

## L02: Logistic Regression

### Mathematical Foundations and Implementation

Methods and Algorithms – MSc Data Science

## The Classification Problem

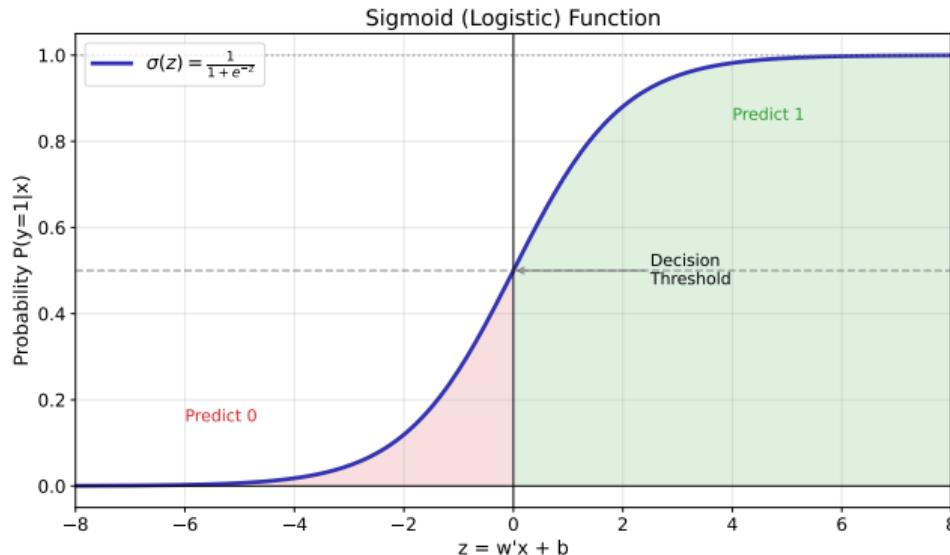
- Given features  $\mathbf{x} \in \mathbb{R}^p$ , predict  $y \in \{0, 1\}$
- Linear regression:  $\hat{y} = \mathbf{w}^T \mathbf{x} + b$  (unbounded)
- Need:  $P(y = 1|\mathbf{x}) \in [0, 1]$

## Solution: The Logistic Function

$$P(y = 1|\mathbf{x}) = \sigma(\mathbf{w}^T \mathbf{x} + b) = \frac{1}{1 + e^{-(\mathbf{w}^T \mathbf{x} + b)}}$$

The logistic function is also called the sigmoid function

# The Sigmoid Function



## Key Properties:

- Range:  $(0, 1)$  – perfect for probabilities
- $\sigma(0) = 0.5$  – threshold for classification
- $\sigma'(z) = \sigma(z)(1 - \sigma(z))$  – simple gradient

## Understanding the Model

- Odds:  $\frac{P(y=1)}{P(y=0)} = \frac{p}{1-p}$
- Log-odds (logit):  $\log\left(\frac{p}{1-p}\right) = \mathbf{w}^T \mathbf{x} + b$

## Coefficient Interpretation

- $w_j$ : change in log-odds per unit increase in  $x_j$
- $e^{w_j}$ : odds ratio – multiplicative effect on odds
- Example:  $w_{\text{income}} = 0.5 \Rightarrow$  each unit increase in income multiplies odds by  $e^{0.5} \approx 1.65$

