

Week 0b: Supervised Learning

The Prediction Challenge

Machine Learning for Smarter Innovation

BSc Innovation & Design Thinking

1 Part 1: The Challenge

2 Part 2: Linear + Regularization

3 Part 3: Nonlinear Methods

4 Part 4: Synthesis

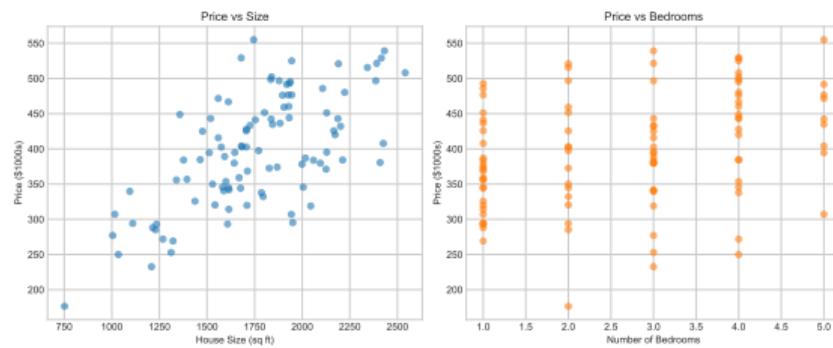
1. Real Estate Price Prediction

The Business Problem

- Predict house prices from features
- Features: size, bedrooms, location, age
- Target: price in thousands
- Training data: 10,000 historical sales

Size	Beds	Age	Price
1200	2	5	250k
2500	4	10	450k
1800	3	2	380k

Sample Data Points



Supervised learning transforms labeled examples into predictive models - regression predicts continuous values from multiple correlated features

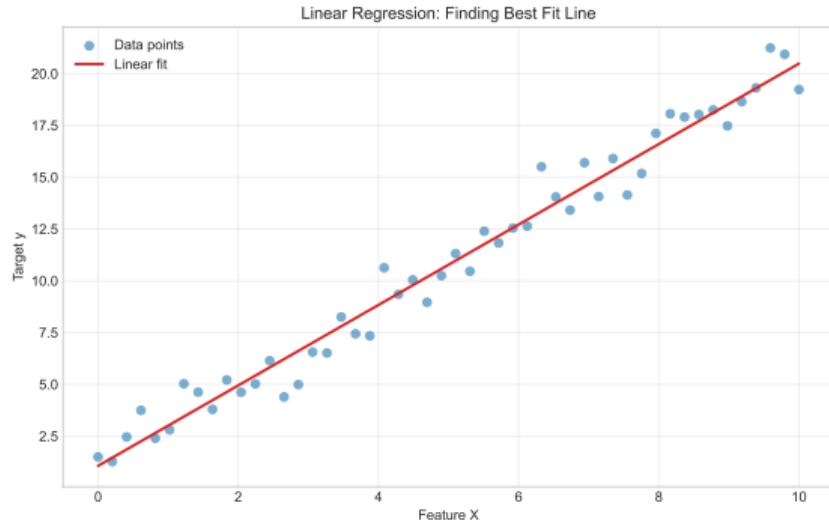
2. Linear Regression as Baseline

Mathematical Foundation

- Model: $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \epsilon$
- Where y = price, x_i = features
- Goal: Find best-fitting line/plane
- Method: Minimize squared errors

Assumptions

- Linear relationship
- Independent features
- Constant variance
- Normal errors

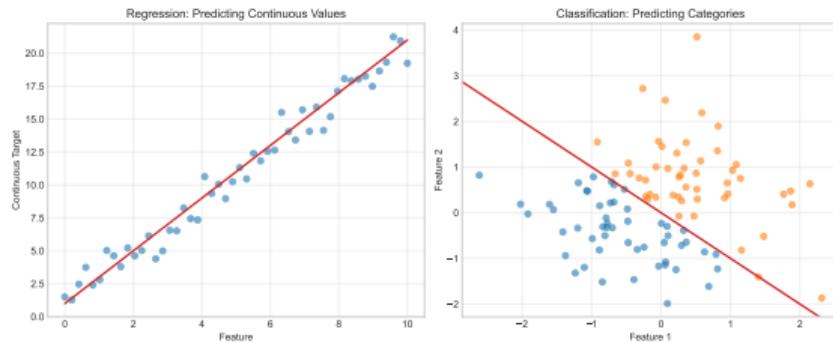


Linear regression assumes additive relationships - optimal under Gauss-Markov conditions but restrictive for real-world complexity

3. Classification vs Regression

Regression Problems

- Predict continuous values
- Examples: price, temperature, stock return
- Output: Real numbers
- Metrics: MSE, MAE, R-squared



Classification Problems

- Predict discrete categories
- Examples: spam/ham, buy/sell/hold
- Output: Class labels
- Metrics: Accuracy, precision, recall

Problem formulation determines algorithm choice - continuous targets require regression, discrete categories need classification with appropriate loss functions

