Unit II XAI Notes

Unit-II: Model Visualization Techniques and Traditional Interpretable Algorithms

1) Model Validation, Evaluation, and Hyperparameters

Core idea

Model validation checks whether a trained model generalizes to unseen data (not just training data). Hyperparameters are user-set values before training (for example: `max_depth`, `C`, `alpha`, learning rate), while model parameters are learned during training.

Key points

- Split data into training, validation, and test sets.
- Use the same split across models for fair comparison.
- Overfitting: very good train performance, weak test performance (high variance).
- Underfitting: poor performance on both train and test (high bias).
- Bias-variance trade-off: increasing complexity lowers bias but can raise variance.
- k-fold cross-validation gives a robust estimate but costs more compute.

Formula

$$E_{cv} = \frac{1}{k}\sum_{i=1}^{k} E_i$$

where `E_i` is fold `i` error.

Important methods

- Holdout split: simple but noisier estimate.
- Grid Search: tries all parameter combinations.
- Random Search: samples combinations; often more efficient in large spaces.
- Bayesian optimization: guided search over hyperparameter space.

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2) Model Selection and Learning/Validation Curves

Core idea

Model selection chooses the model-hyperparameter pair with best validation behavior, not just best training score.

Validation curve

Plots score vs one hyperparameter. - Left side often underfits. - Right side often overfits. - Best point is where validation score peaks.

Learning curve

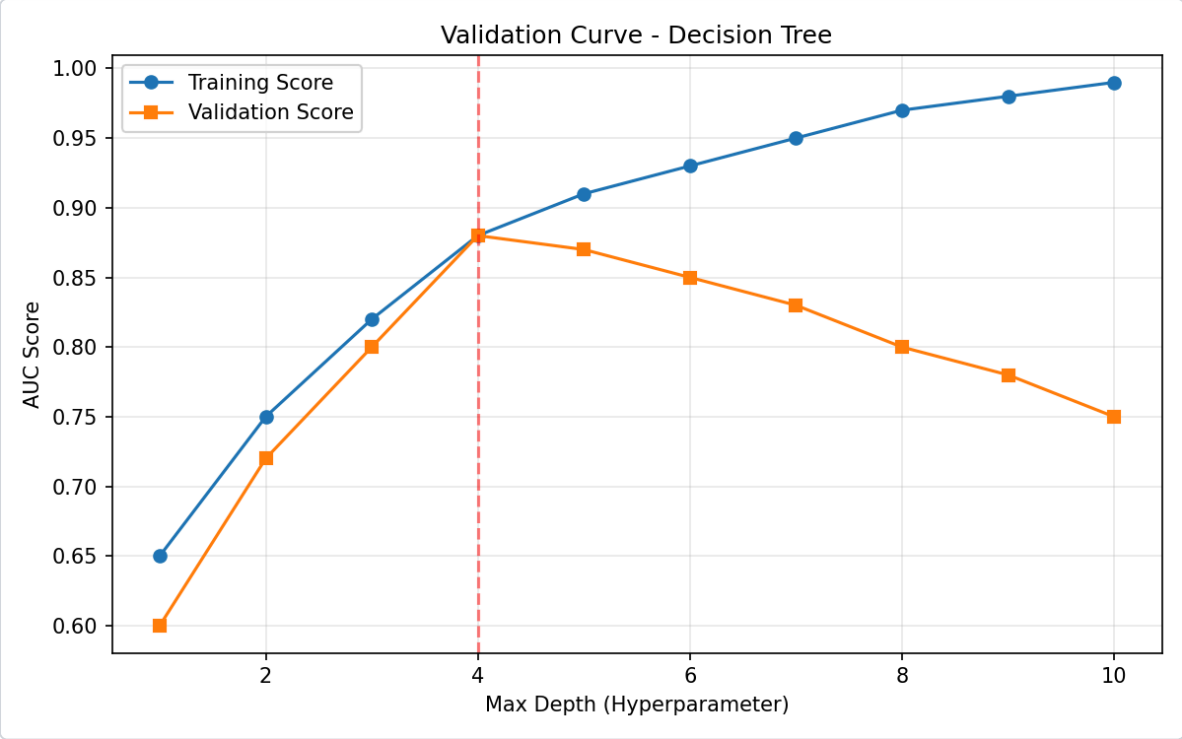
Plots score vs training set size. - Small gap + low scores -> underfitting. - Large train-validation gap -> overfitting. - If validation score keeps improving with more data, collecting data can help.

Steps

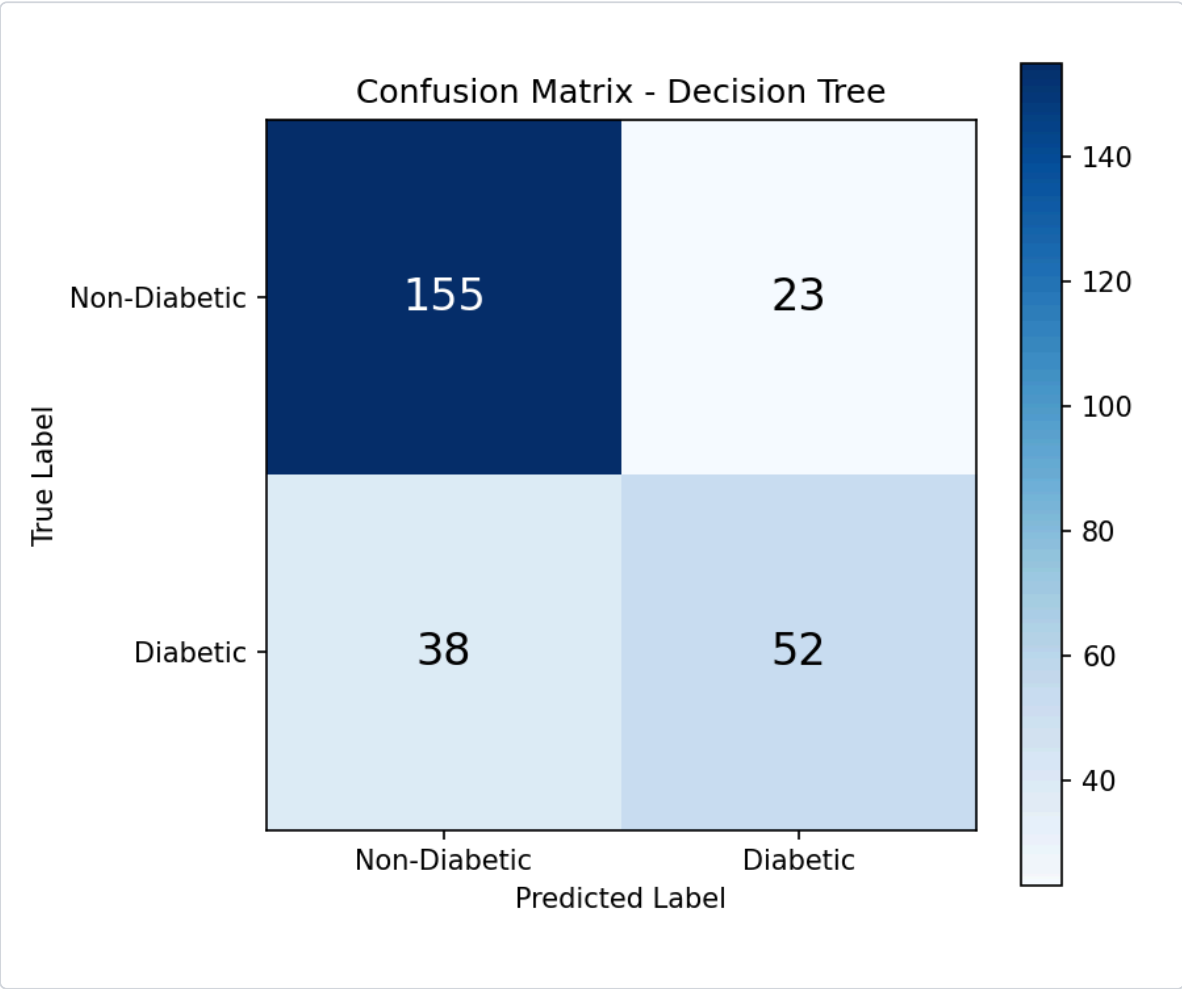
1. Define hyperparameter range.
2. Train and compute cross-validated scores for each value.
3. Plot train vs validation curves.
4. Pick value near best validation score with stable generalization.