Log-odds interpretation is key for regulatory compliance in banking

## The Likelihood Function

For observations  $(x_i, y_i)$ , the likelihood is:

$$L(\mathbf{w}) = \prod_{i=1}^n p_i^{y_i} (1 - p_i)^{1-y_i}$$

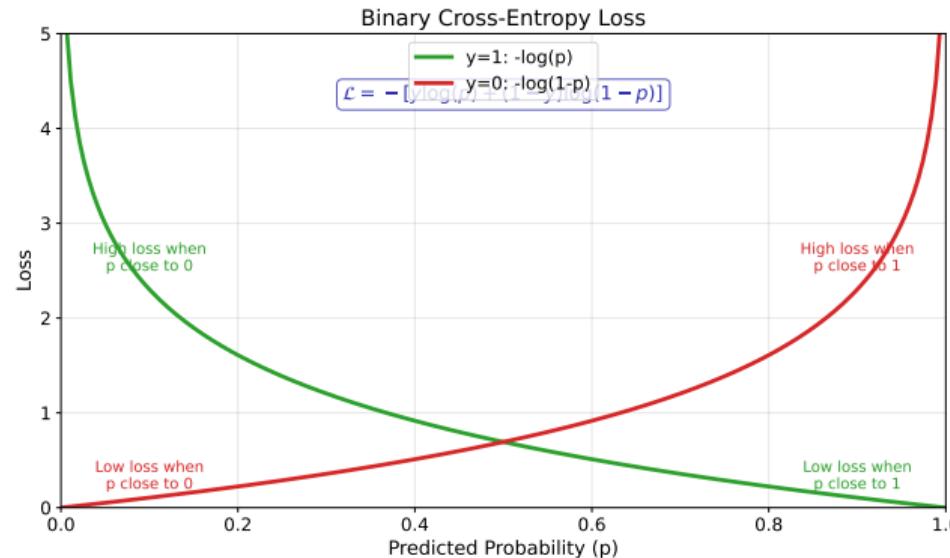
where  $p_i = \sigma(\mathbf{w}^T \mathbf{x}_i + b)$

## Log-Likelihood (easier to optimize)

$$\ell(\mathbf{w}) = \sum_{i=1}^n [y_i \log(p_i) + (1 - y_i) \log(1 - p_i)]$$

Maximize log-likelihood = minimize negative log-likelihood (cross-entropy)

# Binary Cross-Entropy Loss



## Loss Function

$$\mathcal{L} = -\frac{1}{n} \sum_{i=1}^n [y_i \log(p_i) + (1-y_i) \log(1-p_i)]$$

Cross-entropy loss is convex in the weights – guaranteed global optimum

# Gradient Derivation

## Computing the Gradient

For a single sample:

$$\frac{\partial \mathcal{L}}{\partial w_j} = (p - y)x_j$$

## In Matrix Form

$$\nabla_w \mathcal{L} = \frac{1}{n} \mathbf{X}^T (\mathbf{p} - \mathbf{y})$$

where  $\mathbf{p} = \sigma(\mathbf{X}\mathbf{w})$

**Key Insight:** Same form as linear regression gradient!

The elegance of logistic regression: gradient has the same form as linear regression

# Gradient Descent Update

## Update Rule

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \nabla_{\mathbf{w}} \mathcal{L}$$

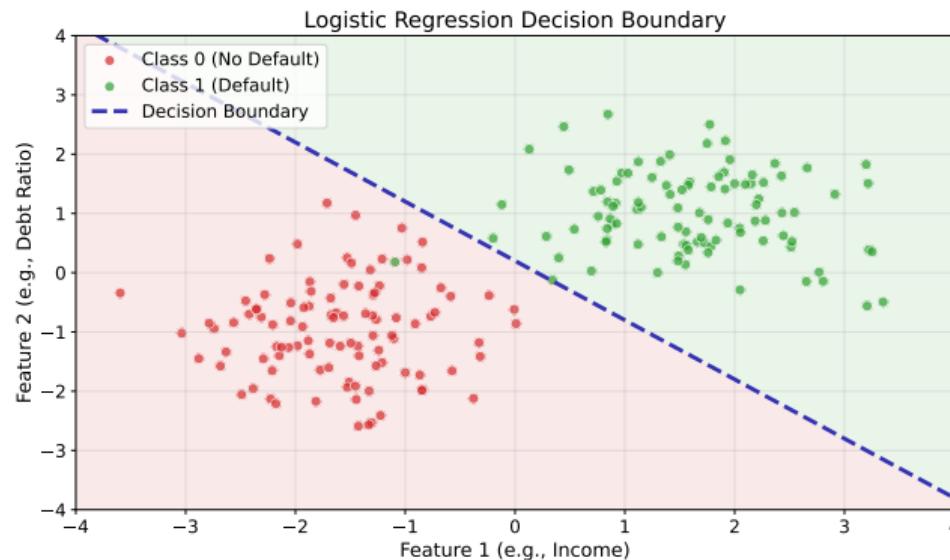
$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \frac{\eta}{n} \mathbf{X}^T (\sigma(\mathbf{X}\mathbf{w}^{(t)}) - \mathbf{y})$$

