf{w}^{(0)} - \eta \nabla \ell$

$$= \begin{bmatrix} 0 \\ 0 \end{bmatrix} - 0.5 \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} = \begin{bmatrix} -0.25 \\ -0.25 \end{bmatrix}$$

# NUMERICAL EXAMPLE: SECOND SGD ITERATION

Randomly select second example:  $(\mathbf{x}^{(3)}, y^{(3)}) = ([1 \ 3], 1)$

Step 1: Forward pass:  $z^{(3)} = \mathbf{x}^{(3)} \mathbf{w}^{(1)} = [1 \ 3] \begin{bmatrix} -0.25 \\ -0.25 \end{bmatrix} = -1.0$

$$\hat{y}^{(3)} = \sigma(-1.0) = \frac{1}{1 + e^{1.0}} \approx 0.269$$

Step 2: Compute error:  $\text{error} = 0.269 - 1 = -0.731$

Step 3: Compute gradient:  $\nabla \ell = -0.731 \begin{bmatrix} 1 \\ 3 \end{bmatrix} = \begin{bmatrix} -0.731 \\ -2.193 \end{bmatrix}$

Step 4: Update weights:  $\mathbf{w}^{(2)} = \begin{bmatrix} -0.25 \\ -0.25 \end{bmatrix} - 0.5 \begin{bmatrix} -0.731 \\ -2.193 \end{bmatrix} = \begin{bmatrix} 0.116 \\ 0.847 \end{bmatrix}$

# NUMERICAL EXAMPLE: CHECKING PROGRESS

After 2 SGD iterations, let's check predictions:

With  $\mathbf{w}^{(2)} = \begin{bmatrix} 0.116 \\ 0.847 \end{bmatrix}$ :

Example 1:  $\hat{y}^{(1)} = \sigma(0.116 + 0.847 \cdot 1) \approx \sigma(0.963) \approx 0.724$

Example 2:  $\hat{y}^{(2)} = \sigma(0.116 + 0.847 \cdot 2) \approx \sigma(1.810) \approx 0.859$

Example 3:  $\hat{y}^{(3)} = \sigma(0.116 + 0.847 \cdot 3) \approx \sigma(2.657) \approx 0.934$

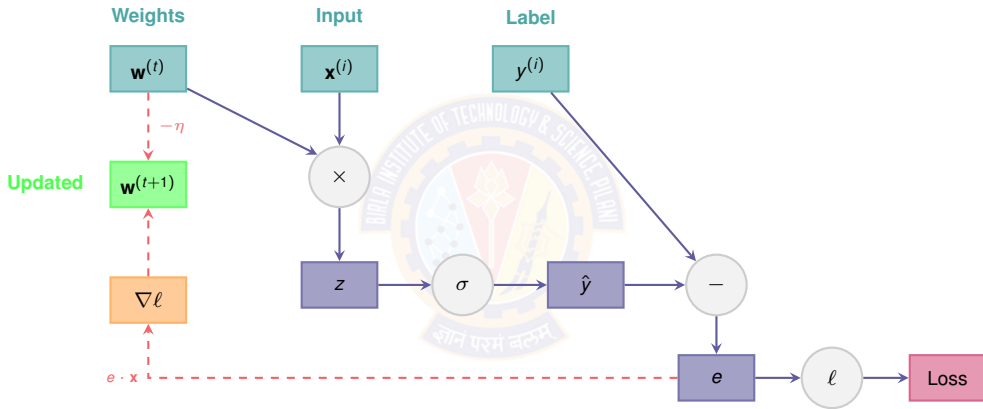
Example 4:  $\hat{y}^{(4)} = \sigma(0.116 + 0.847 \cdot 4) \approx \sigma(3.504) \approx 0.971$

Progress:

- Examples 1, 2 (true label 0): predictions moving toward 0 ✓
- Examples 3, 4 (true label 1): predictions moving toward 1 ✓

Continue SGD for multiple epochs until convergence!

# COMPUTATIONAL GRAPH FOR ONE SGD STEP



Single example used per iteration — much faster than batch GD!

# TABLE OF CONTENTS

## 1 CLASSIFICATION

## 2 BINARY CLASSIFICATION

- Logistic Regression
- The Model: Single Neuron for Binary Classification
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- Binary Classification: Evaluation Metrics

## 3 MULTI-CLASS CLASSIFICATION

- Multi-class Classification Model
- Mini-batch Stochastic Gradient Descent
- Multiclass Classification: Worked Example
- Making Predictions (Inference)
- Multiclass Classification: Evaluation Metrics

## 4 IMPLEMENTATION TIPS AND DEBUGGING

## 5 SUMMARY

# EVALUATING CLASSIFICATION MODELS

Unlike regression, we need different metrics for classification.

Key Questions:

- How often does the model predict correctly? (Accuracy)
- What types of errors does it make? (Confusion Matrix)
- How well does it identify positive cases? (Precision, Recall)

Data Split:

- Training set: Learn weights  $\mathbf{w}$  (typically 90-99%)
- Validation set: Tune hyperparameters (typically 10-15%)
- Test set: Final evaluation (typically 1-10%)

Always evaluate on unseen test data to measure generalization!

# CONFUSION MATRIX

The confusion matrix shows all prediction outcomes:

		Predicted	
		Positive (1)	Negative (0)
Actual	Positive (1)	True Positive (TP)	False Negative (FN)
	Negative (0)	False Positive (FP)	True Negative (TN)

Definitions:

- **TP**: Correctly predicted positive
- **TN**: Correctly predicted negative
- **FP**: Incorrectly predicted positive (Type I error)
- **FN**: Incorrectly predicted negative (Type II error)

# CLASSIFICATION METRICS I

1. **Accuracy:** Overall correctness

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN} \quad (11)$$

2. **Precision:** Of predicted positives, how many are correct?

$$\text{Precision} = \frac{TP}{TP + FP} \quad (12)$$



# CLASSIFICATION METRICS II

3. Recall (Sensitivity): Of actual positives, how many did we find?

$$\text{Recall} = \frac{TP}{TP + FN} \quad (13)$$

4. F1 Score: Harmonic mean of precision and recall

$$F1 = 2 \cdot \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}} \quad (14)$$

# WHEN TO USE WHICH METRIC?

## Accuracy:

- Use when classes are balanced
- **Misleading with imbalanced data!** (e.g., 95% negative class)

## Precision:

- Important when False Positives are costly
- Example: Spam detection (don't want to mark real emails as spam)

## Recall:

- Important when False Negatives are costly
- Example: Disease detection (don't want to miss sick patients)

## F1 Score:

- Use when you need balance between precision and recall
- Good for imbalanced datasets

# EXAMPLE: COMPUTING METRICS

Given predictions:

True	Pred	True	Pred
1	1 (TP)	0	0 (TN)
1	1 (TP)	0	0 (TN)
1	0 (FN)	0	1 (FP)
1	1 (TP)	0	0 (TN)

$$\text{Accuracy} = \frac{3 + 3}{3 + 3 + 1 + 1} = \frac{6}{8} = 0.75$$

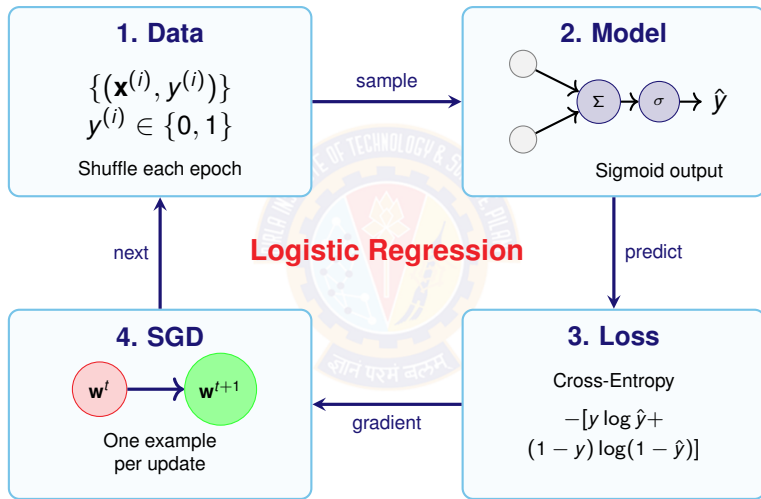
$$\text{Precision} = \frac{3}{3 + 1} = 0.75$$

$$\text{Recall} = \frac{3}{3 + 1} = 0.75$$

$$F1 = 2 \cdot \frac{0.75 \times 0.75}{0.75 + 0.75} = 0.75$$

Counts: TP = 3, TN = 3, FP = 1, FN = 1

# SUMMARY: BINARY CLASSIFICATION



This framework is the foundation for neural networks!

# KEY TAKEAWAYS

- Binary classification predicts discrete categories using  $y \in \{0, 1\}$ .
- Sigmoid activation  $\sigma(z) = \frac{1}{1+e^{-z}}$  maps to probabilities  $[0, 1]$ .
- Logistic regression = linear model + sigmoid activation.
- Cross-entropy loss is the appropriate objective for classification.
- Stochastic Gradient Descent (SGD) updates weights one example at a time — faster and more scalable.
- Feature scaling is essential for convergence and numerical stability.
- Evaluation metrics: Accuracy, Precision, Recall, F1 Score, Confusion Matrix.
- This framework extends naturally to multi-class classification and deep networks.

# TABLE OF CONTENTS

## 1 CLASSIFICATION

## 2 BINARY CLASSIFICATION

- Logistic Regression
- The Model: Single Neuron for Binary Classification
- Binary Classification: Worked Example
- Binary Classification: Evaluation Metrics

## 3 MULTI-CLASS CLASSIFICATION

- Multi-class Classification Model
- Mini-batch Stochastic Gradient Descent
- Multiclass Classification: Worked Example
- Making Predictions (Inference)
- Multiclass Classification: Evaluation Metrics

## 4 IMPLEMENTATION TIPS AND DEBUGGING

## 5 SUMMARY

# WHAT IS MULTI-CLASS CLASSIFICATION?

## DEFINITION

Multi-class classification assigns each input to one of  $K$  classes, where  $K > 2$ .

### Key Characteristics:

- Classes:  $y \in \{1, 2, 3, \dots, K\}$  (or  $\{0, 1, 2, \dots, K - 1\}$ )
- Each example belongs to **exactly one** class
- Output: Probability distribution over all  $K$  classes
- Probabilities sum to 1:  $\sum_{k=1}^K P(y = k|\mathbf{x}) = 1$

### Example:

- Input: Image of a handwritten digit
- Output: Probabilities for each of 10 classes (0, 1, 2, ..., 9)
- Prediction: Class with highest probability

# EXAMPLES OF MULTI-CLASS CLASSIFICATION

## ① Handwritten Digit Recognition (MNIST)

- ▶ Input:  $28 \times 28$  pixel image
- ▶ Output: One of 10 digits (0-9)

## ② Image Classification (ImageNet)

- ▶ Input: Color image
- ▶ Output: One of 1000 object categories (cat, dog, car, plane, ...)

## ③ Text Classification

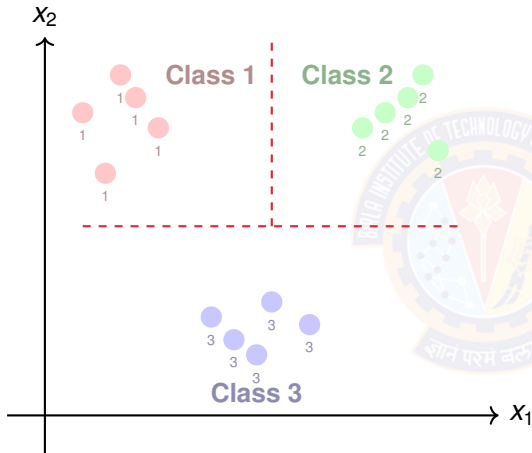
- ▶ Input: News article text
- ▶ Output: Topic category (politics, sports, technology, entertainment, business)

## ④ Speech Recognition

- ▶ Input: Audio features
- ▶ Output: Phoneme class (multiple phonemes in a language)



# MULTI-CLASS CLASSIFICATION: VISUAL EXAMPLE



Key insight: We need **multiple output neurons** (one per class) and a way to convert their outputs into a valid probability distribution.

Decision boundaries separate  $K = 3$  classes in feature space.

# TABLE OF CONTENTS

## 1 CLASSIFICATION

## 2 BINARY CLASSIFICATION

- Logistic Regression
- The Model: Single Neuron for Binary Classification
- Binary Classification: Worked Example
- Binary Classification: Evaluation Metrics

## 3 MULTI-CLASS CLASSIFICATION

- **Multi-class Classification Model**
- Mini-batch Stochastic Gradient Descent
- Multiclass Classification: Worked Example
- Making Predictions (Inference)
- Multiclass Classification: Evaluation Metrics

## 4 IMPLEMENTATION TIPS AND DEBUGGING

## 5 SUMMARY

# THE FOUR COMPONENTS FOR MULTI-CLASS

A complete multi-class classification system consists of:

- ① **Data:** Input features and class labels  $y \in \{1, 2, \dots, K\}$
- ② **Model:** Linear model with  $K$  output neurons (no hidden layers)
- ③ **Activation:** Softmax function to produce probability distribution
- ④ **Objective Function:** Categorical cross-entropy loss
- ⑤ **Learning Algorithm:** Mini-batch stochastic gradient descent

**Note:** We now use **mini-batch SGD** instead of single-example SGD for better efficiency and stability.

# DATA REPRESENTATION

Input Features:

$$\mathbf{X} \in \mathbb{R}^{N \times (d+1)} \quad \mathbf{X} = \begin{bmatrix} 1 & x_1^{(1)} & \dots & x_d^{(1)} \\ 1 & x_1^{(2)} & \dots & x_d^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(N)} & \dots & x_d^{(N)} \end{bmatrix}$$