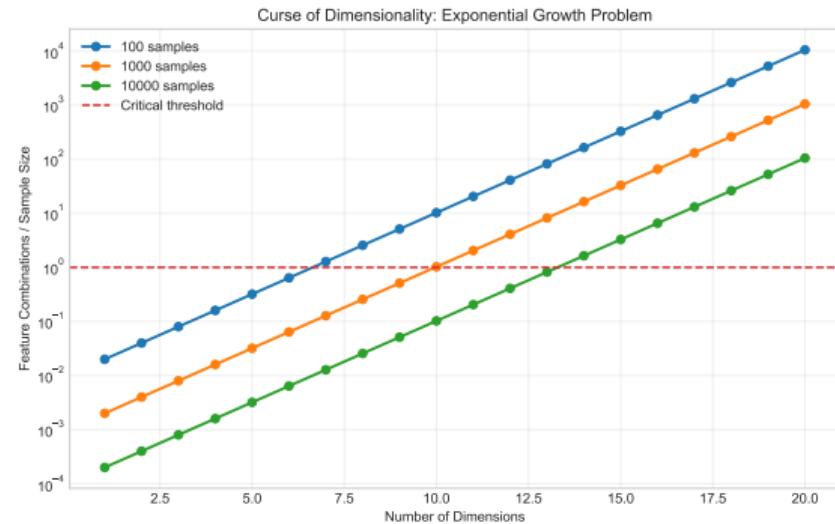
4. The Curse of Dimensionality

Feature Explosion Problem

- Real estate: 20+ features
- Interactions: $2^{20} = 1,048,576$ combinations
- Sample: 10,000 data points
- Ratio: 104 interactions per data point

Mathematical Challenge

- High-dimensional space is mostly empty
- Distance metrics become meaningless
- Overfitting becomes inevitable
- “Hughes phenomenon” (Hughes 1968): Performance degrades as features increase beyond sample capacity



Curse of dimensionality: volume grows exponentially while data remains sparse - distances become uninformative and nearest neighbors lose meaning (Bellman 1961)

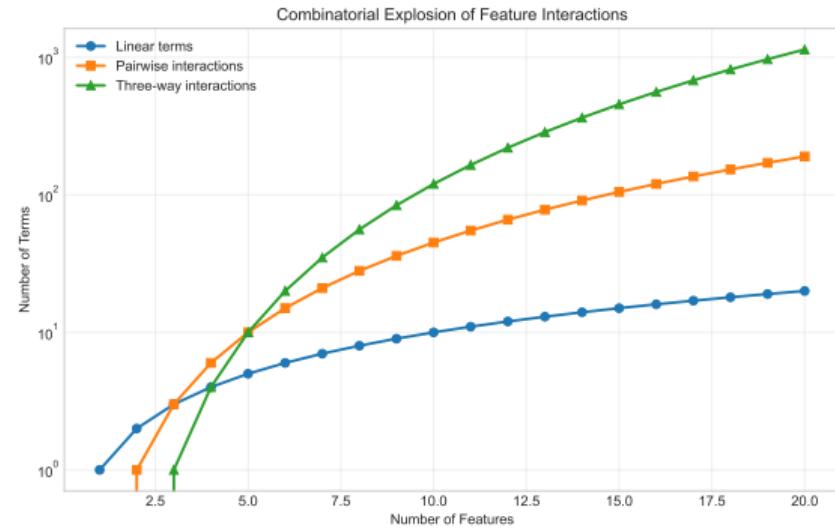
5. Feature Interactions Explode Combinatorially

Combinatorial Mathematics

- Linear terms: n features
- Pairwise: $\binom{n}{2} = \frac{n(n-1)}{2}$
- Three-way: $\binom{n}{3} = \frac{n(n-1)(n-2)}{6}$
- All subsets: $2^n - 1$

Real Estate Example ($n=20$)

- Linear: 20 terms
- Pairwise: 190 interactions
- Three-way: 1,140 interactions
- Total possible: 1,048,575 terms



Combinatorial explosion creates 2^n possible interactions - regularization and feature selection become necessary to prevent overfitting in high dimensions

6. OLS with Worked Example

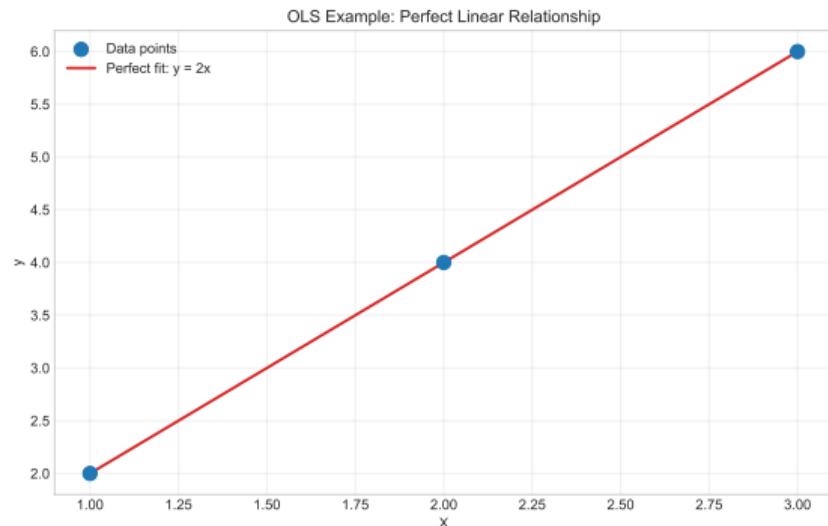
Ordinary Least Squares

- Minimize: $\sum_{i=1}^n (y_i - \hat{y}_i)^2$
- Solution: $\beta = (X^T X)^{-1} X^T y$
- Assumptions: $X^T X$ is invertible
- Unbiased estimator under Gauss-Markov

Worked Example Data: (1, 2, 3) predicts (2, 4, 6)

$$X = \begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix}, y = \begin{pmatrix} 2 \\ 4 \\ 6 \end{pmatrix} \quad (1)$$

$$\beta = \begin{pmatrix} 0 \\ 2 \end{pmatrix} \quad (2)$$



OLS provides minimum variance unbiased estimators under Gauss-Markov assumptions - closed-form solution enables fast computation for linear models