## Practical Considerations

- Feature scaling: standardize inputs for faster convergence
- Learning rate: start with  $\eta = 0.01$ , use line search or decay
- Convergence: monitor loss, check gradient norm ; tolerance

No closed-form solution like normal equation – must use iterative optimization

# Linear Decision Boundary



**Decision Rule:** Predict  $\hat{y} = 1$  if  $\mathbf{w}^T \mathbf{x} + b \geq 0$

The decision boundary is always a hyperplane in the feature space

# Threshold Selection

## Default Threshold: 0.5

- Predict 1 if  $P(y = 1|x) \geq 0.5$
- Equivalent to:  $\mathbf{w}^T \mathbf{x} + b \geq 0$

## Custom Thresholds

- Lower threshold: more sensitive (higher recall)
- Higher threshold: more specific (higher precision)
- Choose based on business costs of FP vs FN

## Example: Fraud Detection

- Cost of missing fraud (FN)  $\ll$  Cost of false alarm (FP)
- Use lower threshold, e.g., 0.3

Optimal threshold depends on the cost matrix of your application

## Polynomial Features

- Original:  $[x_1, x_2]$
- Expanded:  $[x_1, x_2, x_1^2, x_2^2, x_1x_2]$
- Creates curved decision boundaries

## Trade-offs

- More features: more flexible boundaries
- Risk: overfitting to training data
- Solution: regularization

Logistic regression is linear in parameters, but can model non-linear boundaries

## One-vs-Rest (OvR)

- Train  $K$  binary classifiers
- Predict class with highest probability

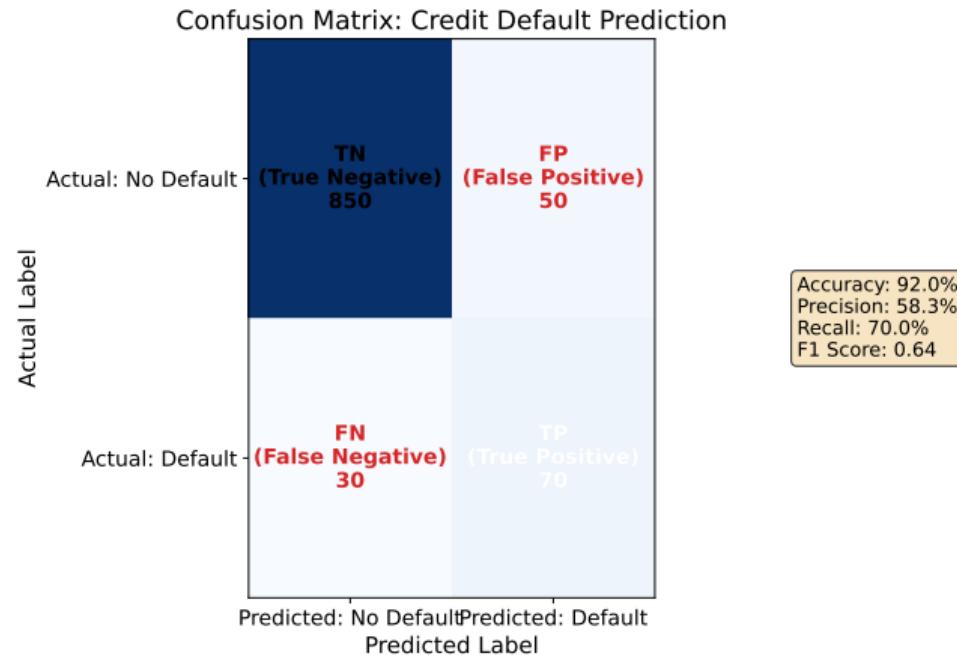
## Multinomial (Softmax) Logistic Regression