Class Labels: Two representations

1. Integer encoding:  $\mathbf{y} \in \{1, 2, \dots, K\}^N$

$$\mathbf{y} = [3 \ 1 \ 2 \ 1 \ 3]^T$$

2. One-hot encoding:  $\mathbf{Y} \in \{0, 1\}^{N \times K}$  (preferred for computation)

# ONE-HOT ENCODING

**Definition:** Convert class label to binary vector of length  $K$

**For class  $k$ :** All zeros except 1 at position  $k$

**Example with  $K = 4$  classes:**

Class 1:  $\mathbf{y} = [1, 0, 0, 0]^T$

Class 2:  $\mathbf{y} = [0, 1, 0, 0]^T$

Class 3:  $\mathbf{y} = [0, 0, 1, 0]^T$

Class 4:  $\mathbf{y} = [0, 0, 0, 1]^T$

**Why one-hot?**

- Treats all classes equally (no implicit ordering)
- Matches the format of softmax output probabilities
- Simplifies loss computation
- Standard in deep learning frameworks

# WEIGHT MATRIX FOR MULTI-CLASS CLASSIFICATION

For  $K$  classes and  $d$  input features:

**Weight Matrix:**  $\mathbf{W} \in \mathbb{R}^{(d+1) \times K}$

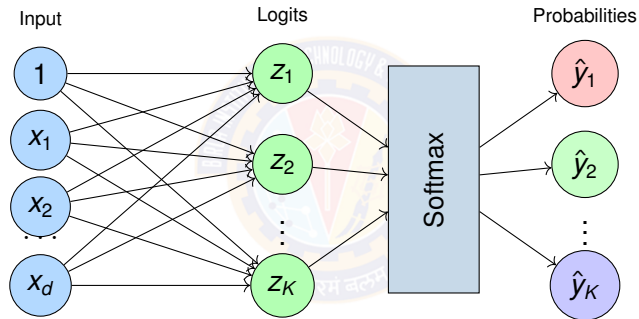
$$\mathbf{W} = \begin{bmatrix} w_{0,1} & w_{0,2} & \cdots & w_{0,K} \\ w_{1,1} & w_{1,2} & \cdots & w_{1,K} \\ w_{2,1} & w_{2,2} & \cdots & w_{2,K} \\ \vdots & \vdots & \ddots & \vdots \\ w_{d,1} & w_{d,2} & \cdots & w_{d,K} \end{bmatrix}$$

- Each **column**  $\mathbf{w}_k$  represents weights for class  $k$
- Each class has its own linear model
- Row 0: Bias terms for all classes
- Total parameters:  $(d + 1) \times K$

Compare to binary: 1 weight vector vs  $K$  weight vectors!

# MULTI-CLASS MODEL ARCHITECTURE

**Architecture:** Multiple output neurons with softmax activation



$$\mathbf{z} = \mathbf{W}^T \mathbf{x} \text{ (linear)} \rightarrow \hat{\mathbf{y}} = \text{softmax}(\mathbf{z}) \text{ (activation)}$$

# LINEAR MODEL: COMPUTING LOGITS

Step 1: Compute logits (pre-activation values)

For a single input  $\mathbf{x}$ :

$$\mathbf{z} = \mathbf{W}^T \mathbf{x} = \begin{bmatrix} \mathbf{w}_1^T \mathbf{x} \\ \mathbf{w}_2^T \mathbf{x} \\ \vdots \\ \mathbf{w}_K^T \mathbf{x} \end{bmatrix} = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_K \end{bmatrix} \quad (15)$$

where  $z_k = \mathbf{w}_k^T \mathbf{x} = w_{0,k} + w_{1,k}x_1 + \dots + w_{d,k}x_d$

For entire dataset (batch):

$$\mathbf{Z} = \mathbf{XW} \in \mathbb{R}^{N \times K} \quad (16)$$

Each row of  $\mathbf{Z}$  contains logits for one example.

Logits are **unbounded** values in  $(-\infty, \infty) \rightarrow$  not probabilities yet!



# THE SOFTMAX FUNCTION

**Purpose:** Convert  $K$  logits into a valid probability distribution

## DEFINITION:

For logit vector  $\mathbf{z} = [z_1, z_2, \dots, z_K]^T$

$$\text{softmax}(\mathbf{z})_k = \frac{e^{z_k}}{\sum_{j=1}^K e^{z_j}} \quad \text{for } k = 1, 2, \dots, K \quad (17)$$

**Output:** Probability vector  $\hat{\mathbf{y}} = [\hat{y}_1, \hat{y}_2, \dots, \hat{y}_K]^T$

$$\hat{y}_k = P(y = k|\mathbf{x}) = \frac{e^{z_k}}{\sum_{j=1}^K e^{z_j}} \quad (18)$$

**Interpretation:**  $\hat{y}_k$  is the predicted probability for class  $k$

# PROPERTIES OF SOFTMAX

## Key Properties:

- ① Output range:  $\hat{y}_k \in (0, 1)$  for all  $k$
- ② Probability distribution:  $\sum_{k=1}^K \hat{y}_k = 1$
- ③ Preserves order: If  $z_i > z_j$ , then  $\hat{y}_i > \hat{y}_j$
- ④ Translation invariant:  $\text{softmax}(\mathbf{z}) = \text{softmax}(\mathbf{z} + c)$  for any constant  $c$
- ⑤ Differentiable: Enables gradient-based learning
- ⑥ Reduces to sigmoid: When  $K = 2$ , softmax is equivalent to sigmoid

The exponential amplifies differences: larger logits get much larger probabilities!

# SOFTMAX EXAMPLE: NUMERICAL COMPUTATION

Given logits:  $\mathbf{z} = [2.0, 1.0, 0.1]^T$  for  $K = 3$  classes

Step 1: Compute exponentials

$$e^{z_1} = e^{2.0} \approx 7.39$$

$$e^{z_2} = e^{1.0} \approx 2.72$$

$$e^{z_3} = e^{0.1} \approx 1.11$$

Step 2: Compute sum

$$\sum_{j=1}^3 e^{z_j} = 7.39 + 2.72 + 1.11 = 11.22$$

Step 3: Normalize

$$\hat{y}_1 = \frac{7.39}{11.22} \approx 0.659$$

$$\hat{y}_2 = \frac{2.72}{11.22} \approx 0.242$$

$$\hat{y}_3 = \frac{1.11}{11.22} \approx 0.099$$

Step 4: Predicted class:

$\arg \max_k \hat{y}_k = 1$  (highest probability)



# COMPLETE FORWARD PASS

For a batch of  $N$  examples  $\mathbf{X}$ :

Step 1: Compute logits  $\mathbf{Z} = \mathbf{XW} \in \mathbb{R}^{N \times K}$  (19)

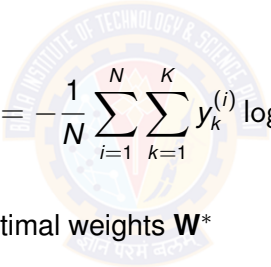
Step 2: Apply softmax  $\hat{\mathbf{Y}} = \text{softmax}(\mathbf{Z}) \in [0, 1]^{N \times K}$  (20)  
(softmax applied row-wise to each example)

Step 3: Predict class  $\hat{k} = \arg \max_k \hat{y}_k$  (21)

Each row of  $\hat{\mathbf{Y}}$  is a probability distribution over  $K$  classes.

