Chapter 5

Regression and Predictive Modeling

Concept and Use of Empirical Models

- Empirical models are models that are based on observed data rather than on theoretical principles.
- These models use past data to establish relationships between variables.
- The primary use of empirical models is to predict future outcomes or to understand the patterns and dynamics of a system based on real-world data to make informed decisions and predictions.

Key Uses:

- Forecasting future trends (e.g., weather predictions, stock prices).
- Identifying relationships between variables (e.g., advertising expenditure and sales).
- Model development for decision-making in business, science, and technology.

Regression and Predictive Analytics

Regression

• **Regression** is a statistical method used to model the relationship between a dependent variable and one or more independent variables.

Use in Predictive Analytics:

- It is used for predictive analytics to predict the value of the dependent variable based on known values of independent variables.
- Regression models are widely employed to predict continuous outcomes, such as sales, temperatures, or stock prices.
- It helps identify factors that impact the dependent variable, providing insights for decision-making.

Differences Between Regression and Classification Tasks

Regression Tasks:

- These tasks involve predicting a continuous value. For example, predicting house prices based on features like size, location, and number of rooms.
- The target variable is continuous, and the output is a numerical value.

Classification Tasks:

- These tasks involve predicting a categorical outcome, where the target variable is a class or category.
- For instance, classifying an email as spam or not spam. The output is a category or label, not a numerical value.

Differences Between Regression and Classification Tasks

Aspect	Regression	Classification
Output	Continuous values (e.g., sales, price)	Discrete categories (e.g., spam/non-spam)
Objective	Predict a numeric value	Classify observations into categories
Algorithms	Linear regression, Polynomial regression	Logistic regression, Decision trees
Evaluation Metrics	MSE, MAE	Accuracy, Precision, Recall, F1- Score

Simple Linear Regression

- Simple linear regression models the relationship between two variables by fitting a linear equation to the observed data.
- The equation of the line is typically represented as:

$$Y=\beta 0+\beta 1X+\epsilon$$

Where:

- Y is the dependent variable (what you're predicting),
- X is the independent variable (the predictor),
- β0 is the intercept (constant),
- β1 is the slope (the change in Y for a unit change in X),
- ε is the error term (the difference between the predicted and actual values).

Simple Linear Regression (contd.)

Assumptions of Simple Linear Regression

- **1. Linearity:** The relationship between independent and dependent variables is linear.
- 2. Independence: Observations are independent.
- 3. Homoscedasticity: Constant variance of errors.
- 4. Normality of Errors: Errors follow a normal distribution.
- **5. No Multicollinearity:** Only one independent variable (for simple regression).

Simple Linear Regression (contd.)

Application:

- Simple linear regression is used when there is a linear relationship between two variables.
- Common applications include
 - Predicting sales based on advertising spend
 - Predicting the price of an item based on its demand, and
 - Predicting the height of a person based on age.

Simple Linear Regression (contd.)

Interpretation:

- The **slope** β1 tells you the expected change in the dependent variable for each unit increase in the independent variable.
- The **intercept** $\beta 0$ represents the value of the dependent variable when the independent variable is zero.

Concept of Least Squares Estimator (LSE)

- Least Squares Estimator (LSE) is a method used to estimate the parameters of a regression model by minimizing the sum of the squared differences (residuals) between the observed data points and the predicted values.
- In linear regression, the objective is to minimize the sum of squared residuals, $\sum_{i=1}^{n} (y_i \hat{y}_i)^2$
 - where y_i is the actual value and \hat{y}_i is the predicted value.

Concept of Least Squares Estimator (LSE)

 The general form for the least squares method in linear regression is to minimize the following cost function:

$$J(heta)=\sum_{i=1}^n(y_i-(eta_0+eta_1x_i))^2$$

- Where $\beta 0$ and $\beta 1$ are the parameters to be estimated, and x_i are the independent variables.
- The least squares solution provides the estimates for β0 and β1 that minimize the sum of squared residuals.