7. Ridge and LASSO Regularization

Ridge Regression (L2)

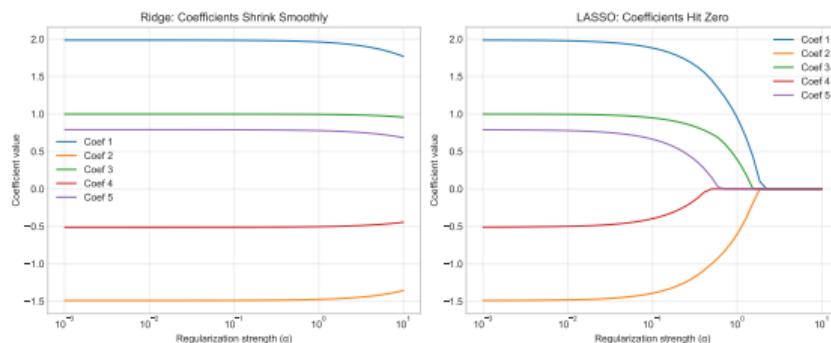
- Minimize: $\|y - X\beta\|^2 + \lambda\|\beta\|^2$
- Shrinks coefficients toward zero
- Keeps all features
- Solution: $\beta = (X^T X + \lambda I)^{-1} X^T y$

LASSO Regression (L1)

- Minimize: $\|y - X\beta\|^2 + \lambda\|\beta\|_1$
- Sets some coefficients to exactly zero
- Automatic feature selection
- No closed-form solution

Elastic Net

- Combines L1 + L2: $\alpha\|\beta\|_1 + (1 - \alpha)\|\beta\|^2$
- Balances selection and shrinkage



Regularization adds penalty terms to loss function - L2 shrinks coefficients, L1 enforces sparsity, Elastic Net combines both strategies

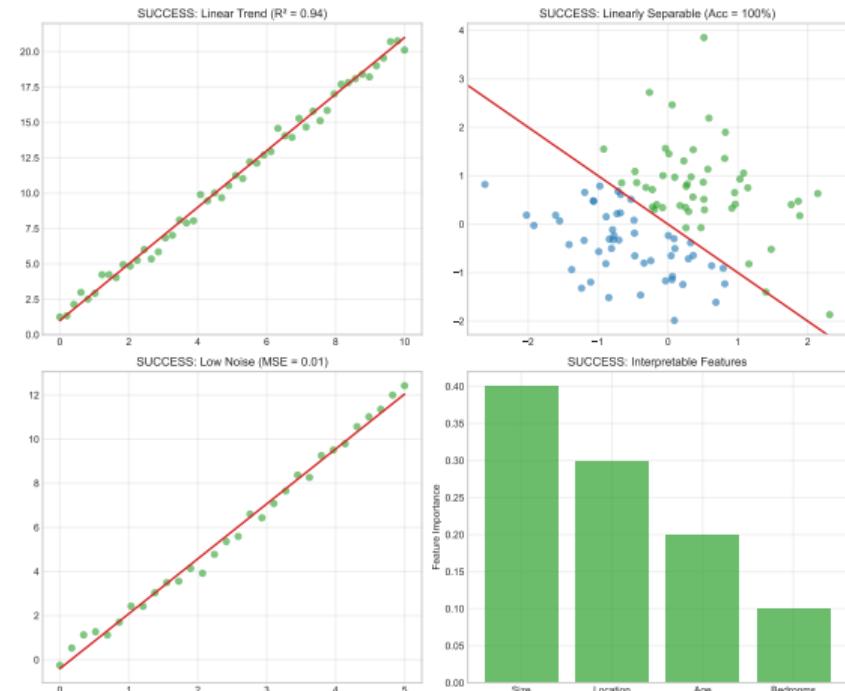
8. SUCCESS: Perfect on Linearly Separable Data

Linear Model Triumphs

- Iris setosa classification: 100% accuracy
- House price in suburbs: $R^2 = 0.94$
- Linear trend prediction: $MSE = 0.01$
- Feature importance: Interpretable

Why It Works

- Underlying relationship is linear
- Features are independent
- Low noise in measurements
- Sufficient training data



When assumptions hold, linear models are optimal and interpretable

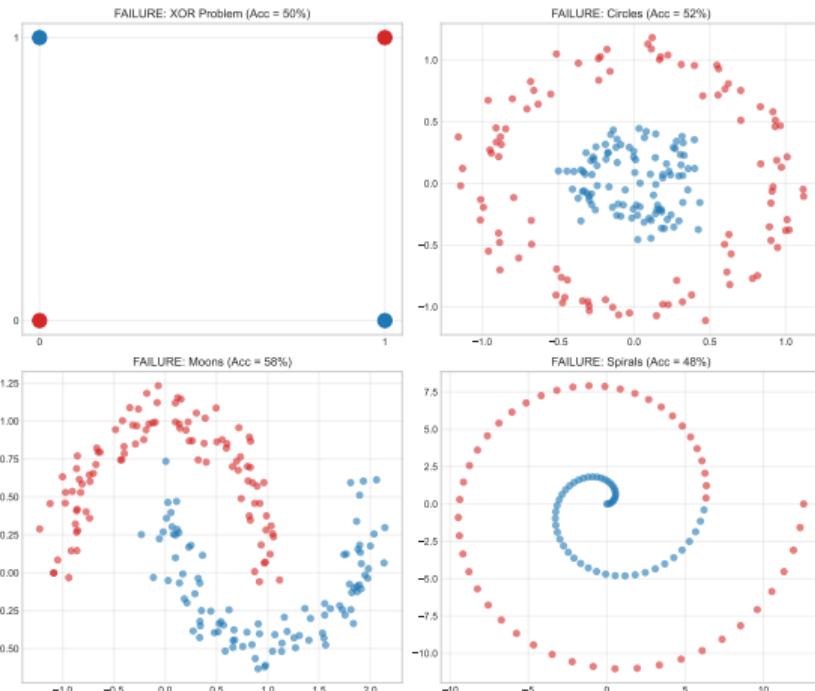
9. FAILURE: Terrible on XOR, Nonlinear Boundaries