# CATEGORICAL CROSS-ENTROPY LOSS

Total loss over dataset:


$$J(\mathbf{W}) = -\frac{1}{N} \sum_{i=1}^N \sum_{k=1}^K y_k^{(i)} \log(\hat{y}_k^{(i)}) \quad (22)$$

**Goal:** Minimize  $J(\mathbf{W})$  to find optimal weights  $\mathbf{W}^*$

# UNDERSTANDING CATEGORICAL CROSS-ENTROPY

Intuition:

- Loss depends only on predicted probability for the **true class**
- Heavily penalizes **confident wrong predictions**
- Encourages high probability for correct class

Example: True class is 2 ( $\mathbf{y} = [0, 1, 0]$ )

Prediction	$\hat{y}_1$	$\hat{y}_2$	Loss = $-\log(\hat{y}_2)$
Good	0.1	<b>0.8</b>	0.22
Medium	0.3	<b>0.5</b>	0.69
Bad	0.7	<b>0.2</b>	1.61
Very bad	0.9	<b>0.05</b>	3.00

Loss increases exponentially as predicted probability for true class decreases!

# WHY CATEGORICAL CROSS-ENTROPY?

## Advantages:

- Probabilistic interpretation: Derived from maximum likelihood
- Appropriate for multi-class: Naturally handles  $K$  classes
- Works well with softmax: Numerically stable gradient
- Penalizes wrong confidence: Heavily penalizes confident mistakes
- Convex: For linear models (like ours)

## Connection to binary cross-entropy:

When  $K = 2$ :

$$\text{Categorical: } - [y_1 \log(\hat{y}_1) + y_2 \log(\hat{y}_2)]$$

$$\text{Binary: } - [y \log(\hat{y}) + (1 - y) \log(1 - \hat{y})]$$

They are equivalent! (with  $y_2 = y$  and  $y_1 = 1 - y$ )

# TABLE OF CONTENTS

## 1 CLASSIFICATION

## 2 BINARY CLASSIFICATION

- Logistic Regression
- The Model: Single Neuron for Binary Classification
- Binary Classification: Worked Example
- Binary Classification: Evaluation Metrics

## 3 MULTI-CLASS CLASSIFICATION

- Multi-class Classification Model
- **Mini-batch Stochastic Gradient Descent**
- Multiclass Classification: Worked Example
- Making Predictions (Inference)
- Multiclass Classification: Evaluation Metrics

## 4 IMPLEMENTATION TIPS AND DEBUGGING

## 5 SUMMARY



# FROM SGD TO MINI-BATCH SGD

## Recap: Gradient Descent Variants

### 1. Batch Gradient Descent:

- Uses **all**  $N$  examples per update
- Slow but stable, accurate gradient

### 2. Stochastic Gradient Descent (SGD):

- Uses **1** random example per update
- Fast but noisy, unstable

### 3. Mini-batch SGD (Best of both worlds):

- Uses **small batch** of  $B$  examples per update ( $1 < B \ll N$ )
- Typical batch sizes:  $B \in \{32, 64, 128, 256, 512\}$
- Good balance of speed and stability
- **Standard in modern deep learning!**

# WHY MINI-BATCH SGD?

## Advantages of mini-batches:

### ① Computational efficiency:

- ▶ Vectorized operations (matrix multiplication)
- ▶ Better GPU utilization
- ▶ Faster than processing examples one-by-one

### ② Gradient estimation:

- ▶ Less noisy than single-example SGD
- ▶ More stable convergence
- ▶ Better approximation of true gradient

### ③ Generalization:

- ▶ Noise helps escape sharp minima
- ▶ Often leads to better test performance

### ④ Memory efficiency:

- ▶ Can handle datasets larger than memory
- ▶ Load and process data in batches

# MINI-BATCH SGD: KEY CONCEPTS

- **Batch size ( $B$ ):** Number of examples per update
  - ▶ Small: 32-64 (more noise, faster iterations)
  - ▶ Medium: 128-256 (balanced)
  - ▶ Large: 512-1024 (less noise, but slower convergence)
- **Iteration:** One weight update (processing one mini-batch)
- **Epoch:** One complete pass through the entire dataset

$$\text{Iterations per epoch} = \left\lceil \frac{N}{B} \right\rceil \quad (23)$$

**Example:**  $N = 60,000$  samples,  $B = 128$

- ▶ Iterations per epoch:  $\lceil 60000/128 \rceil = 469$
- ▶ After 10 epochs:  $469 \times 10 = 4690$  weight updates

# COMPUTING GRADIENTS FOR MINI-BATCH

Gradient for a mini-batch of size  $B$ :

Let  $\mathcal{B}$  be a mini-batch of  $B$  examples:  $\mathcal{B} = \{(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})\}_{i \in \mathcal{I}}$

Average gradient over mini-batch:

$$\nabla J_{\mathcal{B}}(\mathbf{W}) = \frac{1}{B} \sum_{i \in \mathcal{B}} \nabla \ell(\mathbf{W}; \mathbf{x}^{(i)}, \mathbf{y}^{(i)}) \quad (24)$$

For categorical cross-entropy with softmax:

$$\nabla_{\mathbf{W}} J_{\mathcal{B}} = \frac{1}{B} \mathbf{X}_{\mathcal{B}}^T (\hat{\mathbf{Y}}_{\mathcal{B}} - \mathbf{Y}_{\mathcal{B}}) \quad (25)$$

where:

- $\mathbf{X}_{\mathcal{B}} \in \mathbb{R}^{B \times (d+1)}$ : Mini-batch inputs
- $\hat{\mathbf{Y}}_{\mathcal{B}} \in \mathbb{R}^{B \times K}$ : Predicted probabilities
- $\mathbf{Y}_{\mathcal{B}} \in \mathbb{R}^{B \times K}$ : One-hot true labels

# MINI-BATCH SGD UPDATE RULE

Update at iteration  $t$ :

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \nabla J_{\mathcal{B}}(\mathbf{w}^{(t)}) \quad (26)$$

Expanded form:

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \frac{\eta}{B} \mathbf{x}_B^T (\hat{\mathbf{y}}_B - \mathbf{y}_B) \quad (27)$$

