ML_U2

Regression is a **statistical and machine learning technique** used to model and analyze the relationship between a **dependent variable** (target) and one or more **independent variables** (predictors).

Its goal is to predict or estimate the dependent variable based on known values of the independent variables.

- **Dependent Variable (Y):** The value we want to predict (e.g., house price, sales revenue).
- **Independent Variables (X):** The input features used for prediction (e.g., area, location, number of bedrooms).

Need for Regression

Regression is important in many real-life scenarios because it provides both **prediction** and **relationship analysis**.

1. Prediction of future outcomes

• Example: Predicting rainfall based on humidity and temperature.

2. Relationship understanding

• Shows how the dependent variable changes when independent variables change.

3. Forecasting trends

• Example: Estimating future sales from past sales data.

4. Decision-making & planning

- Helps businesses choose strategies (e.g., which features increase product sales).
- 5. Quantifying impact of factors

 Example: Finding which factor most influences customer satisfaction.

Regression and Correlation

Aspect	Regression	Correlation ©
Purpose	Predicts dependent variable from independent variables and shows the nature of relationship.	Measures strength and direction of relationship between two variables.
Direction	One-way (predict Y from X).	No direction; relationship is mutual.
Output	Regression equation ($Y=a+bX$).	Correlation coefficient (r) between -1 and +1.
Variable Types	One dependent (Y) and one/more independent (X).	Two variables treated equally; no dependent/independent distinction.
Application	Used for prediction and forecasting.	Used for measuring degree of association.
Example	Predicting salary from years of experience.	Measuring relationship between salary and years of experience.

Types of Regression

1. Univariate vs. Multivariate Regression

Univariate Regression

A regression model with only one independent variable (X) used to predict a single dependent variable (Y).

Purpose: Helps to understand and quantify the relationship between two variables. **Equation:** Y = a + bX, where a = intercept, b = slope (change in Y per unit change in X). Example: Predicting student marks based on hours studied.

Graph: Straight line in a 2D plot (X vs Y).

Multivariate Regression

A regression model with two or more independent variables (X1, X2, ...) used to predict one dependent variable (Y).

Purpose: Captures more complex relationships and accounts for multiple influencing factors. **Equation:** Y = a + b1X1 + b2X2 + ... + bnXn, where b1, b2 ... = coefficients for each predictor. Example: Predicting house price from size, location,

and age.

Graph: Can be visualized as a plane (for 2 predictors) or hyperplane (for more predictors).

2. Linear vs. Nonlinear Regression

Linear Regression

A regression model where the relationship between dependent and independent variables is linear in the parameters.

Key Point: Variables can be transformed (e.g., polynomial), but coefficients appear in a linear way.

Equation: Y = a + bX. Example: Predicting salary from years of experience.

Advantages: Simple, fast to compute, easy to interpret.

Graph: Straight line in 2D, flat plane in higher dimensions.

Nonlinear Regression

logarithmic, S-shape).

Definition: A regression model where the relationship is nonlinear in parameters. Parameters may appear in exponents, products, or other nonlinear forms. Example: Equation Y $e^{(bX)}$. Example: Modeling population growth using an exponential Advantages: Captures complex, curved patterns. Disadvantages: Harder to compute, may need iterative methods. exponential, Graph: Curved fit line (e.g.,

3. Simple Linear vs. Multiple Linear Regression

Simple Linear Regression (SLR)

Linear regression with one independent variable. **Equation**: Y = a + bX. Example: Predicting marks from hours studied. Interpretation: b tells how much Y changes for a one-unit increase in X. **Graph**: Straight line on 2D plot.

Multiple Linear Regression (MLR)

Linear regression with two or more independent variables.

Equation: Y = a + b1X1 + b2X2 + ... + bnXn. **Example:** Predicting salary based on experience, education level, and skill score. Interpretation: Each bi represents the effect of Xi on Y, keeping other variables constant. Graph: Plane for two predictors, hyperplane for more.

Bias-Variance Trade-Off

The **Bias–Variance Trade-Off** describes the balance between a model's ability to **fit the training data** and its ability to **generalize to unseen data**. The goal is to minimize the **Total Error** (Generalization Error), which comes from three sources:

Total Error=Bias2+Variance+Irreducible Err



High Bias \rightarrow Underfitting \rightarrow Simple model.