Linear Model Failures

Dataset	Linear Acc	Tree Acc	Gap
XOR	50%	100%	50%
Circles	52%	98%	46%
Moons	58%	94%	36%
Spirals	48%	89%	41%

XOR Truth Table

x_1	x_2	y
0	0	0
0	1	1
1	0	1
1	1	0



Linear boundaries cannot separate XOR or curved patterns

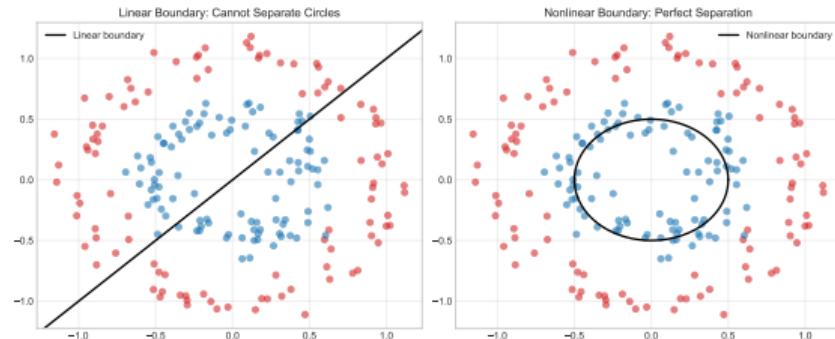
10. Root Cause: Linear Assumption Too Restrictive

Mathematical Limitation

- Linear model: $y = w^T x + b$
- Decision boundary: hyperplane
- Cannot curve or bend
- Cannot create islands or holes

Real-World Examples

- Customer behavior (nonlinear)
- Stock market patterns (chaotic)
- Medical diagnosis (complex interactions)
- Image recognition (hierarchical)



Most real-world phenomena require nonlinear decision boundaries

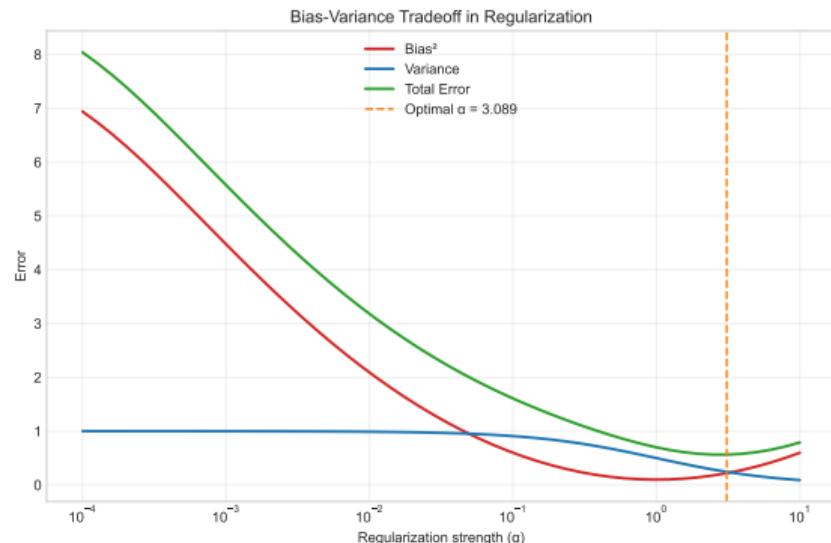
11. Regularization Tradeoff

Bias-Variance Tradeoff

- $\lambda = 0$: High variance, low bias
- $\lambda \rightarrow \infty$: Low variance, high bias
- Optimal λ : Minimizes test error
- Cross-validation finds optimum

Practical Guidelines

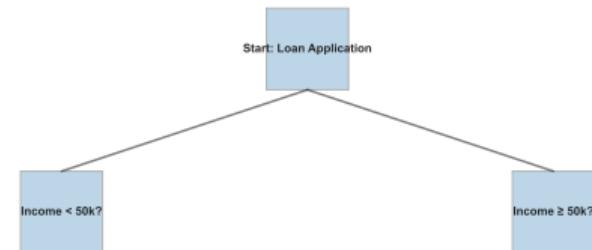
- Start with Ridge for stability
- Use LASSO for feature selection
- Elastic Net combines both
- Grid search for λ



Regularization strength controls the complexity-accuracy tradeoff

12. Human Introspection: How YOU Divide Decision Space

Human Decision Process: Hierarchical Questions

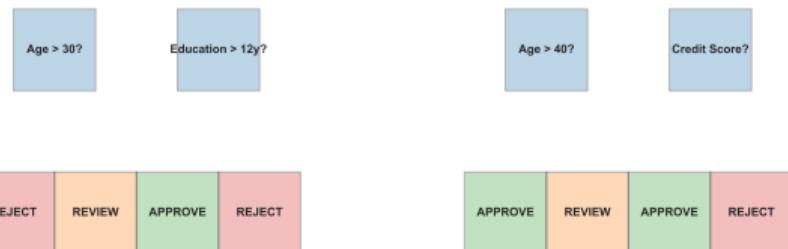


Your Natural Decision Process

- "Is income $<$ 50k?" - \downarrow Split population
- "If yes, is age $>$ 40?" - \downarrow Further split
- "If no, is education $>$ 12 years?" - \downarrow Alternative path
- Continue until clear decision