# MINI-BATCH SGD ALGORITHM

## Algorithm 2: Mini-batch SGD for Multi-class Classification

**Input:** Dataset  $\mathcal{D} = \{(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})\}_{i=1}^N$ , batch size  $B$ , learning rate  $\eta$ , epochs  $T$

**Output:** Learned weight matrix  $\mathbf{W}$

```
1 Initialize  $\mathbf{W} \sim \mathcal{N}(0, 0.01)$  // Small random values
2 for  $epoch = 1$  to  $T$  do
3     Shuffle dataset  $\mathcal{D}$ ;
4     for each mini-batch  $\mathcal{B}$  of size  $B$  do
5         // Forward pass
6          $\mathbf{Z}_{\mathcal{B}} = \mathbf{X}_{\mathcal{B}}\mathbf{W}$  // Compute logits
7          $\hat{\mathbf{Y}}_{\mathcal{B}} = \text{softmax}(\mathbf{Z}_{\mathcal{B}})$  // Apply softmax
8          $\nabla J = \frac{1}{B}\mathbf{X}_{\mathcal{B}}^T(\hat{\mathbf{Y}}_{\mathcal{B}} - \mathbf{Y}_{\mathcal{B}})$  // Compute gradient
9          $\mathbf{W} \leftarrow \mathbf{W} - \eta \nabla J$  // Update weights
10        Optional: Compute total loss for monitoring;
11 return  $\mathbf{W}$ ;
```

# CHOOSING BATCH SIZE

Batch Size	Advantages	Disadvantages
Small (32-64)	<ul style="list-style-type: none"><li>• Fast iterations</li><li>• More updates per epoch</li><li>• Better generalization</li><li>• Escapes sharp minima</li></ul>	<ul style="list-style-type: none"><li>• Noisy gradients</li><li>• Unstable training</li><li>• Poor GPU utilization</li></ul>
Medium (128-256)	<ul style="list-style-type: none"><li>• Good balance</li><li>• Stable training</li><li>• Good GPU usage</li><li>• Standard choice</li></ul>	<ul style="list-style-type: none"><li>• May need tuning</li></ul>
Large (512-1024)	<ul style="list-style-type: none"><li>• Stable gradients</li><li>• Better GPU utilization</li><li>• Faster per-epoch time</li></ul>	<ul style="list-style-type: none"><li>• Slow convergence</li><li>• May generalize worse</li><li>• More memory</li></ul>

# TABLE OF CONTENTS

## 1 CLASSIFICATION

## 2 BINARY CLASSIFICATION

- Logistic Regression
- The Model: Single Neuron for Binary Classification
- Binary Classification: Worked Example
- Binary Classification: Evaluation Metrics

## 3 MULTI-CLASS CLASSIFICATION

- Multi-class Classification Model
- Mini-batch Stochastic Gradient Descent
- **Multiclass Classification: Worked Example**
- Making Predictions (Inference)
- Multiclass Classification: Evaluation Metrics

## 4 IMPLEMENTATION TIPS AND DEBUGGING

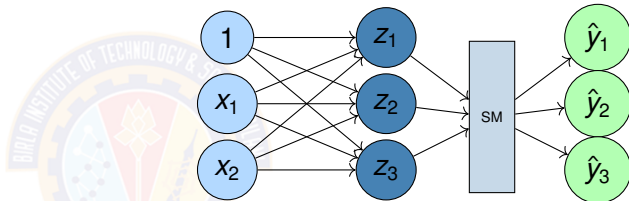
## 5 SUMMARY



# NUMERICAL EXAMPLE: SETUP

**Tiny Dataset:** Classify 4 data points into 3 classes

$x_1$	$x_2$	Class
1	2	1
2	1	2
2	3	1
3	2	3



**Parameters:**

- $K = 3$  classes,  $d = 2$  features,  $N = 4$  examples
- Batch size:  $B = 2$  (mini-batch)
- Learning rate:  $\eta = 0.1$

# NUMERICAL EXAMPLE: DATA REPRESENTATION

Design Matrix: (with bias column)  $\mathbf{X} = \begin{bmatrix} 1 & 1 & 2 \\ 1 & 2 & 1 \\ 1 & 2 & 3 \\ 1 & 3 & 2 \end{bmatrix} \in \mathbb{R}^{4 \times 3}$

One-hot Labels:  $\mathbf{Y} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \in \mathbb{R}^{4 \times 3}$

(class 1)  
(class 2)  
(class 1)  
(class 3)

Weight Matrix: Initialize randomly  $\mathbf{W}^{(0)} = \begin{bmatrix} 0.1 & -0.1 & 0.2 \\ 0.2 & 0.1 & -0.1 \\ -0.1 & 0.2 & 0.1 \end{bmatrix} \in \mathbb{R}^{3 \times 3}$

# NUMERICAL EXAMPLE: FIRST MINI-BATCH (EXAMPLE)

Mini-batch: First 2 examples after shuffling

$$\mathbf{X}_{\mathcal{B}} = \begin{bmatrix} 1 & 1 & 2 \\ 1 & 2 & 1 \end{bmatrix}, \mathbf{Y}_{\mathcal{B}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

Step 1: Compute logits

$$\begin{aligned} \mathbf{Z}_{\mathcal{B}} &= \mathbf{X}_{\mathcal{B}} \mathbf{W}^{(0)} \\ &= \begin{bmatrix} 1 & 1 & 2 \\ 1 & 2 & 1 \end{bmatrix} \begin{bmatrix} 0.1 & -0.1 & 0.2 \\ 0.2 & 0.1 & -0.1 \\ -0.1 & 0.2 & 0.1 \end{bmatrix} \\ &= \begin{bmatrix} 0.1 & 0.4 & 0.3 \\ 0.4 & 0.2 & 0.1 \end{bmatrix} \end{aligned}$$

# NUMERICAL EXAMPLE: SOFTMAX COMPUTATION

Step 2: Apply softmax to each row

Softmax for example 1:  $\hat{\mathbf{y}}^{(1)} \approx \begin{bmatrix} 0.280 \\ 0.378 \\ 0.342 \end{bmatrix}$

Similarly for example 2:  $\hat{\mathbf{y}}^{(2)} \approx [0.387, 0.315, 0.298]^T$

For the entire batch:  $\hat{\mathbf{Y}}_{\mathcal{B}} = \begin{bmatrix} 0.280 & 0.378 & 0.342 \\ 0.387 & 0.315 & 0.298 \end{bmatrix}$