Example Problem:

 Suppose we have data on the number of hours studied and the corresponding exam scores for 5 students:

Hours Studied (X)	Exam Score (Y)
1	2
2	4
3	5
4	4
5	5

• We want to fit a simple linear regression model to this data

The formula for the slope β_1 and the intercept β_0 using the Least Squares method are:

$$eta_1 = rac{n\sum XY - \sum X\sum Y}{n\sum X^2 - (\sum X)^2}$$
 $eta_0 = rac{\sum Y - eta_1\sum X}{n}$

Where:

- n is the number of data points (here, n=5),
- ullet $\sum XY$ is the sum of the product of X and Y,
- ullet $\sum X$ and $\sum Y$ are the sums of the X and Y values, respectively,
- ullet $\sum X^2$ is the sum of the squared X values.

Calculating the necessary sums:

•
$$\sum X = 1 + 2 + 3 + 4 + 5 = 15$$

•
$$\sum Y = 2 + 4 + 5 + 4 + 5 = 20$$

•
$$\sum X^2 = 1^2 + 2^2 + 3^2 + 4^2 + 5^2 = 1 + 4 + 9 + 16 + 25 = 55$$

•
$$\sum XY = (1 \times 2) + (2 \times 4) + (3 \times 5) + (4 \times 4) + (5 \times 5) = 2 + 8 + 15 + 16 + 25 = 66$$

Plugging these values into the formulas:

$$\beta_1 = \frac{5 \times 66 - 15 \times 20}{5 \times 55 - (15)^2} = \frac{330 - 300}{275 - 225} = \frac{30}{50} = 0.6$$
$$\beta_0 = \frac{20 - 0.6 \times 15}{5} = \frac{20 - 9}{5} = \frac{11}{5} = 2.2$$

So, the Least Squares Estimates are:

- $\beta_1 = 0.6$ (slope),
- $\beta_0 = 2.2$ (intercept).

Thus, the regression equation is: Y=2.2+0.6X

Concept of Maximum Likelihood Estimation

- Maximum Likelihood Estimation (MLE) is a method for estimating the parameters of a model.
- The goal of MLE is to find the parameter values that maximize the likelihood function, which measures how well the model explains the observed data.

Concept of Maximum Likelihood Estimation for Model Fitting

• In linear regression, we assume:

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

The likelihood function for MLE becomes:

$$L(eta_0,eta_1,\sigma^2)=\prod_{i=1}^nrac{1}{\sqrt{2\pi\sigma^2}}e^{-rac{(y_i-eta_0-eta_1x_i)^2}{2\sigma^2}}$$

Maximizing this function leads to the familiar formulas for the regression coefficients obtained by minimizing the sum of squared errors.

Comparing MLE and Least Squares in Regression

MLE	Least Squares (LS)
Maximizes the likelihood of observing the data given the model parameters.	Minimizes the sum of the squared differences between observed and predicted values.
Assumes the error terms follow a specific distribution (usually normal).	No strict distribution assumption for the errors; focuses purely on minimizing squared error.

Comparing MLE and Least Squares in Regression

Mathematical Form

MLE Objective: Maximize

$$L(eta_0,eta_1,\sigma^2)=\prod_{i=1}^nrac{1}{\sqrt{2\pi\sigma^2}}e^{-rac{(y_i-eta_0-eta_1x_i)^2}{2\sigma^2}}$$

Least Squares Objective: Minimize

$$ext{SSE} = \sum_{i=1}^n (y_i - \hat{y_i})^2$$

Understanding Multiple Predictors

 Multiple Linear Regression (MLR) is an extension of simple linear regression to include multiple independent variables (predictors). The general form is:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + ... + \beta_p X_p + \epsilon$$

Where:

- Y: Dependent variable (target)
- β_0 : Intercept
- $\beta_1, \beta_2, ..., \beta_p$: Regression coefficients
- $X_1, X_2, ..., X_p$: Independent variables (predictors)
- ε: Error term

