Machine Learning Methods for Supervised Single-Label and Multi-Label Classification

A Foundational Workshop for Education & Social Science Researchers

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Workshop Roadmap

What is Machine Learning?

Traditional Programming:

$$\text{Rules} + \text{Data} \rightarrow \text{Answers}$$

Machine Learning:

$$\text{Data} + \text{Answers} \rightarrow \text{Rules}$$

Instead of telling the computer *how* to classify, we show it *examples* and let it learn the patterns.

The Big Picture: Supervised vs. Unsupervised

Supervised Learning

- **Input:** Features (X) + Labels (Y)
- **Goal:** Learn mapping $f(X) \to Y$
- **Example:** Predicting student pass/fail
- **When:** You have labeled training data

Unsupervised Learning

- **Input:** Features only (X)
- **Goal:** Discover hidden structure
- **Example:** Grouping students by behavior
- **When:** No labels available

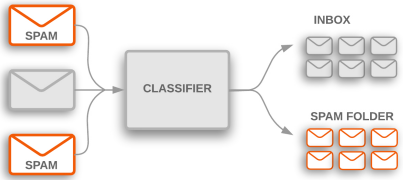
Key Question: Do you know the answer you're looking for?

Why Classification Matters

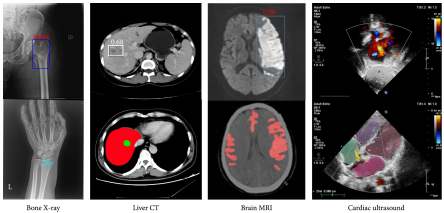
Classification helps us make sense of data by predicting known categories or discovering hidden ones.

Real-World Examples

- **Spam Detection:** Classifying emails as "Spam" vs. "Not Spam".
- **Healthcare:** Diagnosing disease from medical images.
- **Education:** Identifying at-risk students for early intervention.



Email Classification



Medical Diagnosis

Labels Define the Task

The structure of your target variable (Y) determines the model you need.

Binary Classification

One label, two classes (0 or 1)
Example: Pass vs. Fail, Spam vs. Not Spam

Multi-Class Classification

One label, 3+ mutually exclusive classes
Example: Grades (A, B, C, D, F), Iris Species (Setosa, Versicolor, Virginica)

Multi-Label Classification

Multiple labels simultaneously
Example: Movie genres (Comedy **AND** Action), Image tags (Cow **AND** Barn)

Multi-label is fundamentally different and requires special handling!

Visualizing Multi-Label Classification

Consider an image classification task. A single photo can contain:

- A Cow
- A Barn
- Grass
- Sky

Key Concept: These are not mutually exclusive. We need a model that can predict:

$$P(\text{Cow}) > 0.5 \quad \text{AND} \quad P(\text{Barn}) > 0.5$$

Multiple labels can apply simultaneously

From Problem to Evaluation

Different problems need different metrics:

Binary/Multi-Class: Single prediction per observation
$\rightarrow$ Confusion matrix, accuracy, precision, recall

Multi-Label: Multiple predictions per observation
$\rightarrow$ Hamming loss, subset accuracy, F1 per label

Today's focus: Binary and multi-class metrics
(Multi-label evaluation is covered in the Colab session)

The Confusion Matrix

A 2×2 table for binary classification showing predictions vs. actual values:

		Predicted	
		Negative	Positive
Actual	Negative	TN	FP
	Positive	FN	TP

- **True Positive (TP):** Correctly identified positive cases
- **True Negative (TN):** Correctly identified negative cases
- **False Positive (FP):** Type I error (false alarm)
- **False Negative (FN):** Type II error (missed case)

Key Evaluation Metrics

Metric	Formula
Accuracy	$(TP + TN)/(TP + TN + FP + FN)$
Precision	$TP/(TP + FP)$
Recall	$TP/(TP + FN)$
F1 Score	$2 \times [(\text{Precision} \times \text{Recall})/(\text{Precision} + \text{Recall})]$

Choosing the Right Metric: Examples

Scenario 1: Email Spam Detection (99% not spam)

- Accuracy can be misleading (always predicting "not spam" = 99% accurate!)
- Use **Precision** (avoid flagging legitimate emails) and **Recall** (catch actual spam)

Scenario 2: Cancer Screening

- Prioritize **Recall** (don't miss any cases)
- Accept lower precision (false positives can be resolved with follow-up tests)

Scenario 3: Student Pass/Fail (balanced classes)

- **Accuracy** is fine
- Check **F1 Score** to ensure both classes perform well

Logistic Regression (The Baseline)

Type: Supervised, Linear Classifier.