High Variance \rightarrow Overfitting \rightarrow Complex model.

Bias

- Error caused by **overly simplistic assumptions** in the model.
- High bias → **Underfitting** (model misses important patterns).
- Example: Using a straight line to fit non-linear data.

Characteristics of High Bias:

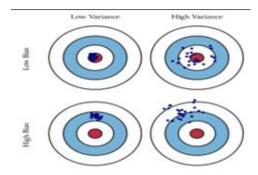
- Poor training accuracy.
- Poor test accuracy.
- Model is too simple.

Variance

- Error caused by too much sensitivity to training data fluctuations.
- High variance → Overfitting (model memorizes training data but fails to generalize).
- Example: Using a high-degree polynomial to fit simple data.

Characteristics of High Variance:

- High training accuracy.
- Low test accuracy.
- Model is too complex.



Overfitting

When a model learns the training data too well, including noise, it performs well on training data but poorly on new (test) data.

- Low training error, high test error
- Predictions follow overly complex curves or patterns

Causes:

- Too many features or parameters
- Too little training data
- Long training without regularization
- Data leakage

Detection:

- Large gap between training and test performance
- High variation in cross-validation scores
- Learning curve shows low training error but high test error

Remedies:

- Add regularization
- Use simpler model
- Prune decision trees or limit depth
- Increase k in k-NN
- Early stopping or dropout (for neural networks)
- Data augmentation or cleaning
- Use cross-validation
- Apply ensembling (bagging)

Underfitting

When a model is too simple to capture the actual pattern in data, it performs poorly on both training and test sets.

- High training error and high test error
- Misses obvious patterns or trends

Causes:

- Model too simple
- Not enough features
- Too much regularization
- Training stopped too early

Detection:

- Learning curve shows both training and test errors are high and close
- Residual plots show clear patterns

Remedies:

- Use a more complex model
- Add more useful features
- Reduce regularization
- Train for longer
- Add interaction terms or nonlinear transformations

Polynomial Regression

Polynomial Regression is an **extension of Linear Regression** that allows us to model **non-linear relationships** between the independent variable(s) XXX and dependent variable YYY.

While **Linear Regression** fits a straight line to the data, Polynomial Regression fits a **curved line** by adding higher-degree terms of the predictor variable.

Why Polynomial Regression?

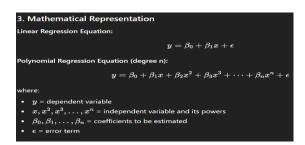
- In real-world problems, relationships are rarely perfectly linear.
- Example: Growth rate of bacteria, housing prices vs. area, learning curves, etc. often follow a curved trend.
- Linear regression would underfit such data because it assumes a constant slope, but polynomial regression can capture bends and curves.

How It Works

- We **transform** the original features by adding polynomial terms.
- Then we perform **Linear Regression** on these transformed features.
- Even though the curve looks non-linear in xxx, the regression is **linear in coefficients**, so it can be solved using the same least squares method.

Choosing the polynomial degree (n) is critical:

- **Too low degree** → Underfitting.
- **Too high degree** → Overfitting.
- Use **cross-validation** to choose optimal n.



Advantages

- ✓ Captures non-linear trends.
 ✓ Easy to implement with existing linear regression algorithms.
- ♥ Works well when the true relationship is polynomial-like.

8. Limitations

- X High-degree polynomials are sensitive to noise
 → Overfitting.
- **X** Can oscillate wildly between points (Runge's phenomenon).
- ➤ Poor extrapolation predictions outside the data range can be unrealistic.

Example: Predicting exam scores based on study hours where improvement rate slows after a certain point.

Stepwise Regression

Stepwise regression is a variable selection method for multiple linear regression that iteratively adds or removes predictors based on statistical criteria such as **p-values**, **AIC**, **BIC**, **or adjusted R**². It aims to find a parsimonious model that explains the data without including unnecessary variables.

Mathematical Expression: Starts with:

$$y=\beta 0+\beta 1X1+\cdots+\beta pXp+\epsilon$$

The algorithm chooses the subset of XXX that minimizes an error metric.

Working:

- 1. **Forward Selection** Start with no variables, add the one with the highest significance until no improvement.
- 2. **Backward Elimination** Start with all variables, remove the least significant one at each step.
- 3. **Stepwise** Combination of both methods.