Graphs

Learning Curve:



Validation Curve:



3) Classification Model Visualization

Core idea

Visual diagnostics for classification include confusion matrix, ROC curve, precision-recall curve, and threshold tuning.

Key metrics and formulas

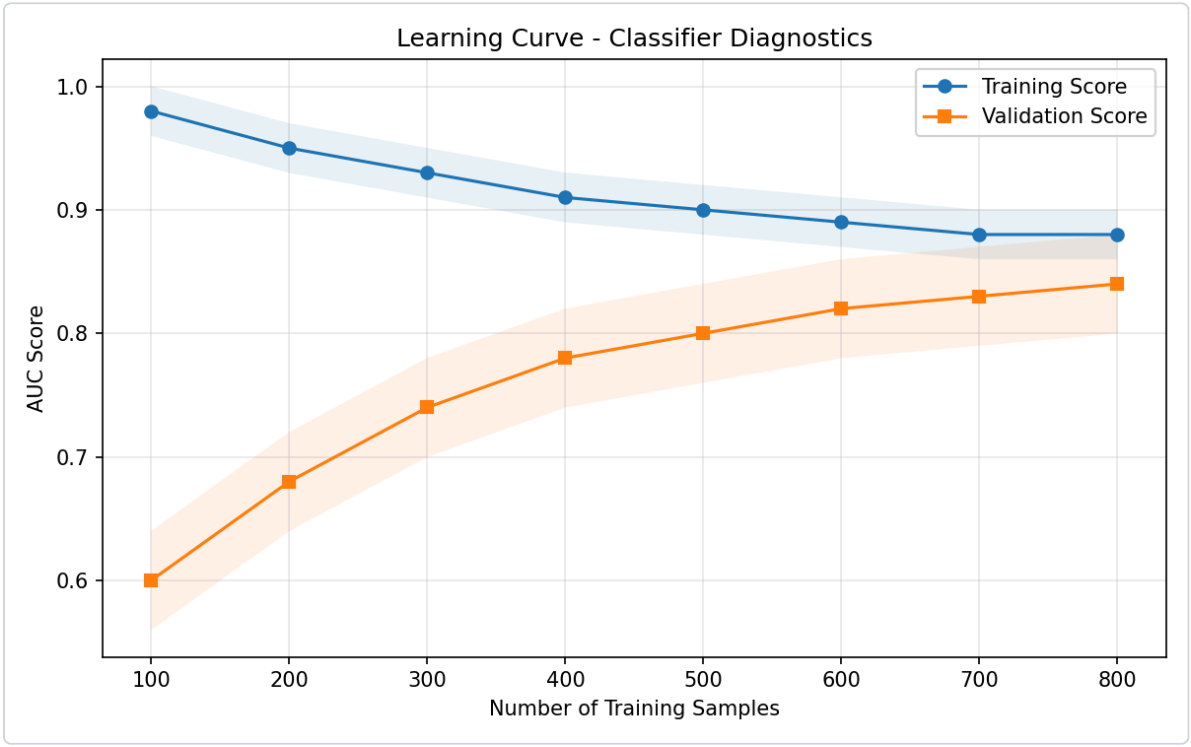
Metric	Formula
Precision	`TP / (TP + FP)`
Recall	`TP / (TP + FN)`
F1 Score	`2 * (Precision * Recall) / (Precision + Recall)`
Accuracy	`(TP + TN) / (TP + TN + FP + FN)`
Specificity	`TN / (TN + FP)`

Interpretation points

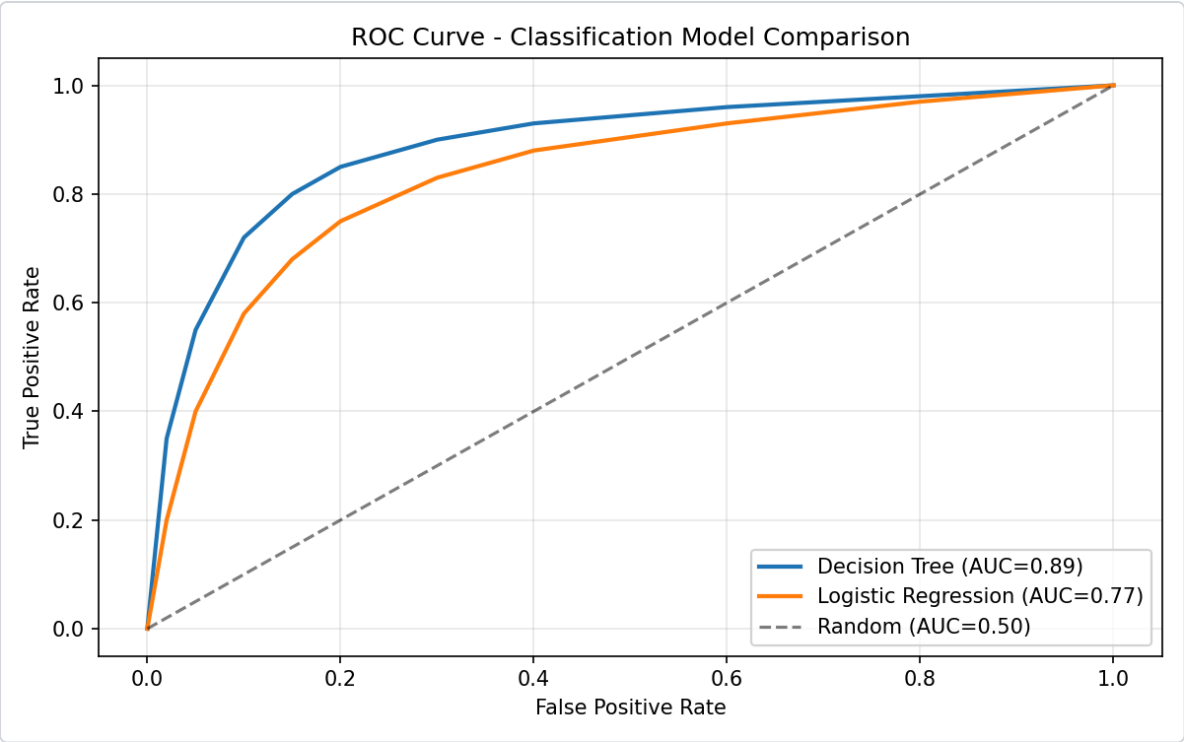
- ROC: plots TPR vs FPR over thresholds; AUC near 1 is better.
- PR curve: better than ROC for imbalanced classes.
- Threshold tuning changes FP/FN trade-off; `0.5` is not always best.