Mechanism

Estimates probability of class membership using the sigmoid function:

$$P(y = 1|\mathbf{x}) = \frac{1}{1 + e^{-z}} \quad \text{where} \quad z = \beta_0 + \beta_1 x_1 + \dots$$

- **Decision Boundary:** Linear (draws a line/plane to separate groups).
- **Pros:** Fast and interpretable.
- **Cons:** Struggles with complex, non-linear boundaries.

Visualizing Logistic Regression

The Sigmoid Function:

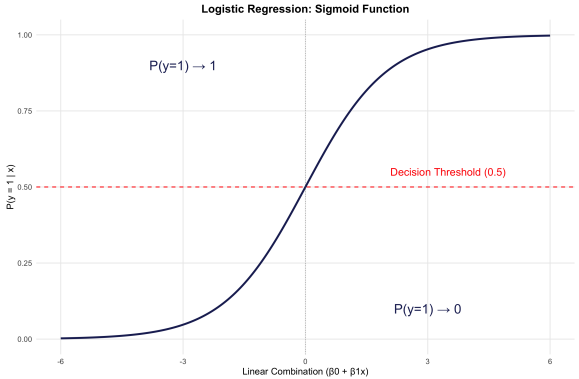
$$P(y = 1|x) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x)}}$$

Key Properties:

- Output: Probability (0 to 1)
- S-shaped curve
- Decision boundary at 0.5

Interpretation:

- $P > 0.5 \rightarrow$ Predict class 1
- $P < 0.5 \rightarrow$ Predict class 0



Multinomial Logistic Regression

Use Case: Multi-Class Classification (> 2 classes).

The Softmax Function

Instead of a single probability, we calculate probabilities for all classes that sum to 1.

$$\sum P(y = k|\mathbf{x}) = 1.0$$

- The model estimates one set of coefficients per class (relative to a reference).
- Decision Rule: Choose the class with the highest probability ($\arg\max P$).

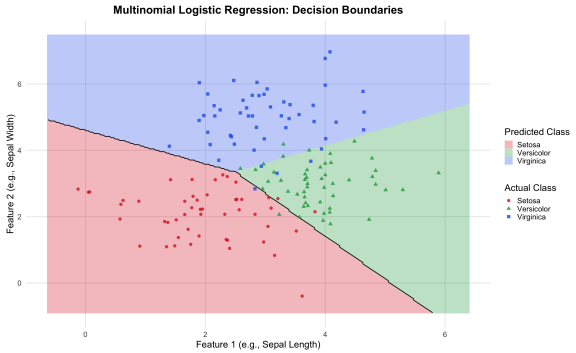
Visualizing Multinomial Logistic Regression

Multiple Decision Boundaries
Unlike binary classification, we now need to separate **3+ classes**.

Example: Iris Species

- Setosa (red)
- Versicolor (green)
- Virginica (blue)

Each region represents where one class has the **highest probability**.



Logistic Regression: When and Why?

Use logistic regression when:

- You need to **interpret** results (which features matter?)
- You have **limited data** (works with small samples)
- Features have **linear relationships** with the log-odds
- You need **fast training and prediction**

Real-world applications:

- Credit scoring (explain why someone was denied)
- Medical diagnosis (interpretable risk factors)
- Social science research (theory testing)

Start here as your baseline model!

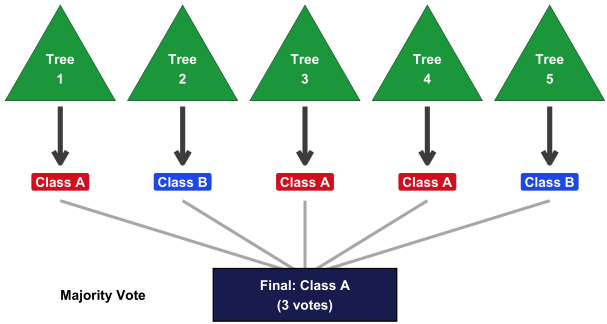
Random Forest (Ensemble Method)

Concept: Combine multiple "weak" decision trees to create one "strong" predictor.

How it works:

1. Randomly sample observations (Bootstrap).
2. Train a tree, but randomly select a subset of features at each split.
3. Aggregate results (Majority Vote).