Advantages:

- Reduces overfitting by eliminating irrelevant variables.
- Automates model building.
- Improves interpretability.

Limitations:

- Can ignore variable interactions.
- May overfit if selection is based solely on training data.
- Unstable when predictors are highly correlated.

Example: Selecting important economic indicators for predicting GDP growth.

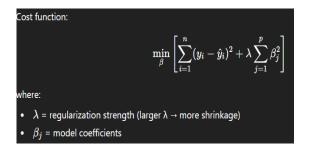
Ridge Regression

Concept:

Ridge Regression is a **regularized form of linear regression** that adds an **L2 penalty** to the loss function.

This penalty shrinks large coefficient values, which helps reduce **overfitting** and handle **multicollinearity** (high correlation between predictors).

It keeps all predictors in the model but with reduced magnitudes.



Working Process:

- 1. Start with the **Ordinary Least Squares** (**OLS**) regression formulation.
- 2. Add an **L2 penalty term** to the cost function.
- 3. Optimize to find coefficients that minimize both **prediction error** and **coefficient magnitude**.

4. Larger $\lambda \to \text{more shrinkage}$; $\lambda = 0$ gives standard linear regression.

Advantages:

- Handles multicollinearity effectively.
- Reduces model complexity and **overfitting**.
- Works well when most predictors have small to moderate effects.

Limitations:

- Does **not** perform feature selection (keeps all predictors).
- Choice of λ requires **cross-validation**.
- Coefficients become biased due to shrinkage.

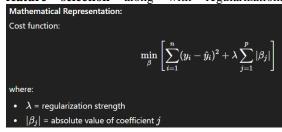
Example:

Predicting **sales** using multiple highly correlated marketing variables (e.g., TV ads, online ads, print ads).

Lasso Regression

Lasso Regression (Least Absolute Shrinkage and Selection Operator) is a regularized linear regression method that uses an L1 penalty on the coefficients.

Unlike Ridge Regression, Lasso can shrink some coefficients **exactly to zero**, effectively performing **feature selection** along with regularization.



Working Process:

- 1. Start with **Ordinary Least Squares (OLS)** regression.
- 2. Add an **L1 penalty term** to the cost function.
- Optimization via coordinate descent or LARS algorithm forces some coefficients to be exactly zero.
- 4. Larger $\lambda \to \text{more coefficients shrink to zero.}$

Advantages:

• Performs automatic feature selection.

- Produces simpler, more interpretable models.
- Useful when only a subset of predictors are important.

Limitations:

- In presence of highly correlated predictors, it tends to select only one and ignore others.
- Choice of λ is critical and requires crossvalidation.
- May be unstable for small datasets.

Example:

Selecting important **genes** from thousands of genomic variables to predict disease risk.

ElasticNet Regression is a hybrid regularization method that combines L1 penalty (from Lasso) and L2 penalty (from Ridge). It performs feature selection like Lasso while maintaining stability in the presence of highly correlated predictors like Ridge.

Mathematical Representation: Cost function:
$$\min_{\beta} \left[\sum_{i=1}^n (y_i - \hat{y}_i)^2 + \lambda_1 \sum_{j=1}^p |\beta_j| + \lambda_2 \sum_{j=1}^p \beta_j^2 \right]$$

Working Process:

- 1. Transform problem into a mix of **L1 and L2 regularization**.
- 2. α controls the balance:
 - \circ $\alpha = 1 \rightarrow pure Lasso$
 - $\alpha = 0 \rightarrow \text{pure Ridge}$
- 3. Solve using coordinate descent or similar optimization methods.
- 4. Select λ using cross-validation.

Advantages:

- Handles **multicollinearity** better than Lasso.
- Performs feature selection while keeping correlated variables.
- More flexible than Ridge or Lasso alone.

Limitations:

- Requires tuning of two parameters (λ and α).
- More computationally intensive than Ridge/Lasso.

Interpretability slightly reduced compared to Lasso.

Example:

Predicting **customer churn** using many correlated customer behavior features where both feature selection and stability are needed.

Bayesian Linear Regression

Bayesian Linear Regression is a **probabilistic approach** to linear regression where model parameters (coefficients) are treated as **random variables** with prior probability distributions. Using **Bayes' theorem**, the model updates these priors into **posterior distributions** after seeing the data, providing both predictions and **uncertainty estimates**.

