Week 0b: Supervised Learning

The Prediction Challenge

Machine Learning for Smarter Innovation

BSc Innovation & Design Thinking

Learning Journey

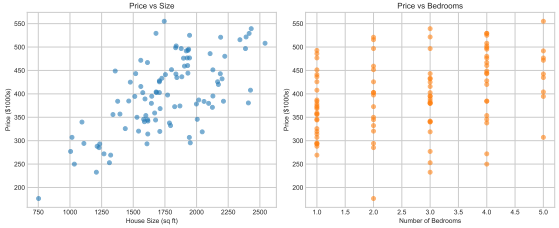
1. Real Estate Price Prediction

The Business Problem

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

Sample Data Points

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



Multiple features create complex relationships requiring mathematical modeling

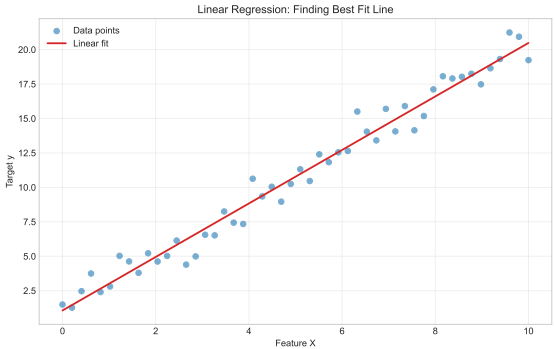
2. Linear Regression as Baseline

Mathematical Foundation

- Model: $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + ... + \epsilon$
- 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 model assumes additive relationships between all features

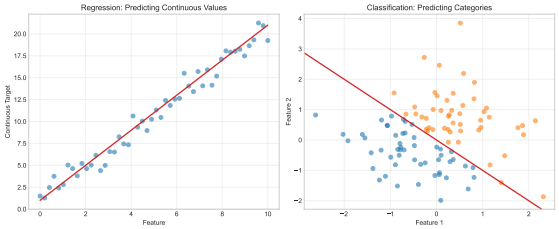
3. Classification vs Regression

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



Different problem types require different algorithms and evaluation metrics

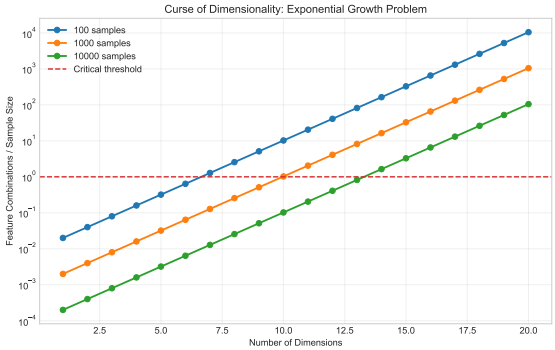
4. The Curse of Dimensionality

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" in pattern recognition



As dimensions increase, all points become equidistant and patterns disappear

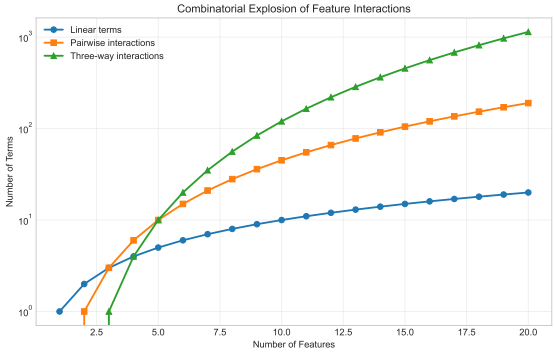
5. Feature Interactions Explode Combinatorially

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



Feature interactions grow exponentially, requiring regularization or feature selection

