

# 1.1.3

# General Introduction

Model selection and performance evaluation techniques

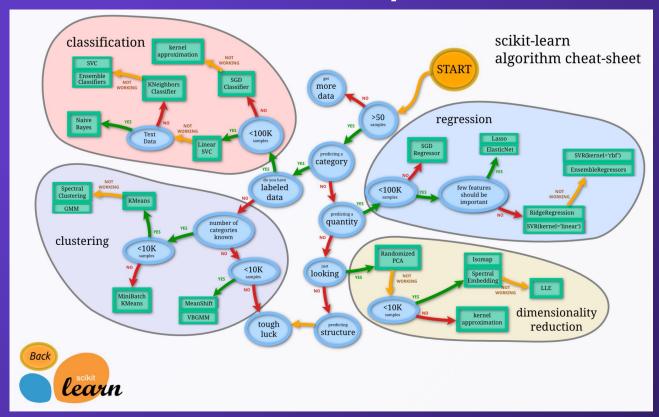


## Model Selection Techniques

- Choosing the right model is crucial for machine learning success
- Performance evaluation helps us understand how well a model performs
- Cross-validation aids in model selection and provides more reliable performance estimates



# Model Selection Techniques





### Model Selection Techniques

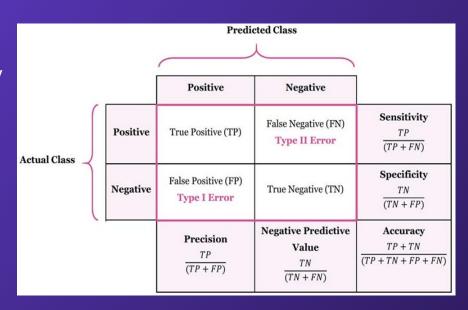
- Choosing the right model depends on the problem and data
- Common Techniques:
  - Understanding the Problem: Classification, Regression, etc.
  - Data Characteristics: Size, Complexity, Feature Types
  - Prior Knowledge and Assumptions
  - Experimentation and Comparison: Trying different models and evaluating their performance
  - Cross-validation: Helps select the best model and prevent overfitting



### Performance Evaluation Metrics

#### Classification Metrics

- Accuracy: The percentage of correctly classified instances.
- Precision: The proportion of true positives within the total predicted positives.
- Recall: The proportion of correctly identified true positives.
- F1-Score: Balances precision and recall, offering a single metric for comparison.
- Confusion Matrix: A table visualizing how well the model predicts each class.





## Choosing Classification Metrics

- Use accuracy when:
  - The classes are balanced and there are equal costs associated with false positives and false negatives
- Use precision when:
  - False positives carry a heavier penalty than false negatives
- Use recall when:
  - Missing an actual positive is substantially more costly than falsely detecting extra positives
- Use the F1 Score when:
  - You need a balance between Precision and Recall.
  - Particularly useful when dealing with imbalanced classes, and both types of errors are important.



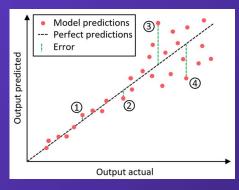
### Performance Evaluation Metrics

#### Regression Metrics

- Mean Squared Error (MSE): Average of the squared differences between predicted and actual values. Lower MSE indicates a better fit.
- Root Mean Squared Error (RMSE): Square root of MSE

 R-squared: The coefficient of determination. Represents the proportion of variance in the target variable explained by the model. Closer to 1 is

better.



$$\begin{split} \mathit{MSE} &= \frac{1}{N} \sum_{i=1}^{N} (y_i - \hat{y})^2 \\ \mathit{RMSE} &= \sqrt{\mathit{MSE}} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (y_i - \hat{y})^2} \\ R^2 &= 1 - \frac{\sum (y_i - \hat{y})^2}{\sum (y_i - \bar{y})^2} \\ \end{split}$$
 Where, 
$$\frac{\hat{y}}{\bar{y}} - \operatorname{predicted} \ value \ of \ y$$
 
$$\frac{\hat{y}}{\bar{y}} - \operatorname{mean} \ value \ of \ y$$

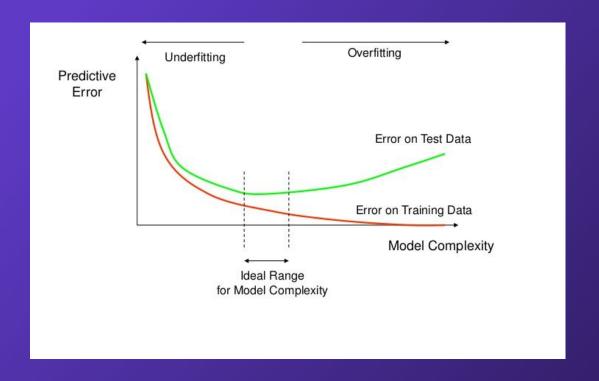


# Choosing Regression Metrics

- Use Root Mean Squared Error (RMSE) when:
  - You want a metric that is in the same units as the dependent variable,
     making interpretation straightforward and penalize large errors.
- Use R-squared (R<sup>2</sup>) when:
  - You need to explain the proportion of variance in the target variable that is predictable from the independent variables and need an intuitive scale from 0 to 1 to compare between models.



# Overfitting, Underfitting, & Cross-validation





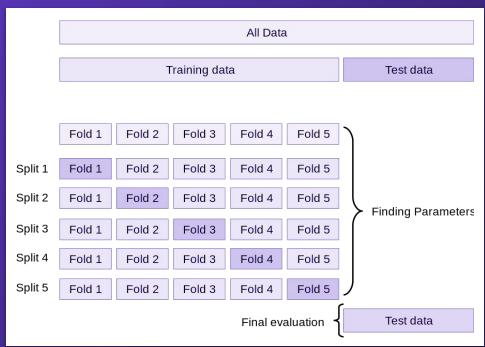
# Overfitting, Underfitting, & Cross-validation

- Overfitting: Model memorizes training data but fails to generalize to unseen data
- Underfitting: Model fails to capture the underlying patterns in the data
- Cross-validation:
  - Splits data into multiple folds
  - Trains and evaluates the model on each fold
  - Helps prevent overfitting
- Techniques to Further Avoid Overfitting:
  - Regularization (L1/L2 penalties)
  - Dropout
  - Early Stopping



## Types of Cross-Validation

- k-Fold Cross-Validation: Data split into k folds; model trained on k-1 folds and tested on the remaining fold
- Leave-One-Out Cross-Validation (LOOCV): A special case of k-fold where k equals the number of data points
- Stratified Cross-Validation:
   Ensures each fold has a similar distribution of classes (useful for imbalanced datasets)





# Model Selection & Evaluation in Practice

- Model selection and performance evaluation are iterative processes
- Start with simpler models and add complexity if needed
- Utilize cross-validation to guide your choices
- Continuously evaluate on real-world data to monitor performance over time
- Don't be afraid to experiment and refine your models