Mathematical

Representation:

Bayes' theorem for regression:

 $p(\beta|X,y) \!\!=\!\! (p(y|X,\!\beta) \!\cdot\! p(\beta))/p(y|X)$

where:

- $p(\beta)$ = prior distribution of coefficients
- $p(y|X,\beta) = likelihood from data$
- $p(\beta|X,y) = posterior distribution after observing data$

Prediction distribution:

 $p(y*|x*,X,y)=\int p(y*|x*,\beta) p(\beta|X,y) d\beta p$

Working Process:

- 1. **Define prior** for coefficients (commonly Gaussian with mean 0).
- 2. **Calculate likelihood** from observed data using the linear model.
- 3. Apply **Bayes' theorem** to obtain the posterior distribution.
- 4. Predict new values using the **posterior mean** (point estimate) or full distribution for uncertainty quantification.

Advantages:

- Produces uncertainty intervals for predictions.
- Can incorporate prior knowledge about parameters.
- Works well with small datasets.
- Naturally prevents overfitting through prior regularization.

Limitations:

- Requires **specifying priors** carefully.
- Computationally expensive for large datasets.
- Analytical solutions may not exist for complex priors (requires approximation methods like MCMC).

Example:

Forecasting **monthly sales** while accounting for uncertainty and prior knowledge about seasonal effects.

1. Mean Squared Error (MSE)

MSE is the average of the squared differences between actual and predicted values. Squaring ensures all errors are positive and penalizes larger errors more heavily.



• Interpretation

- \circ Lower MSE \rightarrow better fit.
- Value is **always** \geq **0**; 0 means perfect predictions.

Advantages

- Easy to compute mathematically.
- Penalizes large errors strongly → useful when big mistakes are costly.

Disadvantages

- Unit is **squared** (not same as target variable).
- Highly sensitive to outliers.

2. Mean Absolute Error (MAE)

• Definition

MAE is the average of the absolute differences between actual and predicted values.

Unlike MSE, it does not square errors, so it treats all errors equally.



• Interpretation

- Measures average magnitude of errors in the same unit as the target variable.
- Gives an idea of how wrong predictions are, on average.

• Advantages

- o Easy to interpret.
- Less sensitive to outliers than MSE

Disadvantages

Does not emphasize large errors
 → may be misleading if big mistakes are important.

3. Root Mean Squared Error (RMSE)

• Definition

RMSE is the square root of MSE. It gives the error in the **same unit** as the target variable.

Formula:
$$ext{RMSE} = \sqrt{rac{1}{n}\sum_{i=1}^n (y_i - \hat{y}_i)^2}$$

• Interpretation

- Shows how far predictions are from actual values, on average.
- Lower RMSE = better model.

Advantages

- Same units as target variable → easy to compare.
- Still penalizes large errors more than MAE.

Disadvantages

Sensitive to outliers.

4. R-squared (R2R^2R2)

Definition

Measures the proportion of variance in the dependent variable explained by the model.

• Formula



• Interpretation

- $R2R^2R2 = 1 \rightarrow perfect fit$
- $R2R^2R2 = 0 \rightarrow \text{model explains}$ none of the variance
- o Can be **negative** if the model is worse than predicting the mean.

Advantages

- Intuitive measure of goodness-offit.
- Easy to compare models on the same dataset.

Disadvantages

- Can increase artificially when adding more variables, even if they are irrelevant.
- Does not indicate bias or overfitting.

5. Adjusted R-squared

• Definition

Modified version of R2R^2R2 that adjusts for the number of predictors in the model. Penalizes adding predictors that don't improve the model.

Formula:	$\text{Adjusted } R^2 = 1 - \left\lceil \frac{(1-R^2)(n-1)}{n-p-1} \right\rceil$
Where:	$\begin{bmatrix} n-p-1 \end{bmatrix}$
• <i>n</i> = number o	f observations
• p = number o	f predictors

Interpretation

- Increases only if the new variable improves the model significantly.
- Useful for comparing models with different numbers of predictors.

Advantages

- Prevents misleading improvement from adding irrelevant predictors.
- Better measure for model selection.

• Disadvantages

- More complex formula.
- Still doesn't guarantee the model is correct.