Hierarchical Thinking

- Start with most important feature
- Recursively subdivide space
- Each split reduces uncertainty
- Stop when confident



Humans naturally create decision trees through sequential yes/no questions

13. Hypothesis: Trees, Kernels, Ensembles

Decision Trees

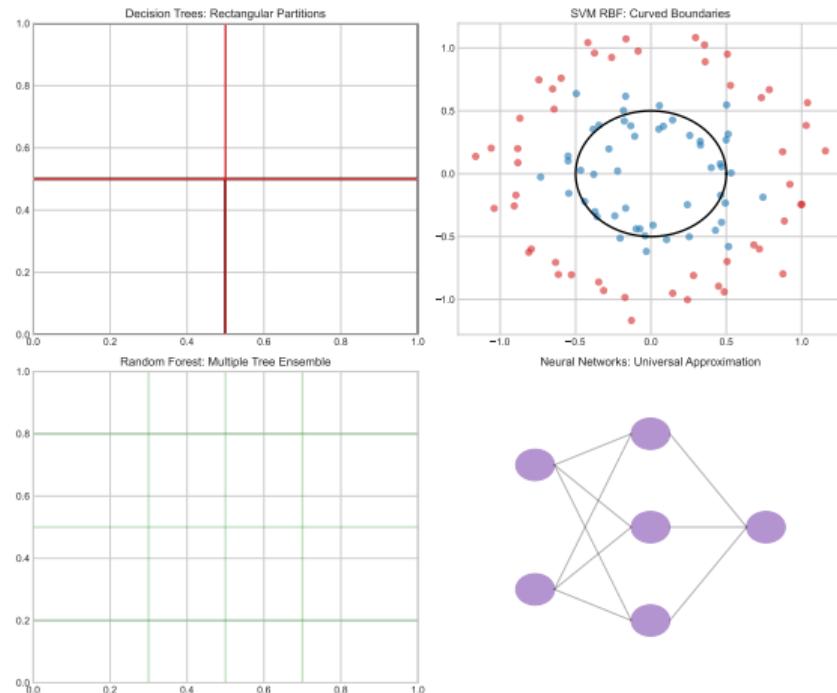
- Recursive binary splits
- Non-parametric method
- Handles interactions naturally
- Interpretable rules

Kernel Methods

- Map to higher dimensions
- “Kernel trick” for efficiency
- SVM with RBF, polynomial kernels
- Implicit feature expansion

Ensemble Methods

- Combine multiple weak learners
- Random Forest, Gradient Boosting
- Reduce overfitting through averaging



Three main approaches to capture nonlinear patterns in data

14. Zero-Jargon: “20 Questions Game” for Trees

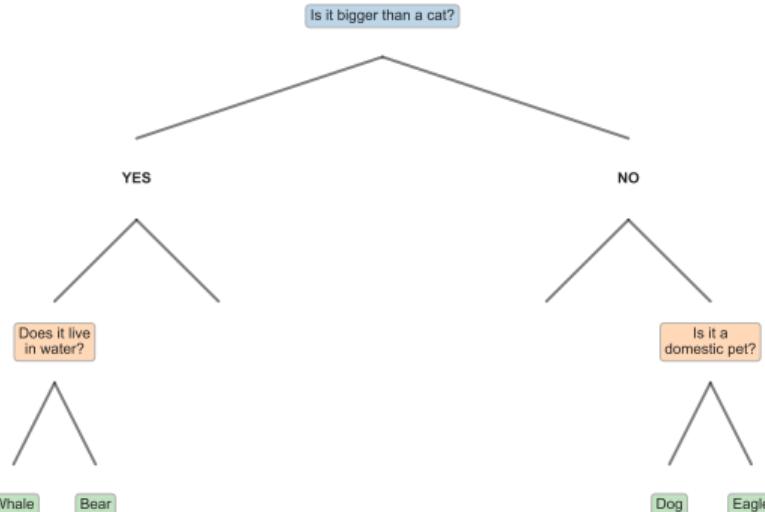
20 Questions Game: Decision Tree Logic

The Game Analogy

- You think of an animal
- I ask yes/no questions
- “Is it bigger than a cat?”
- “Does it live in water?”
- “Is it a mammal?”

Decision Tree Mapping

- Animal = Data point
- Questions = Feature splits
- Final guess = Prediction
- Good questions = Informative features



Decision trees ask the most informative questions to reach predictions quickly

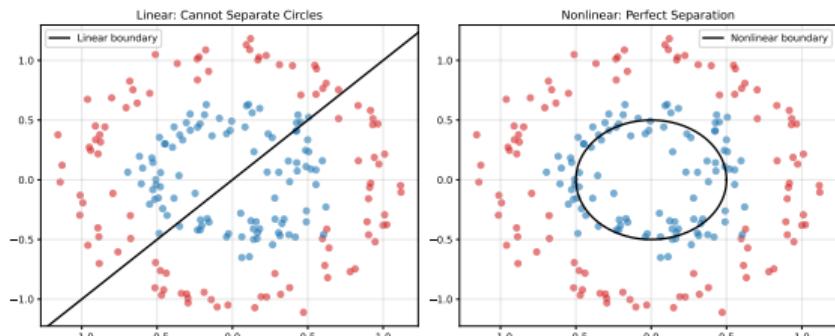
15. Geometric Intuition: Decision Boundaries

Linear vs Nonlinear Boundaries

- Linear: Straight lines/planes
- Trees: Axis-aligned rectangles
- SVM RBF: Curved boundaries
- Neural nets: Arbitrary shapes