Pros: Handles non-linear relationships well; very stable.



Random Forest vs. Logistic Regression

Characteristic	Logistic Regression	Random Forest
Interpretability	High	Low
Handles non-linearity	No	Yes
Feature interactions	Manual	Automatic
Training time	Fast	Slower
Overfitting risk	Low	Medium (with tuning)
Works with missing data	No	Yes (under specific conditions)
Typical accuracy	Good	Better

Rule of thumb: Start with logistic regression for interpretability, move to Random Forest for better predictive performance.

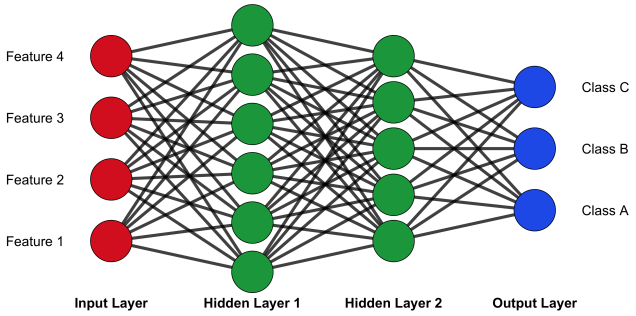
Neural Networks (Deep Learning)

Structure:

- Input Layer (X)
- Hidden Layers (Learn shared patterns)
- Output Layer (Y)

Why use them?

- Captures highly complex, non-linear patterns.
- Can model correlated labels (e.g., if "barn" is present, "grass" is likely present).



Neural Networks for Binary Classification

The Setup

- **Output Structure:** A **single** output neuron.
- **Activation Function:** Sigmoid (σ).
- **Goal:** Predict probability of the positive class ($P(y = 1|X)$).

The Mechanism

- The network maps the final output into a range of $[0, 1]$.
- **Formula:** $\hat{y} = \frac{1}{1+e^{-z}}$

Decision Rule

- We apply a **threshold** (usually 0.5) to classify.
- If $P(y = 1) \geq 0.5 \rightarrow$ Predict Class 1
- If $P(y = 1) < 0.5 \rightarrow$ Predict Class 0

The "Logistic" Connection

This is essentially **Logistic Regression**, but the "features" fed into the final layer are learned by the hidden layers rather than being raw inputs.

Neural Networks for Multi-Class and Multi-Label Tasks

The key difference is in the **Output Layer**.

Multi-Class Classification

- Uses **Softmax** activation
- Probabilities **compete** with each other
- All probabilities sum to 1
- $\sum_{k=1}^{K} P(y = k) = 1.0$

Example:

- $P(\text{Setosa}) = 0.7$
- $P(\text{Versicolor}) = 0.2$
- $P(\text{Virginica}) = 0.1$

Choose one class with highest probability

Multi-Label Classification

- Uses independent **Sigmoids**
- Each label predicted **independently**
- Probabilities don't need to sum to 1
- Each $P(\text{label}) \in [0, 1]$

Example:

- $P(\text{Cow}) = 0.9$
- $P(\text{Barn}) = 0.8$
- $P(\text{Sky}) = 0.1$

Multiple labels can be true simultaneously

When Do You NEED Neural Networks?

Neural networks are usually not needed UNLESS you have:

1. **Unstructured data:** Images, text, audio, video
2. **Very large datasets:** 10,000+ and/or high-dimensional
3. **Complex multi-label tasks:** Correlated labels
4. **Non-linear feature interactions:** That simpler models can't capture

For education/social science research with tabular data:

- Random Forest usually performs as well or better
- Much easier to tune and interpret
- Faster to train on small-medium datasets

Don't use neural networks just because they're trendy!

Shifting Gears: Unsupervised Learning

Everything so far assumed labeled data...

But what if you:

- Don't know what categories exist?
- Want to discover natural groupings?
- Have no labels (too expensive/time-consuming to create)?

Enter: Clustering algorithms

Common research questions:

- Are there distinct types of learners in my classroom?
- Do survey responses cluster into meaningful groups?
- Can I identify subtypes of a phenomenon?

When We Don't Have Labels

Goal: Develop a model that reveals hidden structures or patterns.

- We don't know the categories in advance.
- We want to see what groups "look like".