6. OLS with Worked Example

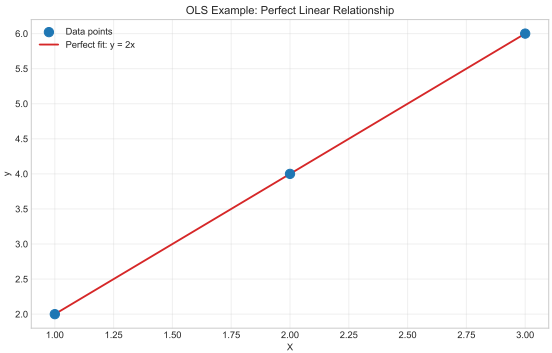
Ordinary Least Squares

- 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 $(2, 4, 6)$

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

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



Perfect fit when relationship is truly linear with minimal noise

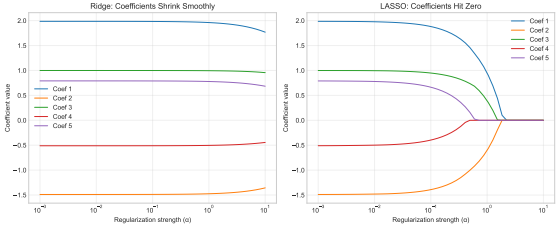
7. Ridge and LASSO Regularization

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



Regularization prevents overfitting by constraining coefficient magnitudes

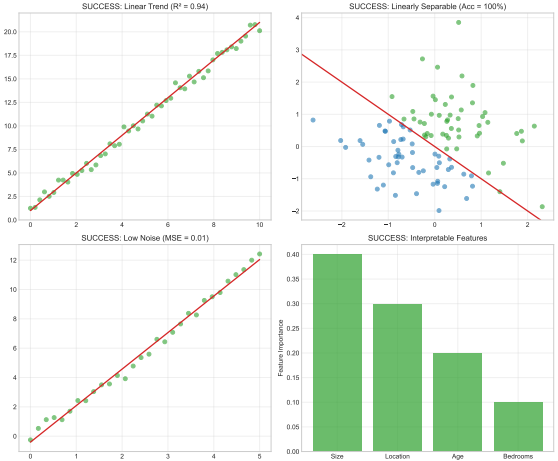
8. SUCCESS: Perfect on Linearly Separable Data

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

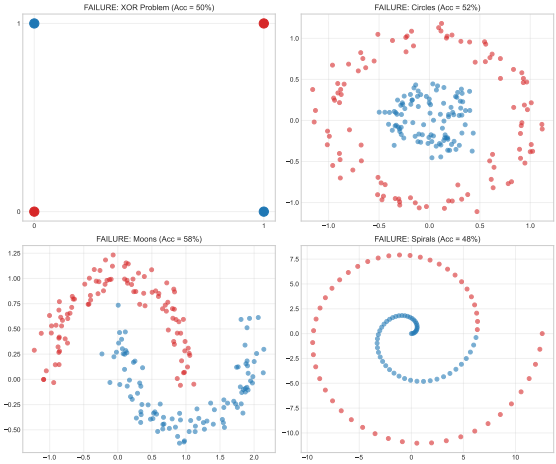
9. FAILURE: Terrible on XOR, Nonlinear Boundaries

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

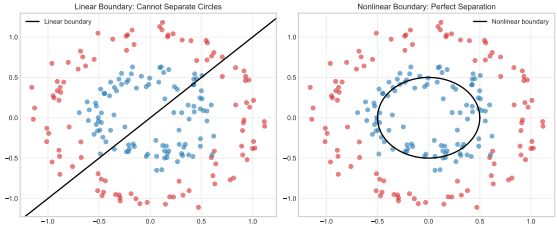
10. Root Cause: Linear Assumption Too Restrictive

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

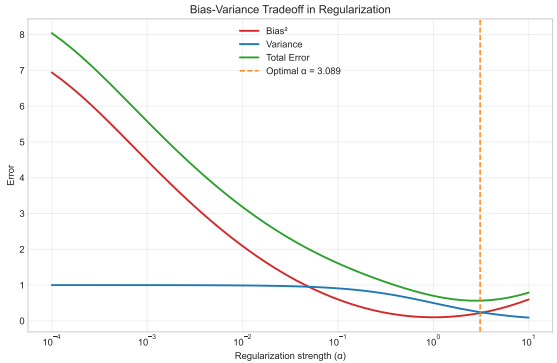
11. Regularization Tradeoff

Bias-Variance Tradeoff

- $\lambda = 0$: High variance, low bias
- $\lambda \to \infty$: 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

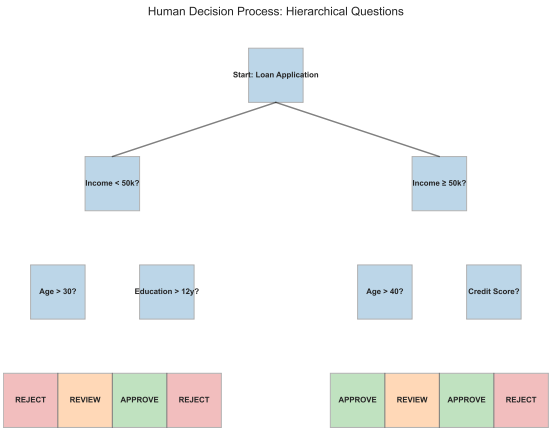
12. Human Introspection: How YOU Divide Decision Space