Graphs

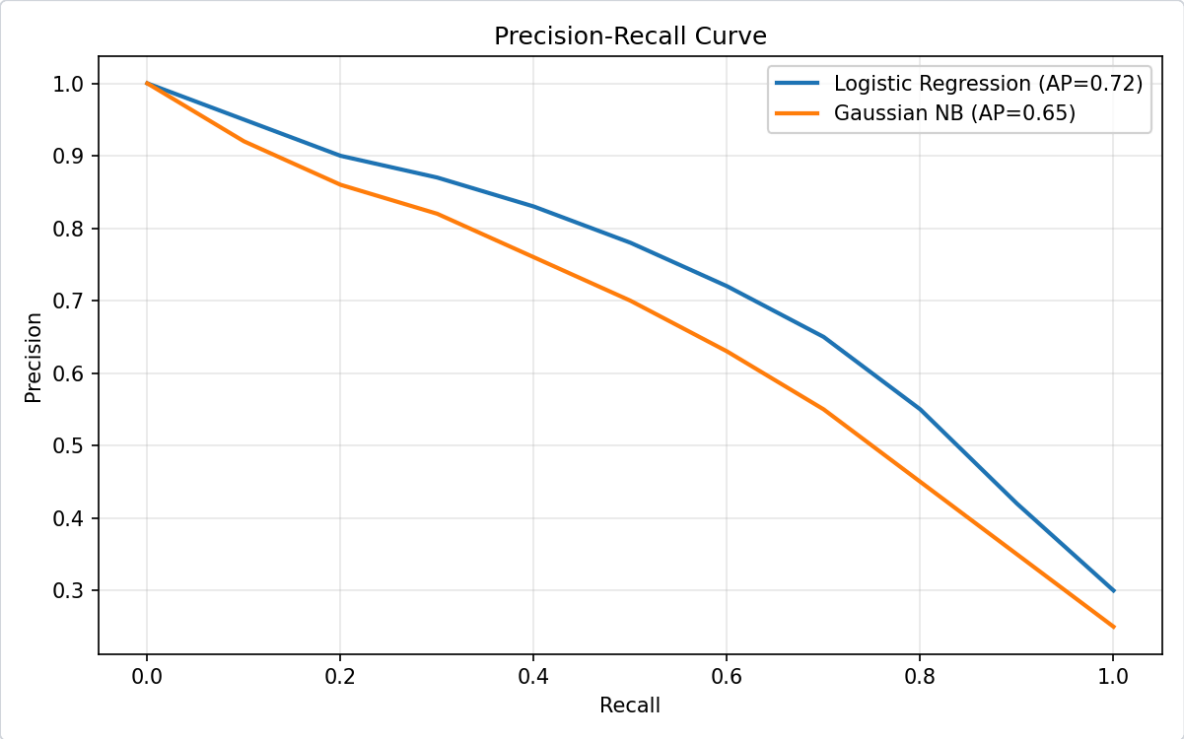
Confusion Matrix:



ROC Curve:



Precision-Recall Curve:



4) Regression Model Visualization

Core idea

Regression diagnostics use residuals, prediction error plots, regularization tuning, and influence analysis.

Key points

- Residual plot (residual vs predicted): should look random around zero.
- Prediction error plot (predicted vs actual): points near 45-degree line indicate better fit.
- Alpha selection: choose regularization strength using CV error curve.
- Cook's Distance: detects influential points.

Formulas

Residual:

$$e = y - \widehat{y}$$

Cook's Distance:

$$D_i = \frac{\sum_{j=1}^{n} (\widehat{y}_j - \widehat{y}_{j(i)})^2}{p \cdot s^2}$$

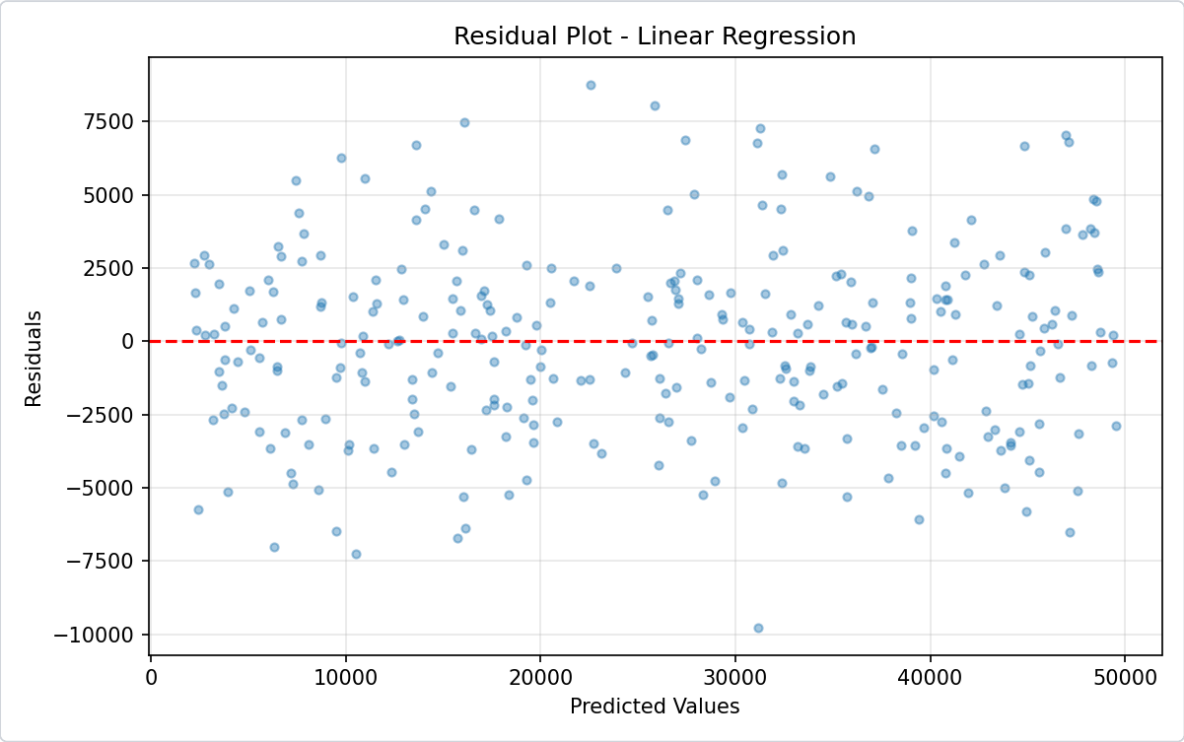
where p is number of parameters, s^2 is MSE.