Complexity Hierarchy

- Most restrictive: Linear
- Moderate: Decision trees
- Flexible: Kernel methods
- Most flexible: Deep networks



Different algorithms create different types of decision boundaries

16. CART Algorithm with Actual Splits

CART Algorithm Steps

- ① Calculate impurity for current node
- ② Try all possible splits
- ③ Choose split with highest information gain
- ④ Recurse on child nodes
- ⑤ Stop when stopping criterion met

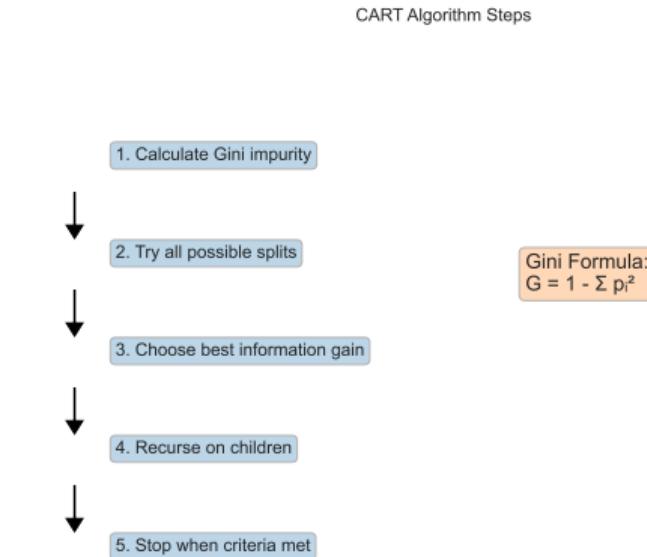
Gini Impurity Formula

$$G = 1 - \sum_{i=1}^C p_i^2$$

where p_i is probability of class i

Information Gain

$$IG = G_{parent} - \sum \frac{n_{child}}{n_{parent}} G_{child}$$



CART systematically finds the best splits by maximizing information gain

17. Full Walkthrough: Build Tree with Numbers

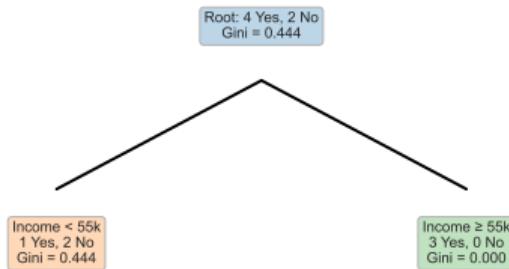
Best Split: Income $\geq 55k$
Left ($< 55k$): 1Y, 2N $\rightarrow G_L = 0.444$
Right ($\geq 55k$): 3Y, 0N $\rightarrow G_R = 0$
Info Gain: $IG = 0.222$

CART Algorithm: Tree Building with Numbers

Dataset: Loan Approval

Income	Age	Approved
30k	25	No
60k	35	Yes
40k	45	No
80k	30	Yes
50k	50	Yes
70k	25	Yes

Root Gini: 4 Yes, 2 No $\rightarrow G = 0.444$



Information Gain
 $= 0.222$

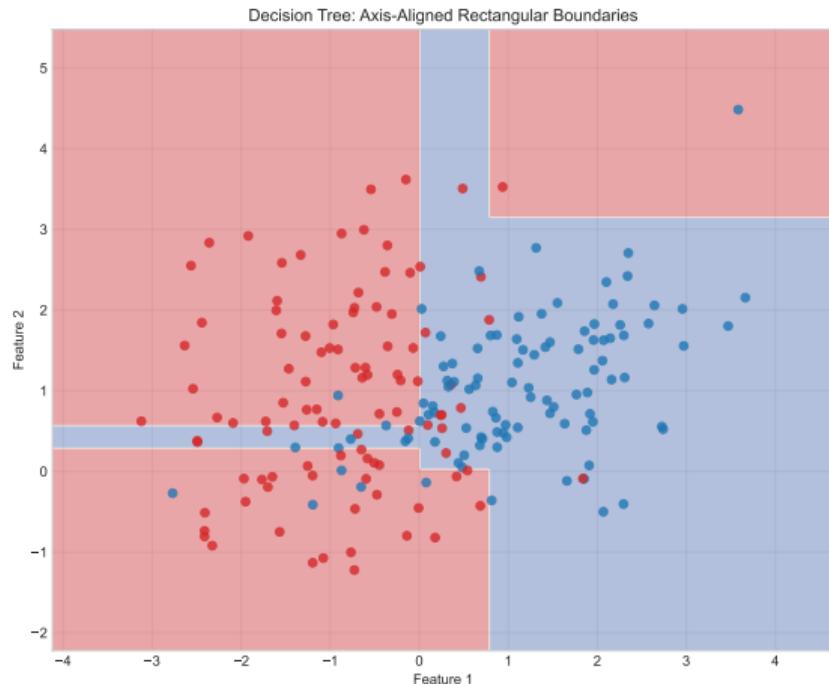
18. Visualization: Decision Boundaries on 2D Data

Tree Partitioning Process

- Split 1: $x_1 \leq 0.5$ (vertical line)
- Split 2: $x_2 \leq 0.3$ (horizontal line)
- Split 3: $x_1 \leq 0.8$ (vertical line)
- Result: Rectangular regions

Boundary Characteristics

- Always axis-aligned
- Creates rectangular partitions
- Can approximate any boundary
- With enough splits