# NUMERICAL EXAMPLE: GRADIENT AND UPDATE

Step 3: Compute gradient

$$\begin{aligned}\nabla J &= \frac{1}{B} \mathbf{X}_B^T (\hat{\mathbf{Y}}_B - \mathbf{Y}_B) \\ \hat{\mathbf{Y}}_B - \mathbf{Y}_B &= \begin{bmatrix} 0.280 & 0.378 & 0.342 \\ 0.387 & 0.315 & 0.298 \end{bmatrix} - \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \\ &= \begin{bmatrix} -0.720 & 0.378 & 0.342 \\ 0.387 & -0.685 & 0.298 \end{bmatrix} \\ \nabla J &= \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} -0.720 & 0.378 & 0.342 \\ 0.387 & -0.685 & 0.298 \end{bmatrix} \\ &\approx \begin{bmatrix} -0.167 & -0.154 & 0.320 \\ -0.024 & -0.496 & 0.469 \\ -0.527 & 0.036 & 0.491 \end{bmatrix}\end{aligned}$$

# NUMERICAL EXAMPLE: WEIGHT UPDATE

## Step 4: Update weights

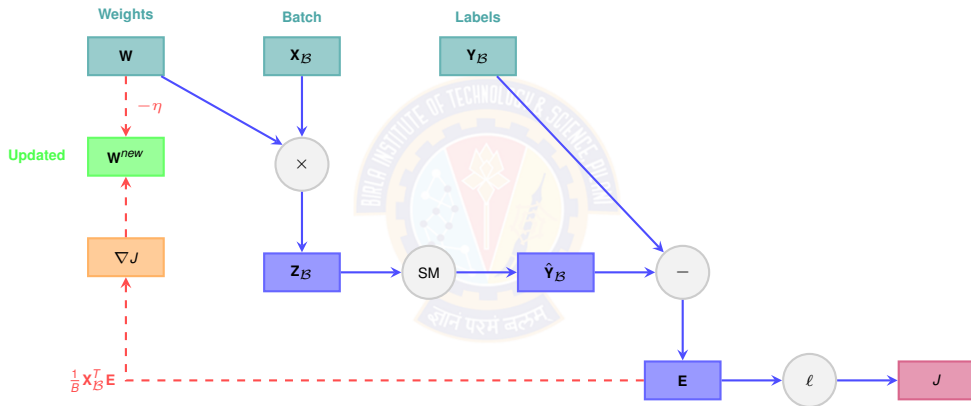
$$\begin{aligned}\mathbf{w}^{(1)} &= \mathbf{w}^{(0)} - \eta \nabla J \\ &= \begin{bmatrix} 0.1 & -0.1 & 0.2 \\ 0.2 & 0.1 & -0.1 \\ -0.1 & 0.2 & 0.1 \end{bmatrix} - 0.1 \begin{bmatrix} -0.167 & -0.154 & 0.320 \\ -0.024 & -0.496 & 0.469 \\ -0.527 & 0.036 & 0.491 \end{bmatrix} \\ &= \begin{bmatrix} 0.117 & -0.085 & 0.168 \\ 0.202 & 0.150 & -0.147 \\ -0.047 & 0.196 & 0.051 \end{bmatrix}\end{aligned}$$

## Progress:

- Weights adjusted based on mini-batch gradient
- Process next mini-batch (examples 3-4) with updated weights
- Continue for multiple epochs until convergence

This completes one iteration of mini-batch SGD!

# COMPUTATIONAL GRAPH FOR MINI-BATCH FORWARD



Mini-batch processes  $B$  examples simultaneously — efficient and stable!

# TABLE OF CONTENTS

## 1 CLASSIFICATION

## 2 BINARY CLASSIFICATION

- Logistic Regression
- The Model: Single Neuron for Binary Classification
- Binary Classification: Worked Example
- Binary Classification: Evaluation Metrics

## 3 MULTI-CLASS CLASSIFICATION

- Multi-class Classification Model
- Mini-batch Stochastic Gradient Descent
- Multiclass Classification: Worked Example
- Making Predictions (Inference)
- Multiclass Classification: Evaluation Metrics

## 4 IMPLEMENTATION TIPS AND DEBUGGING

## 5 SUMMARY



# INFERENCE: MAKING PREDICTIONS

After training, use the model to classify new examples.

Inference process for input  $\mathbf{x}_{\text{new}}$ :

Compute logits:  $\mathbf{z} = \mathbf{W}^T \mathbf{x}_{\text{new}}$  (28)

Apply softmax:  $\hat{\mathbf{y}} = \text{softmax}(\mathbf{z})$  (29)

Predict class:  $\hat{k} = \arg \max_{k=1, \dots, K} \hat{y}_k$  (30)

Optional: Report confidence scores (the probabilities  $\hat{\mathbf{y}}$ )

# INFERENCE EXAMPLE

Trained model with  $K = 3$  classes, new input  $\mathbf{x} = [1, 2.5, 1.8]^T$

Step 1: Compute logits  $\mathbf{z} = \mathbf{W}^T \mathbf{x} = [1.2, 2.5, 0.8]^T$

Step 2: Apply softmax  $e^{1.2} \approx 3.32, \quad e^{2.5} \approx 12.18, \quad e^{0.8} \approx 2.23$

$$\text{Sum} = 3.32 + 12.18 + 2.23 = 17.73$$

$$\hat{\mathbf{y}} = \begin{bmatrix} 3.32/17.73 \\ 12.18/17.73 \\ 2.23/17.73 \end{bmatrix} = \begin{bmatrix} 0.187 \\ 0.687 \\ 0.126 \end{bmatrix}$$

Step 3: Predict class  $\hat{k} = \arg \max_k \hat{y}_k = 2$  (Class 2 with 68.7% confidence)

# TABLE OF CONTENTS

## 1 CLASSIFICATION

## 2 BINARY CLASSIFICATION

- Logistic Regression
- The Model: Single Neuron for Binary Classification
- Binary Classification: Worked Example
- Binary Classification: Evaluation Metrics

## 3 MULTI-CLASS CLASSIFICATION

- Multi-class Classification Model
- Mini-batch Stochastic Gradient Descent
- Multiclass Classification: Worked Example
- Making Predictions (Inference)
- **Multiclass Classification: Evaluation Metrics**

## 4 IMPLEMENTATION TIPS AND DEBUGGING

## 5 SUMMARY

# EVALUATION METRICS FOR MULTI-CLASS

## 1. Accuracy: Overall correctness

$$\text{Accuracy} = \frac{\text{Number of correct predictions}}{N} = \frac{1}{N} \sum_{i=1}^N \mathbb{I}[\hat{y}^{(i)} = y^{(i)}] \quad (31)$$

## 2. Confusion Matrix: $K \times K$ matrix

- Row  $i$ , Column  $j$ : Number of class  $i$  examples predicted as class  $j$
- Diagonal: Correct predictions
- Off-diagonal: Misclassifications

## 3. Per-class Precision and Recall:

- Compute for each class separately (one-vs-all)
- Average across classes (macro-average or weighted average)

# CONFUSION MATRIX FOR MULTI-CLASS

Example: 3-class confusion matrix

		Predicted		
		Class 1	Class 2	Class 3
Actual	Class 1	45	3	2
	Class 2	5	38	7
	Class 3	2	4	44

Interpretation:

- Diagonal (green): Correct predictions (45, 38, 44)
- Off-diagonal (red): Misclassifications
- Row sums: Total actual examples per class (50, 50, 50)
- Column sums: Total predicted examples per class

**Accuracy:**  $(45 + 38 + 44)/150 = 0.847$  or 84.7%

# PER-CLASS METRICS

For each class  $k$ , compute:

**Precision for class  $k$ :** Of all predictions for class  $k$ , what fraction were correct?

$$\text{Precision}_k = \frac{TP_k}{TP_k + FP_k} \quad (32)$$

**Recall for class  $k$ :** Of all actual class  $k$  examples, what fraction did we identify?

$$\text{Recall}_k = \frac{TP_k}{TP_k + FN_k} \quad (33)$$

**F1 Score for class  $k$ :**

$$F1_k = 2 \cdot \frac{\text{Precision}_k \times \text{Recall}_k}{\text{Precision}_k + \text{Recall}_k} \quad (34)$$

# AVERAGING STRATEGIES

How to combine per-class metrics into overall score?