$$P(y = k|x) = \frac{e^{\mathbf{w}_k^T \mathbf{x}}}{\sum_{j=1}^K e^{\mathbf{w}_j^T \mathbf{x}}}$$

- Single model, probabilities sum to 1
- Loss: categorical cross-entropy

scikit-learn: multi\_class='multinomial' for true softmax regression

# Confusion Matrix



Always start evaluation by examining the confusion matrix

## From the Confusion Matrix

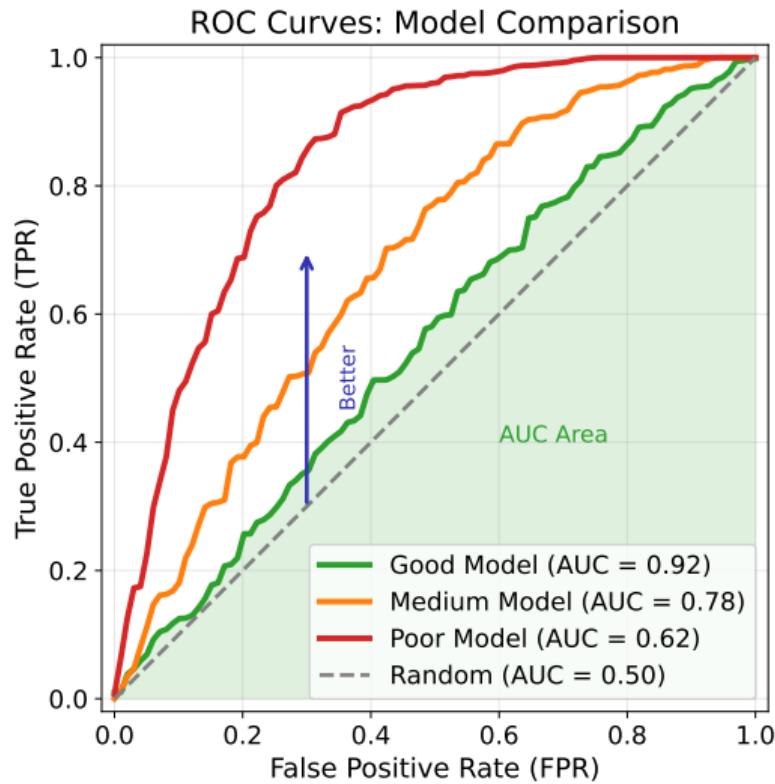
- **Accuracy:**  $\frac{TP+TN}{TP+TN+FP+FN}$  – overall correctness
- **Precision:**  $\frac{TP}{TP+FP}$  – of predicted positives, how many correct?
- **Recall:**  $\frac{TP}{TP+FN}$  – of actual positives, how many found?
- **F1 Score:**  $\frac{2 \cdot \text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$

## When Accuracy Fails

- Imbalanced data: 99% negative class
- Predicting all negatives gives 99% accuracy!