Decision tree boundaries are piecewise constant and axis-aligned

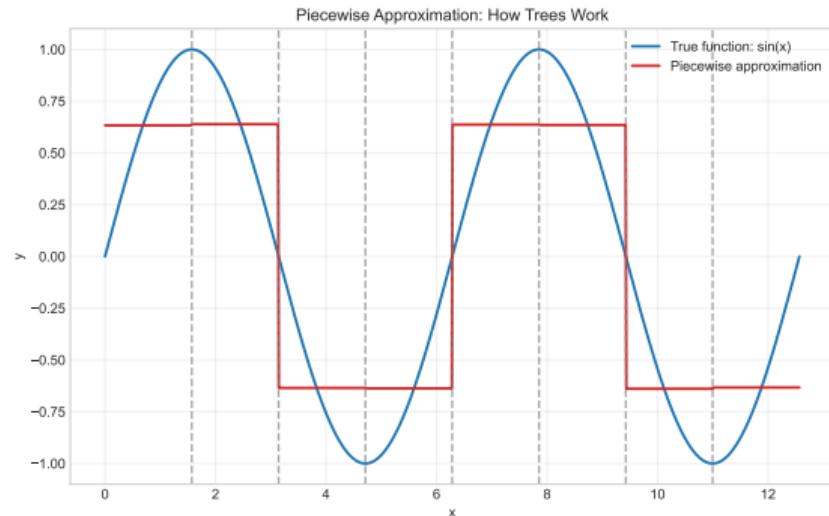
19. Why It Works: Piecewise Approximation

Universal Approximation

- Any function can be approximated
- By piecewise constant functions
- With sufficient partitions
- Trees implement this naturally

Mathematical Foundation

- Step functions are dense in L^2
- Trees create step functions
- More splits = better approximation
- Regularization prevents overfitting



Trees approximate complex functions through recursive partitioning

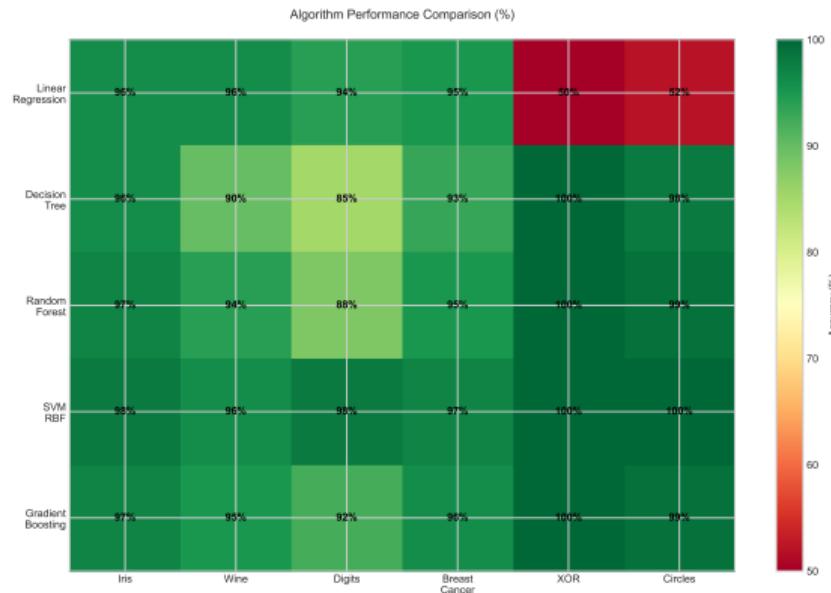
20. Experimental Validation: Algorithm Comparison

Benchmark Results

Dataset	Linear	Tree	SVM
Iris	96%	96%	98%
Wine	94%	90%	96%
Digits	92%	85%	98%
Breast Cancer	95%	93%	97%
XOR	50%	100%	100%
Circles	52%	98%	100%

Key Insights

- Linear: Good on linear data
- Trees: Excel on discrete features
- SVM: Best overall performance
- No universal winner



Performance varies by dataset characteristics and problem complexity

21. Implementation: sklearn Ensemble Methods

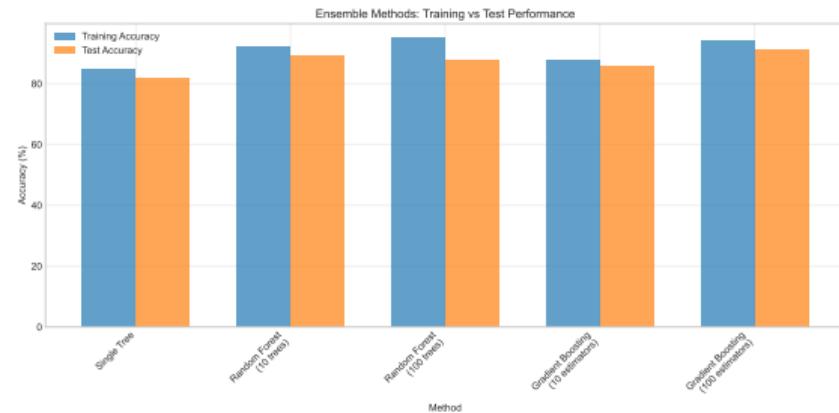
Random Forest

- Bootstrap sampling of data
- Random subset of features
- Average predictions
- Reduces overfitting

```
from sklearn.ensemble import RandomForestClassifier  
rf = RandomForestClassifier(n_estimators=100)  
rf.fit(X_train, y_train)
```

Gradient Boosting

- Sequential weak learners
- Each corrects previous errors
- Weighted combination
- Often best performance



