

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).

General Equation of Regression:

$$Y = f(X) + \epsilon$$

Where:

- $f(X)$ = functional relationship between variables
- ϵ = error term (difference between actual and predicted values)

Example:

Predicting a student's final score (Y) based on hours studied (X).

Simple equation:

$$\text{Score} = a + b \times \text{Hours studied}$$

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 (X_1, X_2, \dots) used to predict one dependent variable (Y).

Purpose: Captures more complex relationships and accounts for multiple influencing factors.

Equation: $Y = a + b_1X_1 + b_2X_2 + \dots + b_nX_n$, where $b_1, b_2 \dots$ = 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

Definition: A regression model where the relationship is nonlinear in parameters. Parameters may appear in exponents, products, or other nonlinear forms.

Equation Example: $Y = a * e^{(bX)}$.

Example: Modeling population growth using an exponential curve.

Advantages: Captures complex, curved patterns.

Disadvantages: Harder to compute, may need iterative methods.

Graph: Curved fit line (e.g., exponential, logarithmic, S-shape).

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: $Y = a + b_1X_1 + b_2X_2 + \dots + b_nX_n$.

Example: Predicting salary based on experience, education level, and skill score.

Interpretation: Each b_i represents the effect of X_i 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

Model Complexity	Bias	Variance	Total Error
Too Simple	High	Low	High
Too Complex	Low	High	High
Optimal	Balanced	Balanced	Low

High Bias → Underfitting → Simple model.

High Variance → Overfitting → 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.

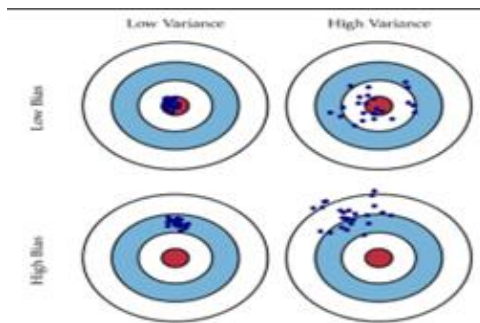
Variance

- 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.

3. Mathematical Representation

Linear Regression Equation:

$$y = \beta_0 + \beta_1 x + \epsilon$$

Polynomial Regression Equation (degree n):

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \dots + \beta_n x^n + \epsilon$$

where:

- y = dependent variable
- x, x^2, x^3, \dots, x^n = independent variable and its powers
- $\beta_0, \beta_1, \dots, \beta_n$ = coefficients to be estimated
- ϵ = error term

Advantages

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

8. Limitations

- ✗ High-degree polynomials are sensitive to noise → Overfitting.
- ✗ 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 R²**. It aims to find a parsimonious model that explains the data without including unnecessary variables.

Mathematical
Starts with:

$$y = \beta_0 + \beta_1 X_1 + \dots + \beta_p X_p + \epsilon$$

Expression:

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.

Decision Tree Regression

Decision Tree Regression is a **non-parametric supervised learning** method used for predicting continuous values. It works by **splitting the dataset into regions** based on decision rules, where each region has similar target values. The final prediction for a region is the **mean** (or sometimes median) of its target values.

Mathematical Representation:

For a region R_m :

$$\hat{y}_{R_m} = \frac{1}{|R_m|} \sum_{x_i \in R_m} y_i$$

The best split minimizes:

$$\text{MSE} = \sum_{m=1}^M \sum_{x_i \in R_m} (y_i - \hat{y}_{R_m})^2$$

Working Process:

1. Start with the full dataset as the root node.
2. Find the feature and split point that **maximally reduces Mean Squared Error (MSE)**.

3. Recursively split each subset into child nodes until stopping criteria are met (max depth, min samples per leaf, or no further improvement).
4. Prediction = **mean target value** of the leaf node where the sample falls.

Advantages:

- Simple to **interpret and visualize**.
- Can capture **non-linear relationships**.
- Works with both numerical and categorical features.
- No need for feature scaling.

Limitations:

- **Prone to overfitting** if grown too deep.
- **High variance** – small changes in data can alter the tree structure.
- Predictions are **piecewise constant**, which may be less smooth than other models.

Example:

Predicting **house prices** based on size, location, and number of bedrooms by splitting data into ranges (e.g., "if size > 1500 sqft and location = city center → higher price").

Random Forest Regression

Random Forest Regression is an **ensemble learning** method that combines predictions from multiple **decision trees** to improve accuracy and reduce overfitting.

It uses **bagging** (Bootstrap Aggregating) and **random feature selection** to create diverse trees and averages their outputs for final prediction.

Mathematical Representation:

If there are T trees $h_t(X)$:

$$\hat{y} = \frac{1}{T} \sum_{t=1}^T h_t(X)$$

Working Process:

1. **Bootstrap Sampling** – Create random samples (with replacement) from the training data.
2. **Random Feature Selection** – At each tree split, consider only a random subset of features.
3. Train each decision tree **without pruning**.
4. For prediction, take the **average** of predictions from all trees.

Advantages:

- **Reduces overfitting** compared to a single decision tree.
- Works well with **non-linear data** and complex relationships.
- Robust to **outliers and noise**.
- Can handle **missing values** effectively.

Limitations:

- Less **interpretable** than a single tree.
- **Computationally expensive** for large datasets.
- Requires careful tuning of parameters (number of trees, max depth, etc.).