1. **Macro-average**: Simple average across classes

$$\text{Precision}_{\text{macro}} = \frac{1}{K} \sum_{k=1}^K \text{Precision}_k \quad (35)$$

- Treats all classes equally
- Good when classes are equally important

2. **Weighted average**: Weight by class frequency

$$\text{Precision}_{\text{weighted}} = \sum_{k=1}^K w_k \cdot \text{Precision}_k \quad w_k = N_k / N \quad (36)$$

- Accounts for class imbalance
- Good when some classes are more common

# TOP-K ACCURACY

For problems with many classes (e.g., ImageNet with 1000 classes):

Top-K Accuracy: Correct if true class is in top  $K$  predictions

$$\text{Top-K Accuracy} = \frac{1}{N} \sum_{i=1}^N \mathbb{I}[y^{(i)} \in \text{Top-K}(\hat{\mathbf{y}}^{(i)})] \quad (37)$$

Example: Image classification with 1000 classes

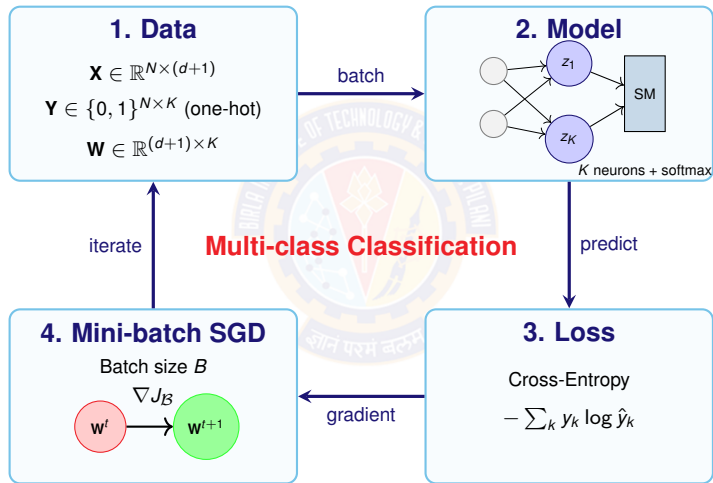
- Top-1 accuracy: Is the highest probability class correct?
- Top-5 accuracy: Is the true class in the top 5 predictions?

Why useful?

- More forgiving metric for large  $K$
- Captures whether model has correct class among top candidates
- Standard in ImageNet challenge



# SUMMARY: MULTICLASS CLASSIFICATION



# TABLE OF CONTENTS

## 1 CLASSIFICATION

## 2 BINARY CLASSIFICATION

- Logistic Regression
- The Model: Single Neuron for Binary Classification
- Binary Classification: Worked Example
- Binary Classification: Evaluation Metrics

## 3 MULTI-CLASS CLASSIFICATION

- Multi-class Classification Model
- Mini-batch Stochastic Gradient Descent
- Multiclass Classification: Worked Example
- Making Predictions (Inference)
- Multiclass Classification: Evaluation Metrics

## 4 IMPLEMENTATION TIPS AND DEBUGGING

## 5 SUMMARY

# IMPLEMENTATION TIPS

- 1. Learning Rate & Epochs:

- ▶ Start:  $\eta \in \{0.01, 0.1, 1.0\}$
- ▶ Typical: 10-100 epochs
- ▶ Use early stopping

- 2. Weight Initialization:

- ▶  $w_j \sim \mathcal{N}(0, 0.01)$
- ▶ Avoid zeros or large values

- 3. Batch Size:

- ▶ Start:  $B \in \{64, 128, 256\}$
- ▶ Powers of 2 preferred
- ▶ Larger: stable, slower
- ▶ Smaller: noisy, faster

- 4. Data Handling:

- ▶ **Always shuffle** each epoch
- ▶ Check class balance

- 5. Feature Scaling: **Essential!**

- ▶ Standardization:  $x'_j = \frac{x_j - \mu_j}{\sigma_j}$
- ▶ Prevents sigmoid saturation

- 6. Numerical Stability:

- ▶ Use:  $\log(\sigma(z))$
- ▶ Stable softmax:  $c = \max_k z_k$
- ▶  $\text{SM}(z)_k = \frac{e^{z_k - c}}{\sum_j e^{z_j - c}}$
- ▶ Log-sum-exp trick
- ▶ Prevents overflow/underflow



# DEBUGGING CHECKLIST

- Loss is NaN/Inf:
  - ▶  $\eta$  too large  $\rightarrow$  decrease
  - ▶ Check  $\log(0)$  in loss
  - ▶ Scale features
  - ▶ Use stable softmax
- Predicts same class:
  - ▶ Check class balance
  - ▶ Verify softmax/loss
  - ▶  $\eta$  might be too small
  - ▶ Verify one-hot encoding
- Loss oscillates:
  - ▶  $\eta$  too large
  - ▶ Use mini-batches
  - ▶ Apply learning rate decay
- Softmax outputs  $\neq 1$ :
  - ▶ Implementation bug
  - ▶ Numerical precision
  - ▶ Use stable softmax
- Loss not decreasing:
  - ▶ Check gradient signs
  - ▶  $\eta$  too small/large
  - ▶ Verify feature scaling
  - ▶ Verify data shuffling
  - ▶ Check one-hot encoding
- High train, low test accuracy:
  - ▶ Overfitting
  - ▶ Add regularization
  - ▶ Get more training data
  - ▶ Simpler model
- Sanity checks:
  - ▶ Tiny dataset  $\rightarrow$  100% accuracy
  - ▶ Verify  $\hat{y} \in [0, 1]$
  - ▶ Verify  $\sum_k \hat{y}_k = 1$
  - ▶ Shuffling improves results
  - ▶ Print confusion matrix