Heuristic threshold:

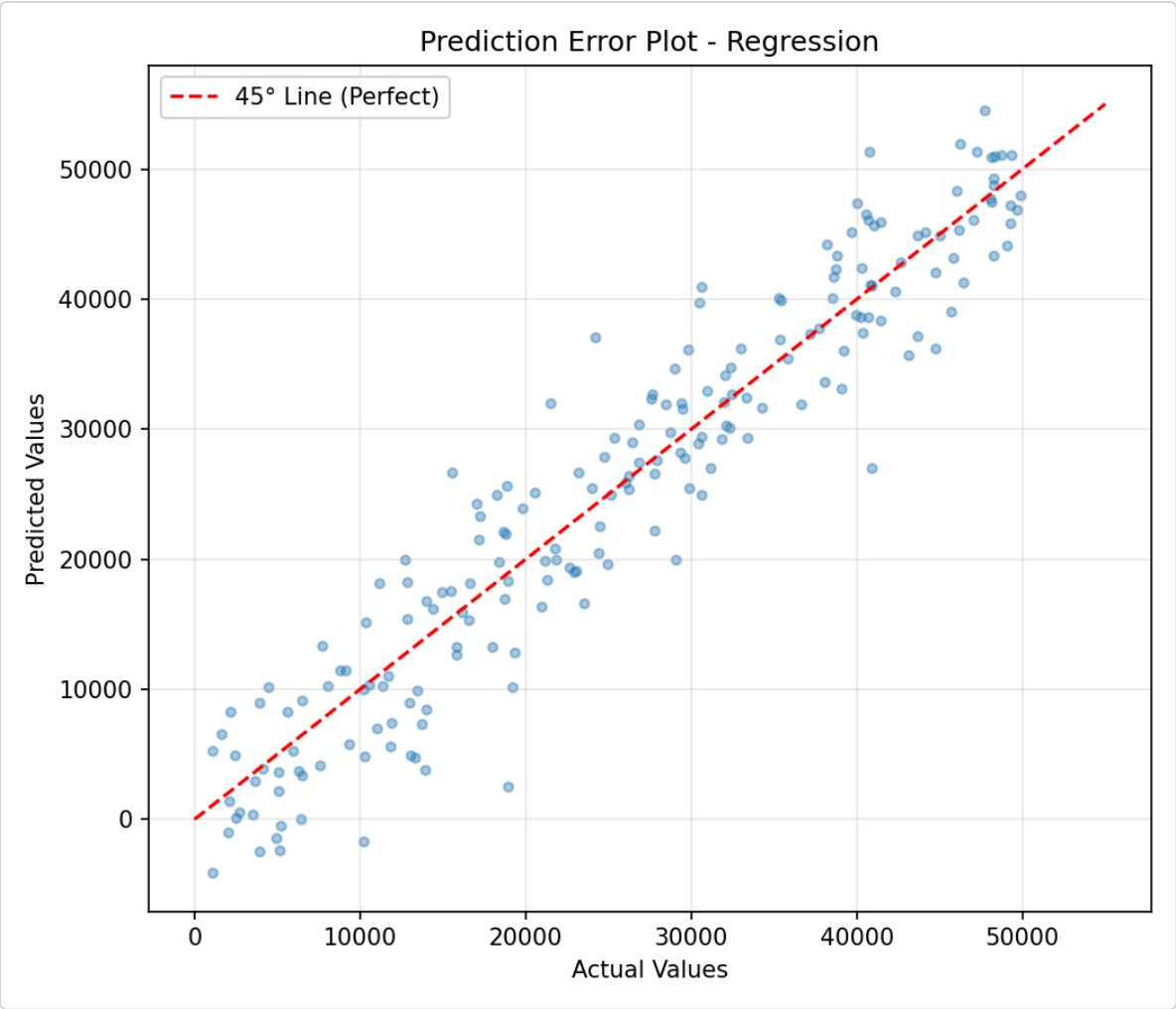
$$D_i > \frac{4}{n}$$

Graphs

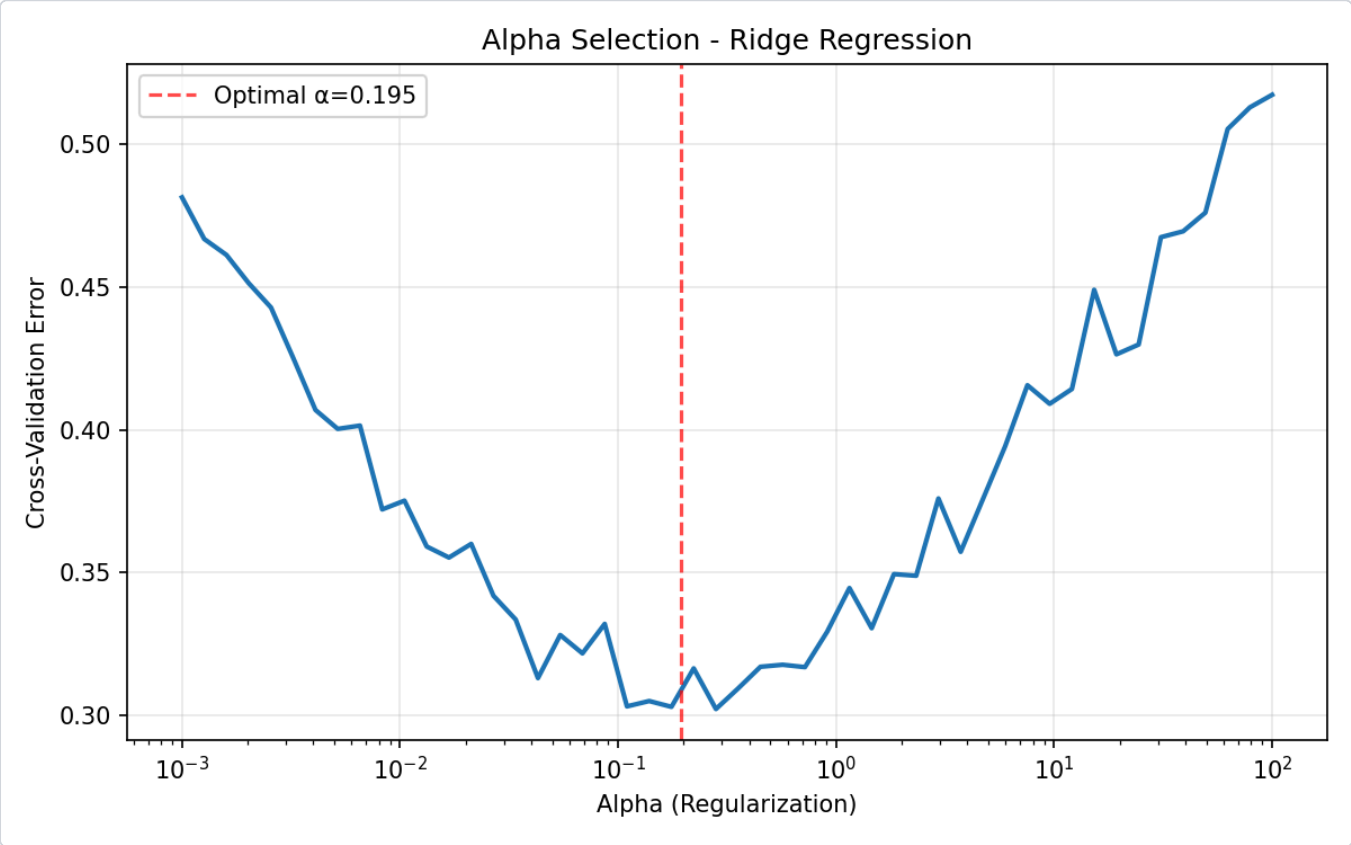
Residual Plot:



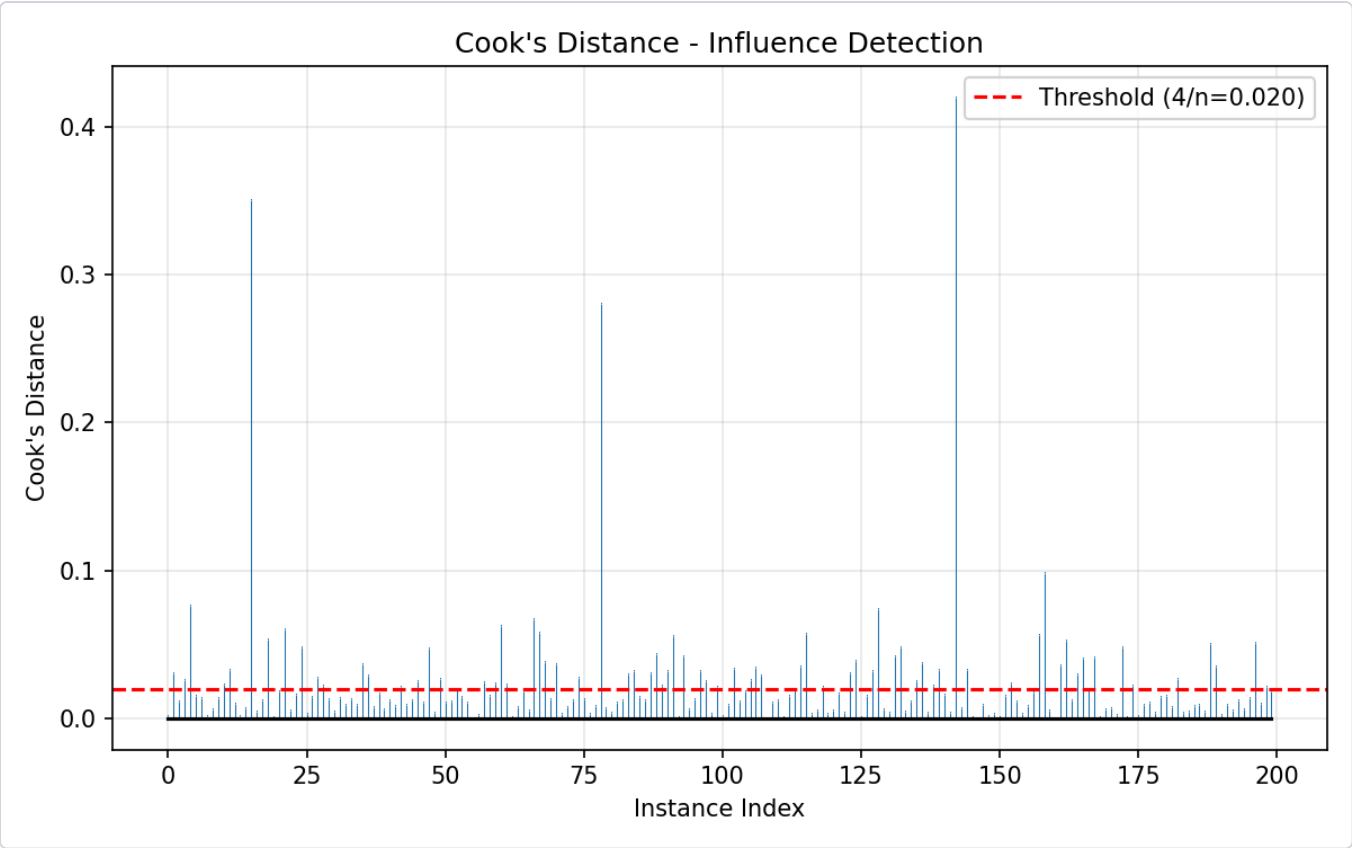
Prediction Error Plot:



Alpha Selection (Ridge):



Cook's Distance:



5) Clustering Model Visualization

Core idea

Since clustering has no labels in many cases, we use internal quality measures and visual diagnostics.

Methods

- Elbow method: choose k near major bend in distortion plot.
- Silhouette coefficient:

$$s = \frac{b - a}{\max(a, b)}$$

a = mean intra-cluster distance, b = mean nearest-cluster distance.