Example:

Predicting **car prices** using multiple features (mileage, age, brand, condition) where each tree learns different patterns and the forest combines them for a stable result.

Support Vector Regression (SVR)

Support Vector Regression is the regression counterpart of **Support Vector Machines (SVM)**. Instead of finding a classification boundary, SVR tries to find a function that fits the data **within an ϵ -margin of tolerance**, ignoring small deviations and penalizing only large errors. It can model **linear and non-linear** relationships using **kernels**.

Mathematical Representation:

Optimization problem:

$$\min \frac{1}{2} \|w\|^2 + C \sum_{i=1}^n (\xi_i + \xi_i^*)$$

subject to:

$$y_i - (w^T x_i + b) \leq \epsilon + \xi_i$$

$$(w^T x_i + b) - y_i \leq \epsilon + \xi_i^*$$

where:

- ϵ = tolerance margin
- C = penalty parameter
- ξ_i, ξ_i^* = slack variables for points outside the margin

Working Process:

1. **Choose a kernel** (linear, polynomial, RBF) to transform data if non-linear.
2. Fit a function such that most data points lie **within $\pm\epsilon$** from it.
3. Penalize only the points lying **outside the ϵ -tube**.
4. Use **support vectors** (critical boundary points) for prediction.

Advantages:

- Effective for **high-dimensional** and **non-linear** data.
- Robust to overfitting due to margin control.
- Uses only support vectors, making it memory efficient for small datasets.

Limitations:

- Requires careful tuning of **C, ϵ , and kernel parameters**.
- Computationally expensive for very large datasets.
- Performance sensitive to choice of kernel.

Example:

Predicting **electricity demand** from temperature and time-of-day where the relationship is complex and non-linear.

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.

Cost function:

$$\min_{\beta} \left[\sum_{i=1}^n (y_i - \hat{y}_i)^2 + \lambda \sum_{j=1}^p \beta_j^2 \right]$$

where:

- λ = regularization strength (larger $\lambda \rightarrow$ more shrinkage)
- β_j = model coefficients

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 $\lambda \rightarrow$ 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.

Mathematical Representation:

Cost function:

$$\min_{\beta} \left[\sum_{i=1}^n (y_i - \hat{y}_i)^2 + \lambda \sum_{j=1}^p |\beta_j| \right]$$

where:

- λ = regularization strength
- $|\beta_j|$ = absolute value of coefficient j

Working Process:

1. Start with **Ordinary Least Squares (OLS)** regression.
2. Add an **L1 penalty term** to the cost function.
3. Optimization via **coordinate descent** or **LARS algorithm** forces some coefficients to be exactly **zero**.
4. Larger $\lambda \rightarrow$ 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 cross-validation.
- May be unstable for small datasets.

Example:

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

ElasticNet

Regression

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:

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

Alternatively, using mixing parameter α ($0 \leq \alpha \leq 1$):

$$\text{Penalty} = \lambda \left[\alpha \sum |\beta_j| + (1 - \alpha) \sum \beta_j^2 \right]$$

Working Process:

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

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

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)

• Definition

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.

Formula:

$$MSE = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

Where:

- n = number of data points
- y_i = actual value
- \hat{y}_i = predicted value

• Interpretation

- Lower MSE → better fit.
- Value is **always** ≥ 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.

Formula:

$$MAE = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i|$$

• 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

- 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:

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

• 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 (R^2)

• Definition

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

• Formula

Formula:

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$$

Where:

- \bar{y} = mean of actual values

- **Interpretation**
 - $R^2 = 1 \rightarrow$ perfect fit
 - $R^2 = 0 \rightarrow$ model explains none of the variance
 - Can be **negative** if the model is worse than predicting the mean.
- **Advantages**
 - Intuitive measure of goodness-of-fit.
 - 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 R^2 that adjusts for the number of predictors in the model. Penalizes adding predictors that don't improve the model.

Formula:

$$\text{Adjusted } R^2 = 1 - \left[\frac{(1 - R^2)(n - 1)}{n - p - 1} \right]$$

Where:

- n = number of observations
- p = number of 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.

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	$Y = \beta_0 + \beta_1 X + \epsilon$	$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_n X_n + \epsilon$
5. Use Case	Predicting sales based on only price.	Predicting sales based on price, advertising spend, and store location together.

Aspect	Ridge Regression	Lasso Regression
1. Regularization Type	Uses L2 regularization ($\lambda \sum \beta_j^2$).	Uses L1 regularization ($\lambda \sum \beta_j $).
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.

2. Regression vs. Correlation (6 Points)

Aspect	Regression	Correlation
1. Definition	Predicts the value of a dependent variable from one or more independent variables.	Measures the degree and direction of relationship between two variables.
2. Purpose	Establishes a predictive equation.	Quantifies strength of association.
3. Direction of Relationship	One variable is dependent, others are independent.	No distinction between dependent and independent variables.
4. Output	Gives a regression equation ($\hat{Y} = \beta_0 + \beta_1 X + \varepsilon$).	Gives a correlation coefficient (r) between -1 and +1.
5. Cause & Effect	Implies a cause-effect relationship (if model assumptions are valid).	Does not imply causation, only association.
6. Use Case	Predicting sales from price and advertising spend.	Measuring how strongly price and sales are related.