Accuracy is misleading for imbalanced datasets

# ROC Curve



ROC = Receiver Operating Characteristic: X-axis FPR, Y-axis TPR

# Area Under ROC (AUC)

## Interpretation

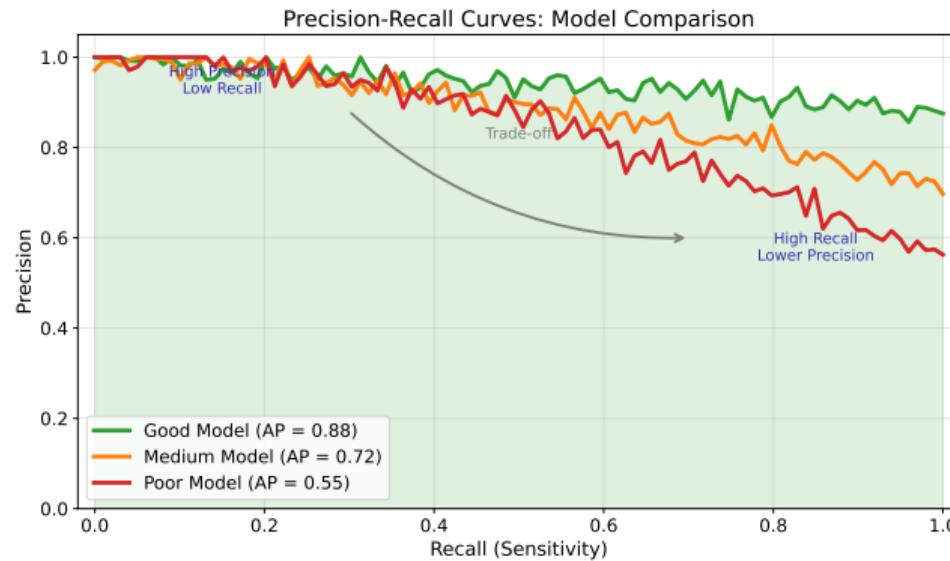
- AUC = 0.5: random guessing
- AUC = 1.0: perfect classifier
- AUC = probability(random positive  $\neq$  random negative)

## Guidelines

- 0.9–1.0: Excellent
- 0.8–0.9: Good
- 0.7–0.8: Fair
- 0.6–0.7: Poor
- 0.5–0.6: Fail

AUC is threshold-independent – summarizes performance across all thresholds

# Precision-Recall Curve



Use PR curves for imbalanced datasets where positive class is rare

# ROC vs Precision-Recall

## When to Use ROC

- Balanced classes
- Care equally about both classes
- Comparing models at specific FPR

## When to Use Precision-Recall

- Imbalanced classes (fraud, disease)
- Positive class is more important
- High precision required

ROC can be overly optimistic with imbalanced data

## What is Calibration?

- Predicted 70% probability should mean 70% actually positive
- Well-calibrated: predicted probabilities match observed frequencies

## Checking Calibration

- Reliability diagram (calibration plot)
- Brier score:  $\frac{1}{n} \sum (p_i - y_i)^2$

## Logistic Regression Advantage

- Naturally well-calibrated (MLE property)
- Unlike trees/random forests that may need calibration

Calibration is crucial when probabilities are used for decision-making

## The Overfitting Problem

- Many features, limited data
- Model fits noise, not signal
- Perfect training accuracy, poor test performance

## Solution: Penalize Large Coefficients

$$\mathcal{L}_{\text{regularized}} = \mathcal{L} + \lambda \cdot \text{penalty}(\mathbf{w})$$

- $\lambda$ : regularization strength (hyperparameter)
- Larger  $\lambda$  = simpler model

Regularization trades bias for variance

# L1 vs L2 Regularization

## L2 (Ridge)

$$\mathcal{L}_{\text{Ridge}} = \mathcal{L} + \lambda \sum_{j=1}^p w_j^2$$

- Shrinks coefficients toward zero
- Keeps all features, reduces magnitude

## L1 (Lasso)

$$\mathcal{L}_{\text{Lasso}} = \mathcal{L} + \lambda \sum_{j=1}^p |w_j|$$

- Some coefficients exactly zero
- Automatic feature selection

L1 for sparse models, L2 when all features likely relevant

# Elastic Net

## Best of Both Worlds

$$\mathcal{L}_{\text{ElasticNet}} = \mathcal{L} + \lambda_1 \sum |w_j| + \lambda_2 \sum w_j^2$$