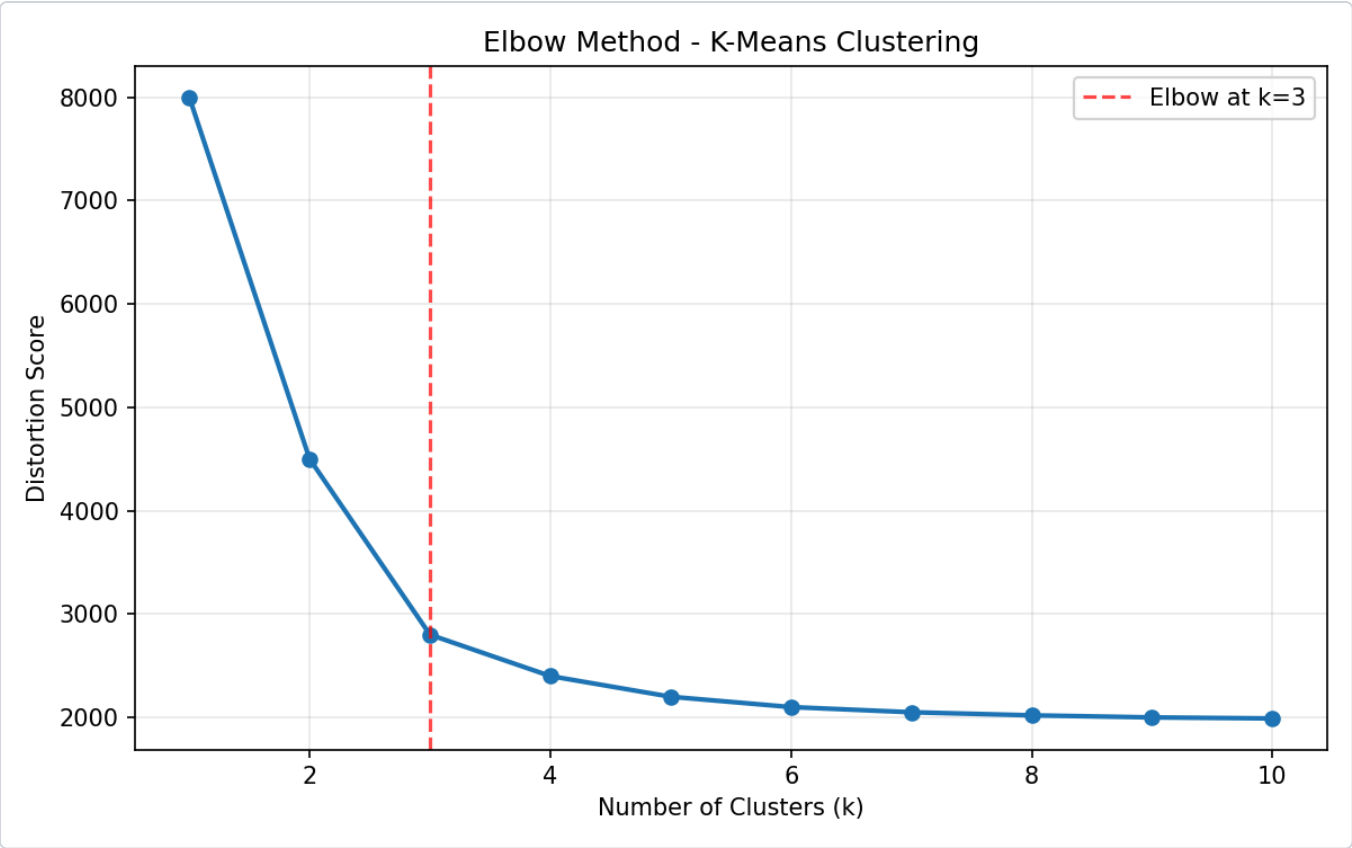
Interpretation: - `s ~ 1`: compact, well-separated clusters. - `s ~ 0`: overlapping clusters. - `s < 0`: likely wrong assignment.

Steps

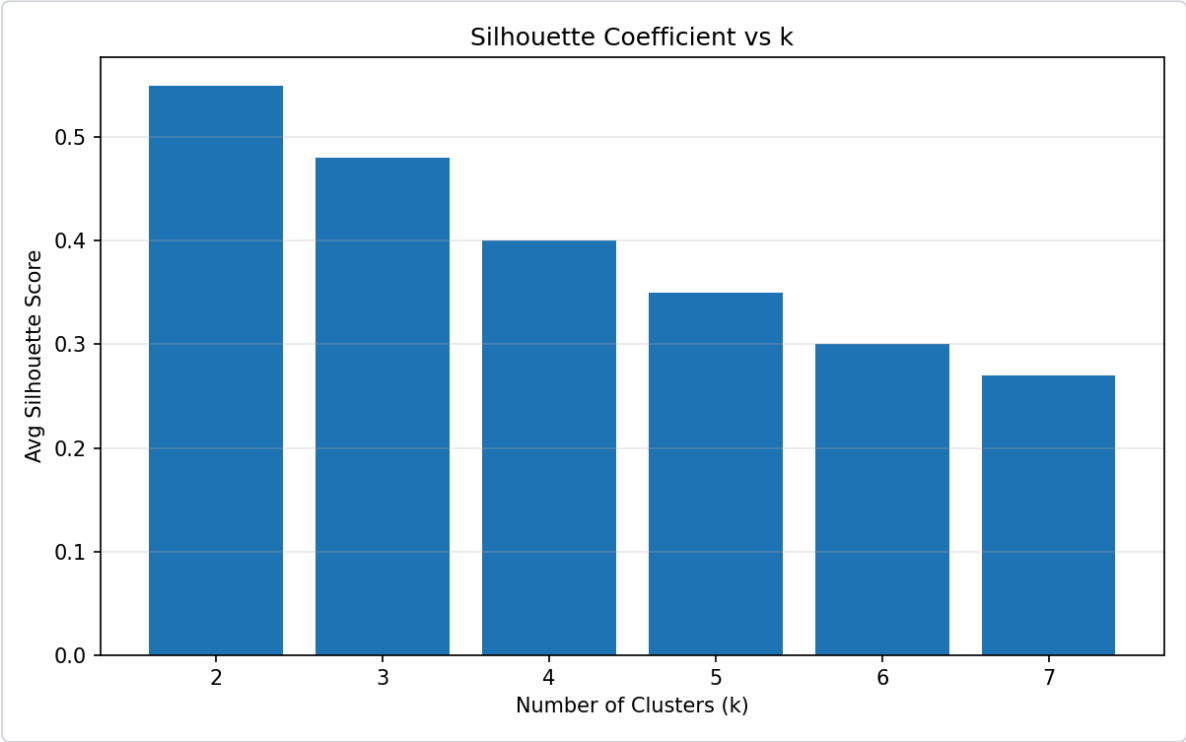
1. Fit clustering for k `= 1..K`.
2. Plot distortion vs k and find elbow.
3. Validate with silhouette scores and distance maps.

Graphs

Elbow Method:



Silhouette Scores:



6) Interpretable ML Properties (Comparison Lens)

Use these properties to compare interpretable algorithms: - Local vs Global explanation - Linearity vs non-linearity - Monotonicity - Feature interactions - Model complexity

Higher interaction capacity usually improves predictive power but reduces interpretability.