Common Algorithms:

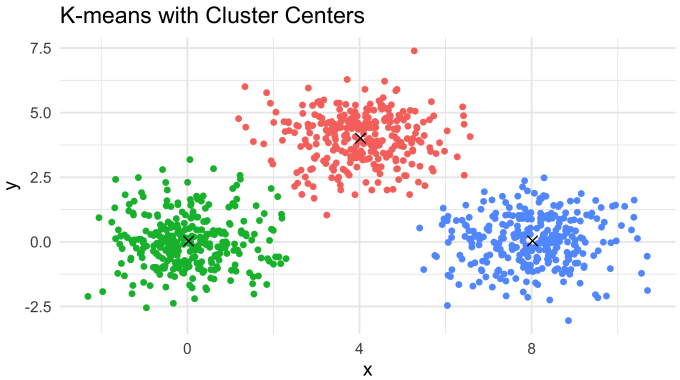
- K-Means Clustering.
- Hierarchical Clustering.
- Gaussian Mixture Models.

K-Means Clustering

Algorithm:

1. Specify K (number of groups)
2. Randomly place K centroids
3. Assign each point to nearest centroid
4. Update centroids to mean of assigned points
5. Repeat steps 3-4 until convergence

Pros: Fast, scalable, simple
Cons: Must choose K; sensitive to outliers; assumes spherical clusters; Sensitive to scale (features must be standardized)



Beyond K-Means: Other Clustering Methods

Hierarchical Clustering

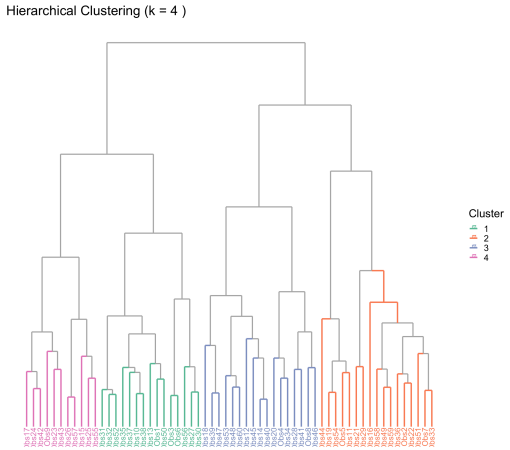
- Creates a tree (dendrogram) of nested clusters
- Can cut tree at different levels

DBSCAN (Density-Based)

- Finds arbitrarily shaped clusters
- Identifies outliers

Gaussian Mixture Models

- Probabilistic clustering (soft assignments)
- Models clusters as overlapping distributions



Which Model Should You Use?

Scenario	Model	Data Size	Interpretable?
Binary/multi-class, need explanation	Logistic Reg.	Small-Large	Yes
Tabular, high accuracy needed	Random Forest	Medium-Large	No
Images, text, complex multi-label	Neural Network	Large	No
No labels, explore structure	K-Means	Any	N/A
Non-spherical clusters	DBSCAN	Medium	N/A

Recommended workflow:

1. Start simple (Logistic Regression)
2. Try Random Forest for better performance
3. Only use Neural Networks if you have sufficient data/complexity

Practical Tips for Research

Before you start:

- Define your research question clearly
- Ensure you have enough data (rule of thumb: 10+ samples per feature)
- Split data: Train (60%), Validation (20%), Test (20%)

During model building:

- Always establish a baseline (e.g., logistic regression)
- Use cross-validation to avoid overfitting
- Check for class imbalance

Common pitfalls to avoid:

- Testing on training data (data leakage!)
- Ignoring class imbalance
- Over-interpreting small accuracy improvements

Feature Scaling and Standardization

Many machine learning algorithms are **sensitive to the scale of your features**.

Why this matters:

- Variables measured on larger scales can dominate the model
- Distance-based methods are especially affected
- Coefficients and regularization depend on scale

Algorithms that REQUIRE scaling:

- K-Means clustering
- K-Nearest Neighbors (KNN)
- Support Vector Machines (SVM)
- Logistic Regression (with regularization)
- Neural Networks

Common approaches:

- **Standardization (Z-score):** $(x - \mu)/\sigma$
- **Min-Max Scaling:** Rescale to [0, 1]

Ready for Hands-On Practice!

What's Next:

Google Colab Session

- Implement logistic regression, random forest, and neural networks
- Compare performance on real datasets
- Explore multi-label classification
- Try K-means clustering

Resources:

- Slides & code: [your link]

Questions after the workshop?

email: yalequan@uw.edu