Univariate Regression vs. Multivariate Regression				
Aspect	Univariate Regression	Multivariate Regression		
1. Number of Independent Variables	Involves only one independent (predictor) variable.	Involves two or more independent (predictor) variables.		
2. Purpose	Examines the relationship between a single predictor and the dependent variable.	Examines the combined effect of multiple predictors on the dependent variable.		
3. Complexity	Simple to model and interpret.	More complex due to multiple predictors and possible interactions.		
4. Equation Form	$Y = \beta_0 + \beta_1 X + \varepsilon$	$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_n X_n + \varepsilon$		
5. Use Case	Predicting sales based on only price.	Predicting sales based on price, advertising spend, and store location together.		

1. Ridge Regression vs. Lasso Regression (6 Points)				
Aspect	Ridge Regression	Lasso Regression		
1. Regularization Type	Uses L2 regularization ($\lambda \sum eta_j^2$).	Uses L1 regularization ((\lambda \sum		
2. Effect on Coefficients	Shrinks coefficients but never exactly zero.	Can shrink some coefficients exactly to zero (feature selection).		
3. Feature Selection	Does not perform feature selection; retains all variables.	Performs automatic feature selection by eliminating irrelevant variables.		
4. Handling Multicollinearity	Good at handling multicollinearity while keeping all predictors.	Can remove redundant predictors entirely when they are highly correlated.		
5. Equation Bias	Adds small bias to reduce variance.	Adds bias but can also create sparse models.		
6. Best Use Case	Best when most features are useful but may have small effects.	Best when many features are irrelevant or dataset is high-dimensional.		

Techniques to Reduce Overfitting in Regression

1. Cross-Validation

- Instead of splitting data into just training and testing, use **k-fold cross-validation**.
- The dataset is divided into *k* subsets. The model trains on (k-1) subsets and validates on the remaining one.
- Helps ensure the model generalizes well and not just fits a single train-test split.

2. Simpler Model

- Reduce model complexity.
- In regression:
 - Use lower-degree polynomials instead of very high-degree ones.
 - Avoid adding unnecessary interaction terms.
- This helps to reduce variance and prevents memorizing training data.

3. Regularization

Regularization introduces a penalty term in the cost function to prevent coefficients from becoming too large.

• Ridge Regression (L2 Regularization): Adds penalty = $\lambda \Sigma (\beta_i^2)$. Shrinks coefficients but never makes them exactly zero. Good for multicollinearity.

- Lasso Regression (L1 Regularization): Adds penalty = $\lambda \Sigma |\beta_i|$. Can shrink some coefficients to exactly zero, performing feature selection.
- Elastic Net (Combination of L1 + L2): Balances Ridge and Lasso. Works well when there are many correlated features.

4. Feature Selection / Dimensionality Reduction

- Too many irrelevant or correlated features increase model variance.
- Solutions:
 - Use feature selection techniques (Forward selection, Backward elimination).
 - Use dimensionality reduction methods like PCA (Principal Component Analysis).
- This reduces noise and improves generalization.

5. Increase Training Data

- With more data, the model learns the true pattern better and noise effect reduces.
- Especially useful when the dataset is small and the model tends to memorize.
- Data augmentation (in images, text, etc.) can also be applied when collecting more data is hard

6. Early Stopping (for iterative optimization models)

- In gradient descent-based models (like polynomial regression with iterative solvers), monitor error on validation set.
- If validation error starts increasing while training error decreases → stop training.
- Prevents the model from over-learning noise.

Decision Tree Regression

- Decision Tree Regression is a supervised learning technique used for predicting continuous numerical values.
- Unlike classification trees (which predict categories), regression trees predict a real

number output (e.g., predicting house prices).

2. Working

1. Splitting the Data:

- The input space is divided into smaller regions by asking a sequence of "if-else" questions (based on feature values).
- Example: "Is area < 1000 sq.ft?"
 → split into two groups.

2. Recursive Partitioning:

 The tree keeps splitting data into subsets until a stopping criterion is met (e.g., maximum depth, minimum samples per leaf).

3. Prediction at Leaves:

 For regression, the value predicted at each leaf node is usually the mean (or median) of the target values in that region.