7) Traditional Interpretable Algorithms

7.1 Linear Regression

Model:

$$y = w_0 + w_1 x_1 + \cdots + w_d x_d$$

Training error:

$$E_{train}(w) = \frac{1}{N} \parallel Xw - y \parallel^2$$

Normal equation:

$$w_{opt} = (X^T X)^{-1} X^T y$$

Ridge:

$$w_{opt} = (X^T X + \lambda I)^{-1} X^T y$$

Lasso:

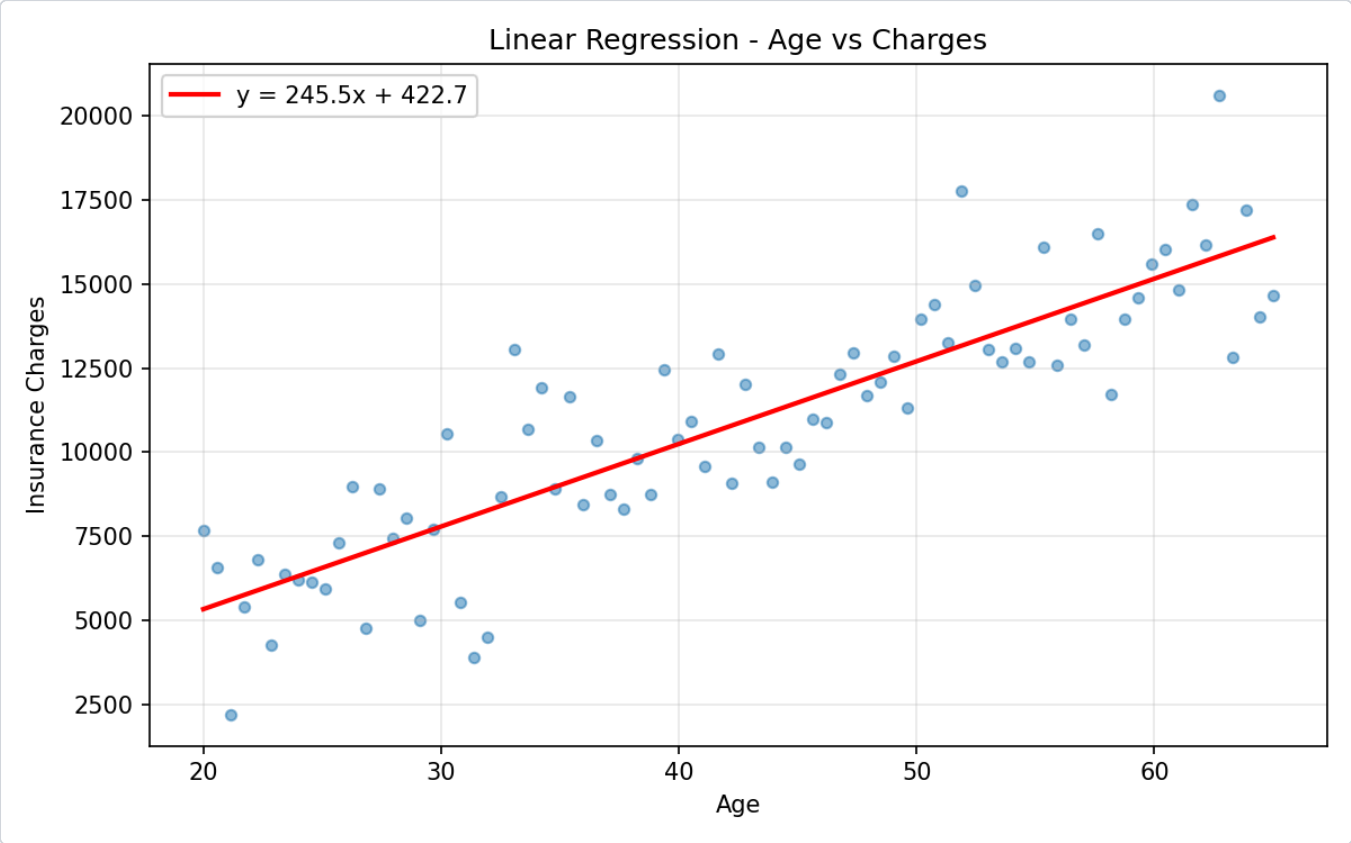
$$w_{opt} = \underset{w}{\operatorname{argmin}} E_{train}(w) + \lambda \parallel w \parallel_1$$

Elastic Net:

$$w_{opt} = \underset{w}{\operatorname{argmin}} E_{train}(w) + \lambda_1 \parallel w \parallel_1 + \lambda_2 w^T w$$

Assumptions: linearity, constant variance, low multicollinearity, near-normal residuals.

Graph:



7.2 Logistic Regression

Hypothesis:

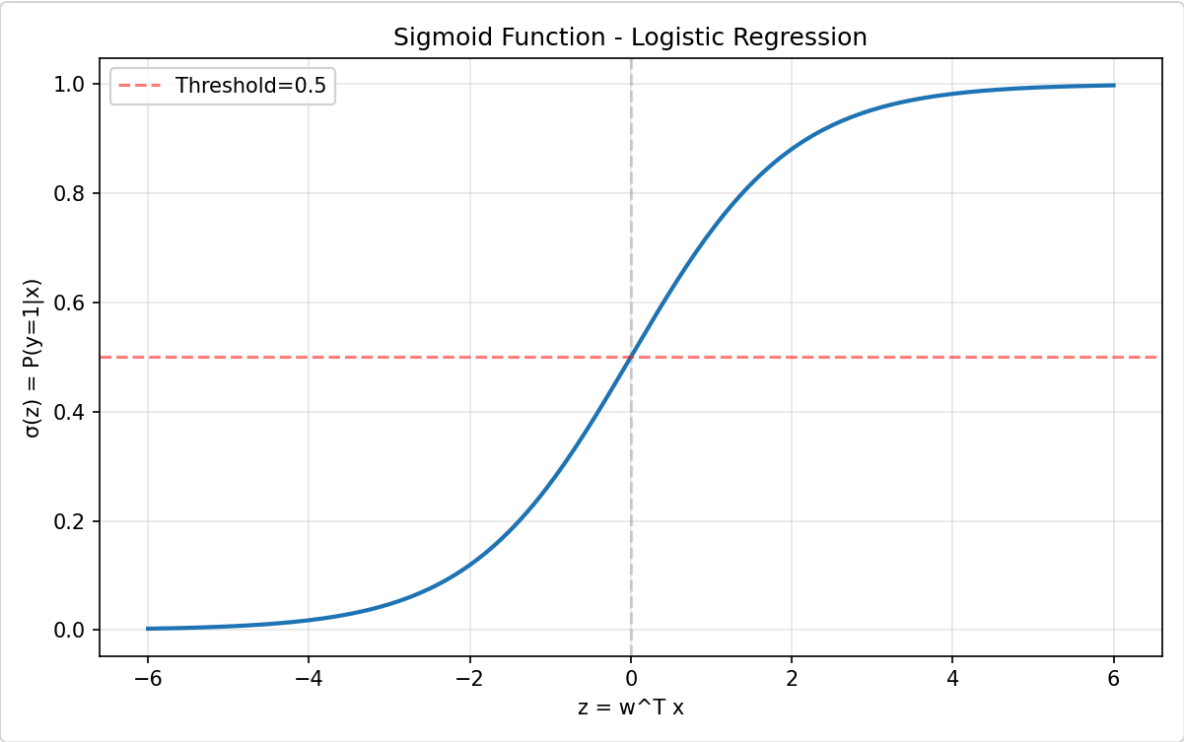
$$P(y = 1|x) = \sigma(w^T x) = \frac{\exp(w^T x)}{1 + \exp(w^T x)}$$

Odds form:

$$\frac{P(y = 1|x)}{P(y = -1|x)} = \exp(w^T x)$$

Each unit increase in feature `x_i` multiplies odds by `\exp(w_i)`.