Matrix Notation for MLR

• In matrix form, the equation becomes:

$$Y=X\beta+\epsilon$$

Where:

- Y is an n×1 vector of target values,
- X is an n×(p+1) design matrix (including a column of 1's for the intercept),
- β is a (p+1)×1 vector of coefficients,
- ε is an n×1 vector of error terms.

$$\mathbf{X} = egin{bmatrix} 1 & X_{11} & X_{12} & \dots & X_{1p} \ 1 & X_{21} & X_{22} & \dots & X_{2p} \ dots & dots & dots & \ddots & dots \ 1 & X_{n1} & X_{n2} & \dots & X_{np} \end{bmatrix}$$

Assumptions and Diagnostics in MLR

- Linearity: The relationship between predictors and the response is linear.
- 2. Independence: Observations are independent of each other.
- Homoscedasticity: Constant variance of residuals across all levels of predictors.
- 4. Normality: Residuals follow a normal distribution.
- 5. No multicollinearity: Predictors should not be highly correlated.

Diagnostics:

- Residual plots: To check homoscedasticity and linearity.
- Q-Q plots: To assess normality of residuals.

Derivation of Regression Coefficients Using Matrix Algebra

To estimate the regression coefficients in MLR, we minimize the sum of squared errors (SSE):

$$SSE = (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})$$

The optimal solution is obtained by setting the gradient equal to zero and solving for β :

$$\frac{\partial SSE}{\partial oldsymbol{eta}} = -2\mathbf{X}^T(\mathbf{Y} - \mathbf{X}oldsymbol{eta}) = 0$$

Thus,

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y}$$

Computational Advantages of the Matrix Approach

- 1. Compact Representation: The matrix approach handles multiple predictors elegantly and compactly.
- 2. Efficiency: Matrix operations are optimized
- 3. Generalization: Extending to higher dimensions is straightforward using matrix algebra.

Extending Linear Regression to Nonlinear Relationships

Fitting Polynomial Models to Data

 A polynomial regression model is simply a linear regression where the predictors are polynomial terms of the original variable:

$$Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \dots + \beta_d X^d + \epsilon$$

Steps to Fit Polynomial Models:

- 1. Create polynomial features from the original data.
- 2. Fit a linear regression model using these features.
- 3. Evaluate the fit using metrics like RMSE.

Avoiding Overfitting in Polynomial Regression

Overfitting occurs when the model captures noise instead of the underlying pattern. To avoid overfitting:

- 1. Regularization: Use Ridge or Lasso regression.
- 2. Cross-validation: Validate the model on unseen data.
- **3. Limit polynomial degree:** Choose a reasonable degree for the polynomial.
- 4. Feature selection: Use only relevant features.

Categorical Regressors and Handling Categorical Variables in Regression Models

Categorical variables must be encoded into numerical values to be used in regression models. Two common techniques are:

- **1. One-Hot Encoding:** Create binary columns for each category. Example: "Color" with categories ["Red", "Blue", "Green"] becomes three columns: "Red", "Blue", "Green."
- **2. Label Encoding:** Assign an integer to each category. Example: "Red" = 1, "Blue" = 2, "Green" = 3.
- 3. Ordinal Encoding: Explicitly assigns integer values based on a meaningful order of categories. Suitable for ordinal (ordered) categories. Example: Education Level: High School = 1, Bachelor's = 2, Master's = 3, PhD = 4

Use of Indicator (Dummy) Variables

 Indicator (dummy) variables represent categorical data in regression models. Each category is assigned a binary variable (0 or 1).

Feature Selection Techniques

• Forward Selection: This technique starts with no features and adds features one by one based on their contribution to model performance.

Steps

- 1. Train models with each individual feature.
- 2. Select the feature with the highest performance (e.g., R² for regression).
- 3. Add this feature to the model.
- 4. Repeat until adding more features doesn't improve performance.