## Advantages

- Handles correlated features better than Lasso alone
- Can select groups of correlated features
- More stable feature selection

## In scikit-learn

- `LogisticRegression(penalty='elasticnet', solver='saga', l1_ratio=0.5)`

Elastic Net: `l1_ratio = 1` is pure L1, `l1_ratio = 0` is pure L2

# Choosing $\lambda$

## Cross-Validation

- Try grid of  $\lambda$  values: [0.001, 0.01, 0.1, 1, 10, 100]
- Use k-fold CV to estimate test performance
- Select  $\lambda$  with best CV score

## scikit-learn Convenience

- LogisticRegressionCV: automatic  $\lambda$  search
- Cs: inverse of  $\lambda$  (larger C = less regularization)

LogisticRegressionCV does cross-validation internally

## Algorithm: Gradient Descent

```
1: Input:  $\mathbf{X}$ ,  $\mathbf{y}$ , learning rate  $\eta$ , max iterations  $T$ 
2: Initialize  $\mathbf{w} = \mathbf{0}$ 
3: for  $t = 1$  to  $T$  do
4:    $\mathbf{p} = \sigma(\mathbf{X}\mathbf{w})$ 
5:    $\nabla = \frac{1}{n}\mathbf{X}^T(\mathbf{p} - \mathbf{y})$ 
6:    $\mathbf{w} = \mathbf{w} - \eta\nabla$ 
7:   if  $\|\nabla\| < \epsilon$  then
8:     break
9:   end if
10: end for
11: return  $\mathbf{w}$ 
```

In practice, use quasi-Newton methods (L-BFGS) for faster convergence

## Basic Usage

- `from sklearn.linear_model import LogisticRegression`
- `model = LogisticRegression()`
- `model.fit(X_train, y_train)`
- `y_pred = model.predict(X_test)`
- `y_proba = model.predict_proba(X_test)`

## Key Parameters

- `C: inverse regularization strength (default=1.0)`
- `penalty: 'l1', 'l2', 'elasticnet', 'none'`
- `solver: 'lbfgs', 'liblinear', 'saga'`
- `class_weight: 'balanced' for imbalanced data`

`predict_proba` returns  $[P(y=0), P(y=1)]$  – use `[:, 1]` for positive class

# Handling Class Imbalance

## The Problem

- 99% negatives, 1% positives
- Model predicts all negatives: 99% accuracy!

## Solutions

- **Class weights:** `class_weight='balanced'`
- **Oversampling:** SMOTE, random oversampling
- **Undersampling:** random undersampling
- **Threshold tuning:** optimize for F1 or business metric

## Weighted Loss

$$\mathcal{L}_{\text{weighted}} = - \sum_i w_{y_i} [y_i \log p_i + (1 - y_i) \log(1 - p_i)]$$

`class_weight='balanced'` sets  $w_k \propto 1/n_k$

## For Logistic Regression

- **Standardization:** mean=0, std=1 for all features
- **Missing values:** impute or create indicator variable
- **Categorical:** one-hot encoding (drop one level)
- **Interactions:**  $x_1 \times x_2$  if domain suggests
- **Non-linearity:** binning or polynomial features

## Credit Scoring Example

- Age: may have non-linear effect (bin into groups)
- Debt-to-income ratio: interaction of two features
- Employment length: indicator for  $\geq 2$  years

Feature engineering often matters more than model selection

## Coefficient Analysis

- Sign: direction of effect
- Magnitude: strength (after standardization)
- Odds ratio  $e^{w_j}$ : multiplicative effect