Graph:



7.3 Generalized Linear Models (GLM)

General form:

$$g(E(y|x)) = w_0 + w_1x_1 + \cdots + w_dx_d$$

Poisson (log link):

$$E(y|x) = \exp(w_0 + w_1x_1 + \cdots + w_dx_d)$$

Logistic regression is a binomial GLM with logit link.

7.4 Generalized Additive Models (GAM)

$$g(E(y|x)) = w_0 + f_1(x_1) + f_2(x_2) + \cdots + f_d(x_d)$$

Smoothing spline objective:

$$\min \frac{1}{N}\sum_{i=1}^{N}(y_i - f(x_i))^2 + \lambda \int (f''(x))^2\,dx$$

GAM captures non-linear single-feature effects but usually not interactions (unless extended variants are used).

7.5 Naive Bayes

Decision rule:

$$h(x) = \arg\max_{y \in \{0,1\}} P(Y = y)\prod_{j=1}^{d} P(X_j = x_j|Y = y)$$

Gaussian conditional:

$$P(X = x|Y = y) = \frac{1}{\sqrt{2\pi\sigma_k^2}}\exp\left(-\frac{(x-\mu_k)^2}{\sigma_k^2}\right)$$

Very fast and simple; main limitation is feature-independence assumption.

7.6 Bayesian Networks

DAG-based probabilistic model with conditional dependencies. Counterfactual influence check:

$$\max_{A,A'}\left|P(Y|X_1,\ldots,X_n,A) - P(Y|X_1,\ldots,X_n,A')\right|$$

Supports local and global reasoning; structure learning can be expensive.

7.7 Decision Trees (CART)

Gini impurity:

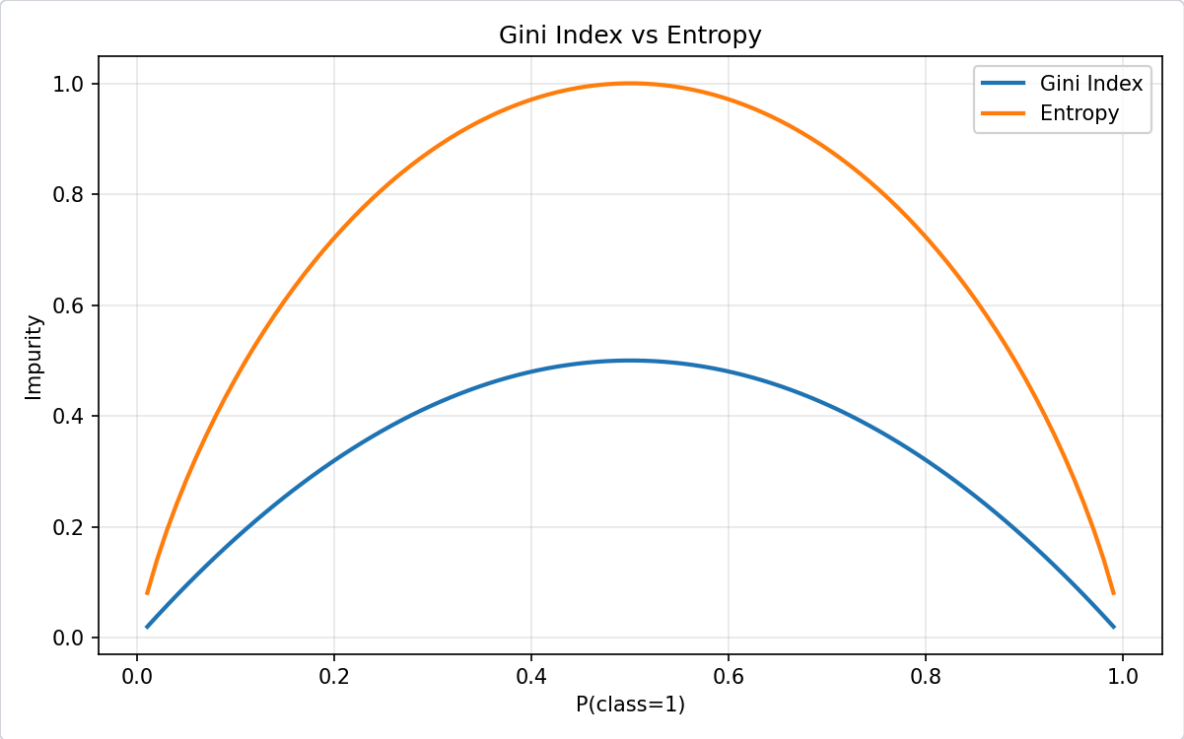
$$\text{Gini} = 1 - \sum_j p_j^2$$

Entropy:

$$H = -\sum_j p_j \log_2(p_j)$$

Interpretable rule paths, handles interactions/non-linearity, but can overfit without pruning.

Graph:



7.8 Rule Induction (CN2)

Separate-and-conquer strategy: 1. Learn one high-quality rule. 2. Remove covered instances. 3. Repeat until positives are covered. 4. Prune to control overfitting.

Good interpretability via explicit IF-THEN rules; rule ordering affects prediction.

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8) Quick Comparison Table

Algorithm	Scope	Linearity	Monotonicity	Feature Interactions	Complexity
Linear Regression	Global	Linear	Yes	No	Low
Logistic Regression	Global	Linear	Yes	No	Low
GLM	Global	Linear (in link space)	Yes	No	Low-Medium
GAM	Global	Non-linear (additive)	Usually yes	Limited	Low-Medium
Naive Bayes	Global + Local	Usually linear boundary (variant-dependent)	Usually yes	No	Low
Bayesian Network	Global + Local	Non-linear	Not guaranteed	Yes	Medium
Decision Tree (CART)	Global	Non-linear	Partial	Yes	Medium-High
Rule Induction (CN2)	Global + Local	Non-linear	Partial	Yes	Medium-High