Your Natural Decision Process

- "Is income ¿ 50k?" -¿ Split population
- "If yes, is age ¿ 40?" -¿ Further split
- "If no, is education ¿ 12 years?" -¿ 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

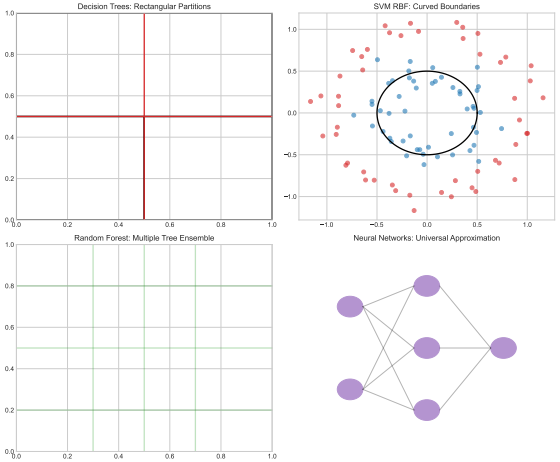
- Recursive binary splits
- Non-parametric method
- Handles interactions naturally
- Interpretable rules

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

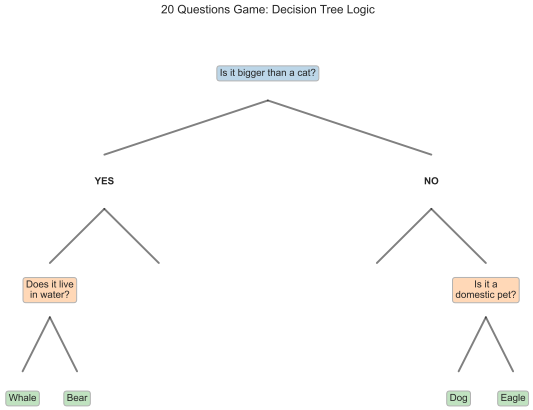
14. Zero-Jargon: "20 Questions Game" for Trees

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

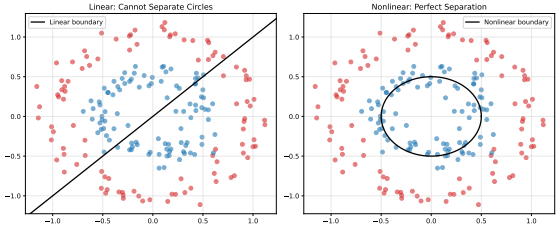
15. Geometric Intuition: Decision Boundaries

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

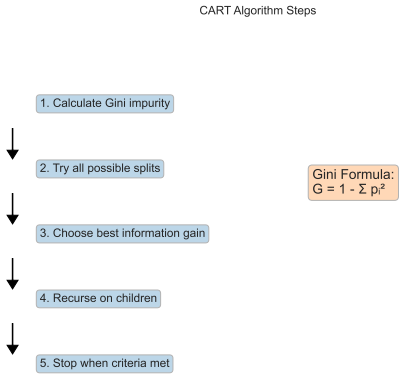
Gini Impurity Formula

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

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

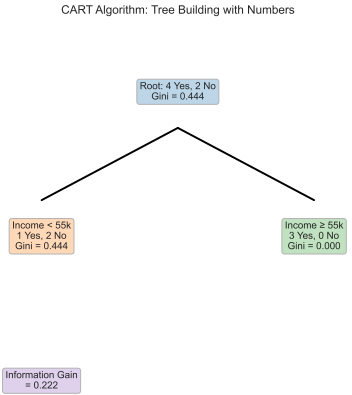
17. Full Walkthrough: Build Tree with Numbers

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 $\rightarrow G = 0.444$

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: $IG = 0.222$



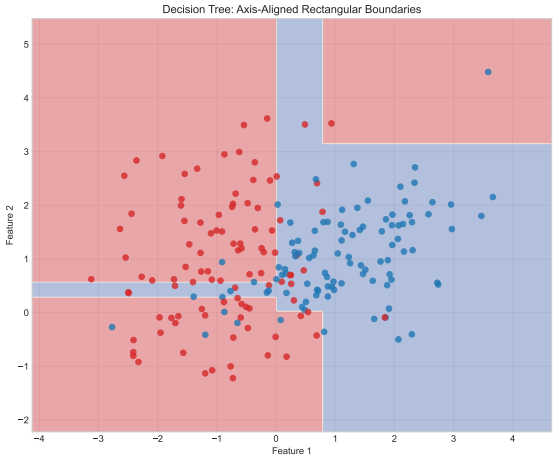
18. Visualization: Decision Boundaries on 2D Data