Example

Dataset Example:

Feature A	Feature B	Feature C	Target
1	2	3	10
2	1	5	15
3	2	7	21
4	3	9	28

Step 1: Evaluate individual features

- Train separate models using each feature and compute their performance (R² values for regression).
- **Feature A:** $R^2 = 0.70$
- **Feature B:** $R^2 = 0.40$
- **Feature C:** $R^2 = 0.80$

Step 2: Select the best feature

• Feature C has the highest R² (0.80), so **select Feature C**.

Step 3: Add one more feature

- Try combining Feature C with each remaining feature:
 - **C** + **A**: $R^2 = 0.95$
 - **C** + **B**: $R^2 = 0.85$

Step 4: Select the best combination

• Select Feature A (C + A) because it gives the highest R^2 (0.95).

Step 5: Check for further improvement

- Add the remaining feature (B):
 - C + A + B: $R^2 = 0.96$
- Since adding Feature B provides only a minor improvement, stop the process.

Final Selected Features:

- Feature C and Feature A
- This is how forward selection efficiently chooses the most impactful features step by step.

Feature Selection Techniques (contd.)

 Backward Elimination: This technique starts with all features and removes the least significant ones iteratively.

Steps

- 1. Train the model using all features.
- 2. Remove the feature with the least statistical significance or importance.
- 3. Retrain the model and repeat until no insignificant features remain.

Step 1: Train the model with all features (A, B, C)

Compute the model's R² and check the significance (using metrics like p-values).

- R² for (A, B, C) = 0.99
- Feature significance (example p-values):
 - Feature A: 0.02
 - Feature B: 0.10
 - Feature C: 0.01

Step 2: Remove the least significant feature

- Feature B has the highest p-value (0.10), indicating low significance.
- Remove Feature B.

Step 3: Train the model with remaining features (A, C)

- R² for (A, C) = 0.98
- Feature significance:
 - Feature A: 0.03
 - Feature C: 0.01

Both features are now statistically significant.

Step 4: Check for further elimination

No features have high p-values, so no further removal is necessary.

Final Selected Features:

Feature A and Feature C

This backward elimination process removes the least significant features step by step.

Feature Selection Techniques (contd.)

• Stepwise Selection: Stepwise selection combines forward and backward approaches by adding features and potentially removing less significant ones at each step.

Steps

- 1. Start with no features.
- 2. Add features one by one based on improvement in performance.
- 3. At each step, evaluate if any included feature should be removed.
- 4. Repeat until no further improvement is possible.

Step 1: Start with No Features (Empty Model)

• Evaluate each feature individually to find the one with the highest predictive power.

Correlation with the target:

• Feature A: 0.99

• Feature B: 0.85

• Feature C: 1.00

Select Feature C because it has the highest correlation (1.00).

Step 2: Add the Next Best Feature

Evaluate the combinations:

• C + A: Correlation = 1.00

• C + B: Correlation = 0.95

Select Feature A (C + A) as it maintains the highest predictive power.

Step 3: Perform Backward Elimination

Check if removing any feature improves the model:

- Removing Feature A reduces the correlation from 1.00 to a lower value.
- So keep **Feature A**.

Step 4: Add the Remaining Feature

Try adding **Feature B**:

• C + A + B: Correlation remains at 1.00.

Since adding Feature B does not improve the correlation, do not add it.

Final Selected Features:

Feature C and Feature A

Model Performance

1. Residuals Analysis: Residuals are the differences between the observed and predicted values:

- Normality: Residuals should ideally be normally distributed.
- **Homoscedasticity**: Residuals should have constant variance across the predicted values.

2. Mean Squared Error (MSE)

$$MSE = rac{1}{n} \sum_{i=1}^{n} (Actual_i - Predicted_i)^2$$

Penalizes larger errors more than smaller ones.

3. Root Mean Squared Error (RMSE)

$$RMSE = \sqrt{MSE}$$

Easier to interpret than MSE.

4. Mean Absolute Error (MAE)

$$MAE = rac{1}{n} \sum_{i=1}^{n} |Actual_i - Predicted_i|$$

Less sensitive to outliers compared to MSE and RMSE.