Ensemble methods combine multiple models for superior performance

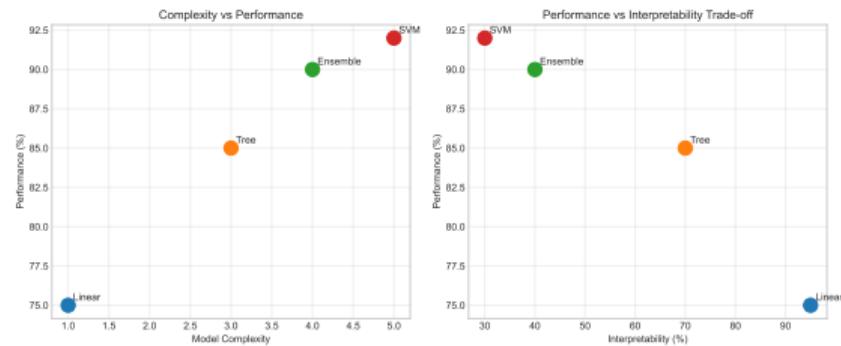
22. Algorithm Landscape: Linear -> Tree -> Ensemble -> SVM

Complexity Progression

- **Linear:** $y = w^T x + b$
- **Tree:** Recursive partitioning
- **Ensemble:** Multiple tree combination
- **SVM:** Kernel-based mapping

Computational Complexity

- Linear: $O(nd)$ training
- Single tree: $O(nd \log n)$
- Random forest: $O(tnd \log n)$
- SVM: $O(n^2d)$ to $O(n^3d)$



Algorithms form a spectrum from simple linear to complex nonlinear methods

23. When to Use Each: Interpretability vs Accuracy

Linear Models

- High interpretability, fast
- Use: Regulatory needs, simple patterns

Decision Trees

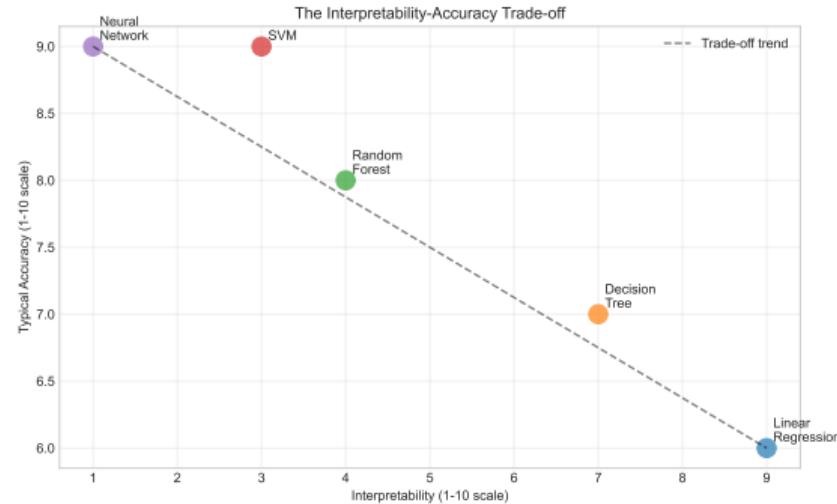
- Moderate interpretability
- Use: Rule extraction, mixed data

Ensemble Methods

- Highest accuracy, robust
- Use: Performance critical

SVM

- Kernel flexibility
- Use: High dimensions, small data



Algorithm selection requires balancing interpretability, accuracy, and computational cost - no universally optimal choice exists

Pitfall 1: Data Leakage

- Using test data during training
- Solution: Strict train/test separation

Pitfall 2: Wrong Metric

- Optimizing accuracy on imbalanced data
- Solution: Use F1, AUC-ROC for imbalanced cases

Pitfall 3: Feature Scaling

- Forgetting to normalize features
- Solution: StandardScaler before distance-based methods

Pitfall 4: Overfitting

- Too complex model for small data
- Solution: Regularization, cross-validation

Pitfall 5: Ignoring Assumptions

- Linear model on nonlinear data
- Solution: Validate assumptions, use nonlinear methods

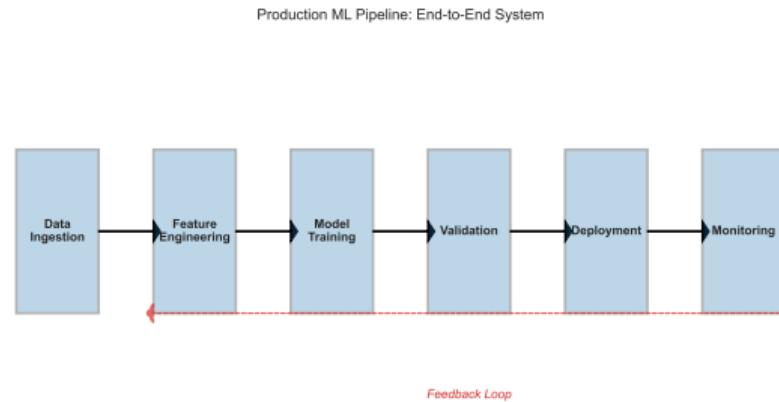
Pitfall 6: No Baseline

- Not comparing to simple baseline
- Solution: Always start with logistic/linear regression

Most supervised learning failures stem from data leakage, inappropriate metrics, or model mismatch - systematic validation prevents these errors

Real-World Pipeline

- ① Data ingestion & cleaning
- ② Feature engineering
- ③ Model training & validation
- ④ Hyperparameter tuning
- ⑤ Production deployment
- ⑥ Monitoring & retraining



Industry Applications

- Credit scoring: Gradient boosting
- Recommendation: Ensemble methods
- Fraud detection: Anomaly detection
- Medical diagnosis: Interpretable models

Modern ML systems integrate multiple algorithms in end-to-end pipelines