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

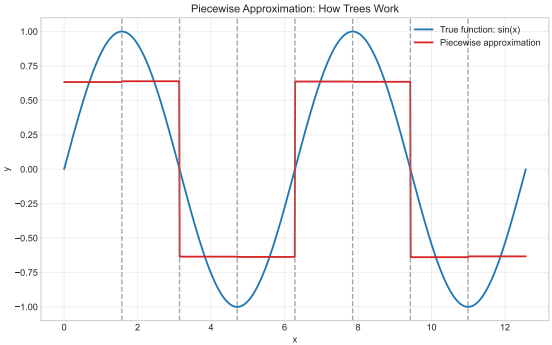
19. Why It Works: Piecewise Approximation

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

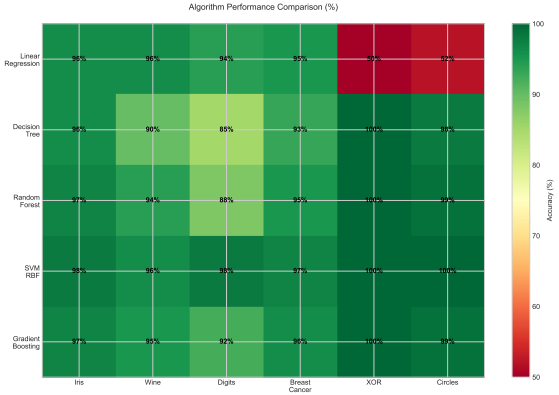
20. Experimental Validation: Algorithm Comparison

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

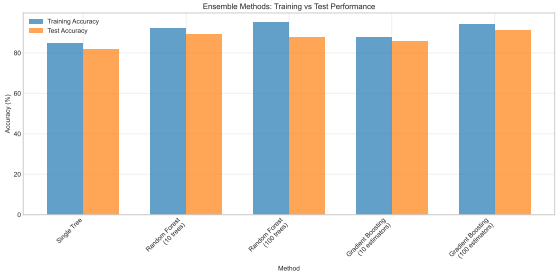
Random Forest

- 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

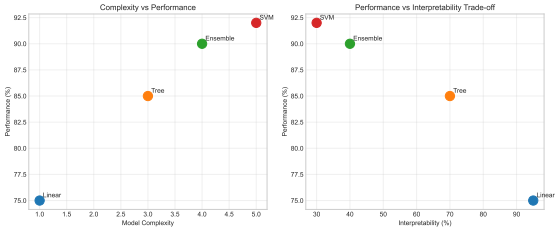
22. Algorithm Landscape: Linear -¿ Tree -¿ Ensemble -¿ SVM

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: $O(n^2 d)$ to $O(n^3 d)$



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

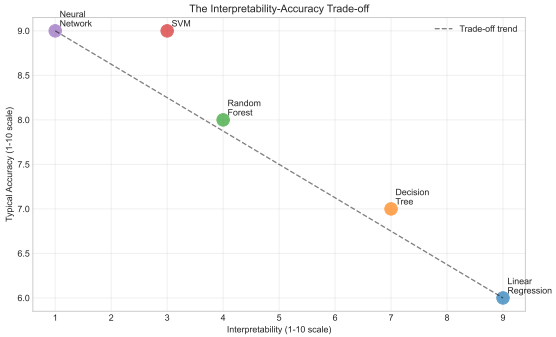
- Moderate interpretability
- Use: Rule extraction, mixed data

Ensemble Methods

- Highest accuracy, robust
- Use: Performance critical

SVM

- Kernel flexibility
- Use: High dimensions, small data



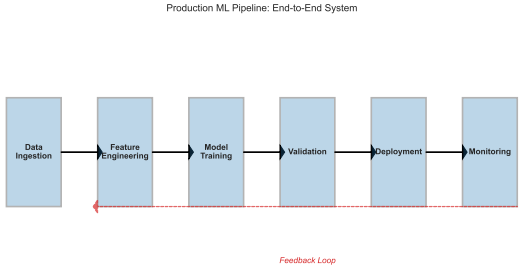
24. Modern Applications: Production ML Pipelines

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

25. Summary & Preview: Unsupervised Learning

Supervised Learning Recap

- Linear: Fast, interpretable
- Regularization prevents overfitting
- Nonlinear for complexity
- Ensembles: Best performance

Key Takeaways

- Start simple, validate on unseen data
- Balance interpretability vs accuracy

Next: Unsupervised Learning

- No labels - pattern discovery
- Clustering, dimensionality reduction

Applications

- Customer segmentation
- Anomaly detection
- Data visualization