## Example Interpretation

- $w_{\text{income}} = 0.5$ : each \$1000 income increase multiplies odds of approval by  $e^{0.5} = 1.65$
- $w_{\text{debt\_ratio}} = -1.2$ : each 0.1 increase in debt ratio multiplies odds by  $e^{-0.12} = 0.89$  (11% decrease)

This interpretability makes logistic regression preferred in regulated industries

## Available Solvers in scikit-learn

- `lbfgs`: default, works for L2 and no penalty
- `liblinear`: fast for small data, supports L1
- `saga`: supports all penalties, works for large data
- `newton-cg`: similar to `lbfgs`
- `sag`: stochastic, for very large data

## Guidelines

- L1 penalty: use `liblinear` or `saga`
- Large data: `saga` or `sag`
- Default (L2): `lbfgs`

`solver='saga'` is the most versatile but may be slower for small datasets

## Warning: “Convergence Warning”

- Model did not converge in max\_iter iterations
- May mean poor solution

## Solutions

- Increase max\_iter (default=100)
- Standardize features
- Increase regularization (smaller C)
- Use different solver

Always check for convergence warnings in production code

## Strengths of Logistic Regression

- Interpretable coefficients
- Well-calibrated probabilities
- Fast training and prediction
- Works well with few samples

## Limitations

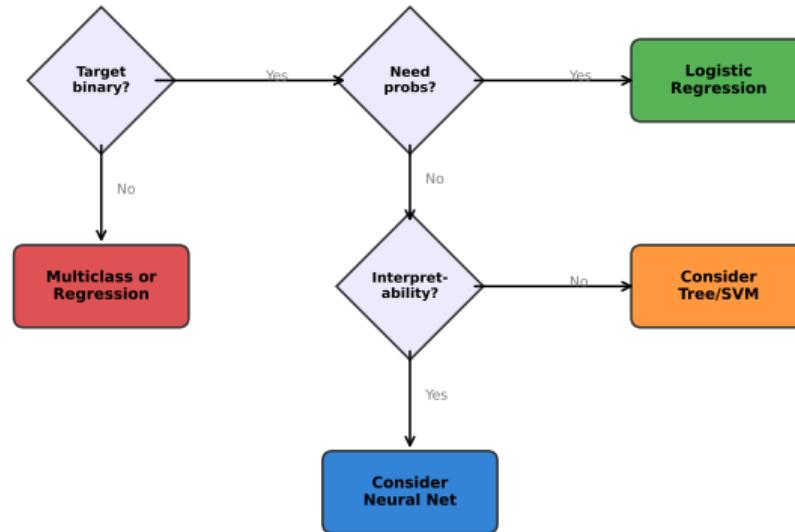
- Linear decision boundary
- May underfit complex patterns
- Sensitive to outliers (compared to trees)

## When to Choose Alternatives

- Complex patterns: Random Forests, Gradient Boosting
- High-dimensional: SVM with RBF kernel
- Interpretability not required: Neural Networks

Start with logistic regression as baseline, then try more complex models

## Logistic Regression Decision Guide



Logistic regression: first choice for binary classification with interpretability

# Key Takeaways

## Mathematical Foundation

- Sigmoid function maps linear combination to probability
- Maximum likelihood estimation via gradient descent
- Cross-entropy loss is convex, guaranteed global optimum

## Evaluation

- Use confusion matrix, precision, recall, F1
- ROC/AUC for balanced data, PR curve for imbalanced
- Calibration matters when using probabilities

## Practice

- Regularization prevents overfitting
- Class weights handle imbalance
- Coefficients are directly interpretable

Logistic regression: simple, fast, interpretable, and often competitive

## Textbooks

- James et al. (2021). *ISLR*, Chapter 4: Classification
- Hastie et al. (2009). *ESL*, Chapter 4: Linear Methods

## Documentation

- scikit-learn: LogisticRegression user guide
- statsmodels: Logit for statistical inference

## Next Lecture

- L03: KNN and K-Means
- From parametric to non-parametric methods