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## 5 SUMMARY

# ACTIVATION FUNCTIONS

Property	Identity	Sigmoid	Softmax
Formula	$f(z) = z$	$\sigma(z) = \frac{1}{1+e^{-z}}$	$\text{SM}(z)_k = \frac{e^{z_k}}{\sum_j e^{z_j}}$
Output Range	$(-\infty, \infty)$	$[0, 1]$	$[0, 1]^K, \sum_k = 1$
Use Case	Regression	Binary classification	Multi-class
# Outputs	1	1	$K$ (coupled)

# LOSS FUNCTIONS

Aspect	MSE	Binary CE	Categorical CE
Formula	$\frac{1}{N} \sum_{i=1}^N (\hat{y}^{(i)} - y^{(i)})^2$	$-\frac{1}{N} \sum_{i=1}^N [y^{(i)} \log \hat{y}^{(i)} + (1 - y^{(i)}) \log(1 - \hat{y}^{(i)})]$	$-\frac{1}{N} \sum_{i=1}^N \sum_{k=1}^K y_k^{(i)} \log \hat{y}_k^{(i)}$
Task	Regression	Binary classification	Multi-class classification
Output Type	Continuous value	Probability (2 classes)	Probability distribution ( $K$ classes)
Target $y$	Real number	$\{0, 1\}$	One-hot vector
Prediction $\hat{y}$	Any real number	Probability $[0, 1]$	Probability vector, $\sum_k \hat{y}_k = 1$
Activation	Identity	Sigmoid	Softmax
Penalizes	Distance from target	Confident wrong predictions	Wrong class probability
Properties	Convex, Quadratic penalty	Convex, Probabilistic, Logarithmic penalty	Convex, Extends binary CE, Multi-class penalty

# GRADIENT DESCENT VARIANTS

Aspect	Batch GD	Stochastic GD	Mini-batch GD
Examples/update	All $N$	1	$B$ (batch size)
Gradient	$\nabla J = \frac{1}{N} \sum_{i=1}^N \nabla \ell_i$	$\nabla \ell_i$ for random $i$	$\nabla J_B = \frac{1}{B} \sum_{i \in B} \nabla \ell_i$
Update rule	$\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla J$	$\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla \ell_i$	$\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla J_B$
Iterations/epoch	1	$N$	$\lceil N/B \rceil$
Speed per iteration	Slow	Fast	Medium
Convergence	Smooth, deterministic	Noisy, oscillating	Balanced
Memory	High (all data)	Low (1 example)	Medium ( $B$ examples)
Gradient quality	Exact	Noisy estimate	Good estimate
Advantages	Stable, Precise gradient, Reproducible	Fast iterations, Online learning, Escapes local minima	<b>Best balance</b> , GPU efficient, Stable & fast
Disadvantages	Slow for large $N$ , High memory, NO online	Very noisy, Unstable, Hard to parallelize	Extra hyperparameter ( $B$ ), Needs tuning
Best for	Small datasets	Online learning	<b>Deep learning (std)</b>
Typical $B$	$N$ (all data)	1	32, 64, 128, 256



# COMPARISON OF LINEAR MODELS

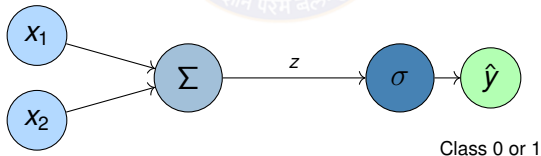
Aspect	Regression	Binary	Multi-class
Output	Continuous $y \in \mathbb{R}$	Discrete $y \in \{0, 1\}$	Discrete $y \in \{1, \dots, K\}$
Activation	Identity: $f(z) = z$	Sigmoid: $\sigma(z)$	Softmax: $\text{SM}(\mathbf{z})$
Loss Function	Mean Squared Error	Binary Cross-Entropy	Categorical Cross-Entropy
Output Range	$(-\infty, \infty)$	$[0, 1]$	$[0, 1]^K, \sum_k = 1$
Interpretation	Predicted value	$P(y = 1 \mathbf{x})$	$P(y = k \mathbf{x})$ for all $k$
Output neurons	1	1	$K$
Weights	Vector $\mathbf{w} \in \mathbb{R}^{d+1}$	Vector $\mathbf{w} \in \mathbb{R}^{d+1}$	Matrix $\mathbf{W} \in \mathbb{R}^{(d+1) \times K}$
Evaluation	MSE, RMSE, $R^2$	Accuracy, Precision, Recall, F1	Confusion matrix, Top-K
Learning	Batch GD or SGD	SGD or Mini-batch	Mini-batch SGD
Examples	House prices, temperature	Spam detection, diagnosis	Digit recognition, ImageNet

# RECAP: BINARY CLASSIFICATION

## LOGISTIC REGRESSION

**Key insight:** Sigmoid maps linear combination to probability; optimized by minimizing cross-entropy loss.

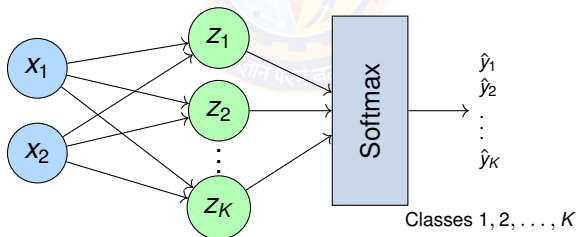
- **Problem:** Classify into two classes:  $y \in \{0, 1\}$
- **Model:** Single neuron with sigmoid activation
- **Output:** Probability  $\hat{y} = P(y = 1|\mathbf{x}) \in [0, 1]$
- **Loss:** Binary cross-entropy
- **Training:** Stochastic Gradient Descent (SGD)



# RECAP: MULTI-CLASS CLASSIFICATION

**Key insight:** Multiple outputs coupled through softmax create valid probability distribution over all classes.

- **Problem:** Classify into  $K$  classes:  $y \in \{1, 2, \dots, K\}$
- **Model:**  $K$  output neurons with softmax activation
- **Output:** Probability distribution  $\hat{\mathbf{y}} = [\hat{y}_1, \dots, \hat{y}_K]^T$ , where  $\sum_{k=1}^K \hat{y}_k = 1$
- **Loss:** Categorical cross-entropy
- **Training:** Mini-batch Stochastic Gradient Descent



# REFERENCES

- Zhang, A., Lipton, Z. C., Li, M., & Smola, A. J. (2023). *Dive into Deep Learning*. Cambridge University Press. Chapter 4 (Linear Neural Networks for Classification). <https://d2l.ai/>
- Goodfellow, I., Bengio, Y., & Courville, A. (2016). *Deep Learning*. MIT Press. Chapter 6 (Deep Feedforward Networks). <https://www.deeplearningbook.org/>
- Bishop, C. M. (2006). *Pattern Recognition and Machine Learning*. Springer. Chapter 4 (Linear Models for Classification).
- Murphy, K. P. (2022). *Probabilistic Machine Learning: An Introduction*. MIT Press. Chapter 10 (Logistic Regression). <https://probml.github.io/pml-book/>

# Thank You!