3. Objective Function

- At each split, the algorithm chooses the feature and threshold that minimizes the prediction error.
- Common error measure: **Mean Squared Error** (**MSE**)

$$MSE = rac{1}{N} \sum_{i=1}^N (y_i - \hat{y})^2$$

- Here, y_i = actual values,
- \hat{y} = mean of values in that region,
- N = number of samples in that region.

4. Example

Suppose we want to predict **house prices** based on "Size of House":

- Root Node: *Is size* < 1000 sq.ft?
 - o If **Yes:** Average price = ₹25 lakh.
 - o If **No:** Next split \rightarrow *Is size* < 2000 *sq.ft?*
 - If **Yes:** Average price = ₹45 lakh.

If **No:** Average price = ₹70 lakh.

Thus, predictions are made by following the path in the tree.

5. Advantages

- Easy to understand and interpret.
- Handles both numerical and categorical features.
- Non-linear relationships can be captured.
- No need for feature scaling (works directly on raw data).

6. Limitations

- Can easily overfit if tree depth is not controlled.
- Predictions are piecewise constant (not smooth).
- Small changes in data can lead to very different trees.

Random Forest Regression

- Random Forest Regression is a supervised ensemble learning method used for predicting continuous values.
- It combines the predictions of multiple decision trees to improve accuracy and reduce overfitting.
- Instead of relying on a single decision tree, it builds many trees and averages their outputs.

2. Working Principle

1. Bootstrap Sampling (Bagging):

- From the training dataset, multiple random samples are taken with replacement.
- Each sample is used to build a separate decision tree.

2. Random Feature Selection:

- At each split in the tree, a random subset of features is chosen (not all features).
- This ensures trees are diverse and not highly correlated.

3. Tree Building:

- Each decision tree is grown (often without pruning).
- Trees may overfit individually, but randomness + averaging reduces this effect.

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4. Prediction: 
• For regression, the final output is the average of predictions from all the decision trees. \hat{y} = \frac{1}{T} \sum_{t=1}^T \hat{y}_t
• Where T = number of trees, 
• \hat{y}_t = prediction of the t^{th} tree.
```

3. Example

Suppose we want to predict **house prices**:

- Tree 1 predicts ₹42 lakh,
- Tree 2 predicts ₹45 lakh,
- Tree 3 predicts ₹44 lakh.
- Final prediction = (42 + 45 + 44)/3 = ₹43.67 lakh.

4. Advantages

- Reduces overfitting compared to a single decision tree.
- Works well for both linear and non-linear relationships.
- Handles large datasets and highdimensional features effectively.
- Robust to missing values and noisy data.

5. Limitations

- More **complex and computationally expensive** than a single tree.
- Less interpretable (harder to visualize than one decision tree).
- Requires tuning (number of trees, max depth, etc.).

Support Vector Regression (SVR)

- Support Vector Regression (SVR) is a supervised machine learning algorithm used for predicting continuous values.
- It is based on the principles of Support Vector Machines (SVM) but adapted for regression tasks.
- SVR tries to fit the best line (or hyperplane) within a predefined margin of tolerance,

rather than minimizing error for every data point.

2. Working Principle

1. Margin of Tolerance (ε-insensitive loss):

 SVR introduces a margin (epsilon, ε) where errors within this boundary are ignored.

2. Support Vectors:

- Only data points lying outside the ε margin (errors beyond tolerance) influence the model.
- These critical points are called support vectors, as they define the regression function.

3. Kernel Trick:

- SVR can use different kernels (linear, polynomial, RBF, etc.) to handle both linear and non-linear relationships.
- Kernels map the input data into higher dimensions where a linear regression hyperplane can be fitted.

3. Example

Suppose we want to predict house prices:

- The true prices vary slightly around ₹44 lakh.
- SVR defines a margin (say ε = ₹1 lakh).
- Predictions within ₹43–45 lakh are considered acceptable (no penalty).
- Only points outside this band affect the model fitting.

4. Advantages

- Effective in **high-dimensional spaces**.
- Works well for both linear and non-linear regression using kernels.
- **Robust to outliers** (small effect, since only support vectors outside the margin matter).
- Provides good generalization due to margin maximization.

5. Limitations

• Computationally expensive, especially for large datasets.

- Requires careful **parameter tuning** (C = penalty parameter, ε = margin, kernel choice).
- Performance is sensitive to **scaling of data** (feature normalization often required).