5. Coefficient of Determination (R²)

$$R^2 = 1 - rac{SS_{Residual}}{SS_{Total}}$$

Where:

- $SS_{Residual} = \sum_{i=1}^{n} (Actual_i Predicted_i)^2$ (Sum of squared errors)
- $SS_{Total} = \sum_{i=1}^{n} (Actual_i Acar{t}ual)^2$ (Total variation in the data)
- Actual is the mean of the observed values.

Interpretation:

- ullet $R^2=0$: The model explains none of the variance in the dependent variable.
- ullet $R^2=1$: The model perfectly explains all the variance in the dependent variable.
- $R^2 < 0$: Happens if the model fits worse than a horizontal line (mean prediction).

6. Adjusted R²

$$Adjusted \ R^2=1-\left(1-R^2
ight)rac{n-1}{n-p-1}$$

- Accounts for the number of predictors in the model.
- Helps prevent overfitting by penalizing unnecessary features.

7. Akaike Information Criterion (AIC)

$$AIC = 2k - 2\ln(L)$$

Where:

- *k* is the number of parameters
- L is the likelihood function
- Lower AIC indicates a better fit.

8. Bayesian Information Criterion (BIC)

$$BIC = k \ln(n) - 2 \ln(L)$$

- Penalizes models with a higher number of parameters more than AIC.
- Lower BIC suggests a better model.

Multiple Linear Regression (MLR): Numerical (up to 3 variables)

S.N.	X1	X2	X3	Y
1	1	2	3	10
2	2	3	4	20
3	3	4	5	30

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon} \qquad \boldsymbol{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

Step 1: Define the Matrices

Matrix **Y** (Dependent Variable):

$$\mathbf{Y} = egin{bmatrix} 10 \\ 20 \\ 30 \end{bmatrix}$$

Matrix \mathbf{X} (Design Matrix):

$$\mathbf{X} = \begin{bmatrix} 1 & 1 & 2 & 3 \\ 1 & 2 & 3 & 4 \\ 1 & 3 & 4 & 5 \end{bmatrix}$$

$$\mathbf{X}^T \mathbf{X} = \begin{bmatrix} 3 & 6 & 9 & 12 \\ 6 & 14 & 20 & 26 \\ 9 & 20 & 29 & 38 \\ 12 & 26 & 38 & 50 \end{bmatrix}$$

$$\mathbf{X}^T\mathbf{X} = egin{bmatrix} 3 & 6 & 9 & 12 \ 6 & 14 & 20 & 26 \ 9 & 20 & 29 & 38 \ 12 & 26 & 38 & 50 \end{bmatrix} \qquad (\mathbf{X}^T\mathbf{X})^{-1} = egin{bmatrix} 1.5 & -0.5 & 0 & 0 \ -0.5 & 0.5 & 0 & 0 \ 0 & 0 & 0.5 & -0.5 \ 0 & 0 & -0.5 & 0.5 \end{bmatrix}$$

$$\mathbf{X}^T\mathbf{Y} = egin{bmatrix} 60 \ 140 \ 200 \ 260 \end{bmatrix}$$

$$oldsymbol{eta} = egin{bmatrix} 20 \\ 40 \\ -30 \\ 30 \end{bmatrix}$$

Final Regression Equation

The regression equation is:

$$Y = 20 + 40X_1 - 30X_2 + 30X_3$$

Logistic Regression

- Logistic Regression is a statistical and machine learning model used for binary classification tasks, where the goal is to predict the probability of an instance belonging to one of two classes (e.g., yes/no, spam/not spam).
- It is a fundamental algorithm in supervised learning and is widely used due to its simplicity, interpretability, and effectiveness.

Differences Between Linear and Logistic Regression

1. Purpose:

- Linear Regression: Predicts continuous outcomes (e.g., house prices, temperature).
- Logistic Regression: Predicts probabilities for classification usually binary(e.g., spam vs. not spam).

2. Model Equation:

• Linear: Uses a linear equation:

$$y = \beta_0 + \beta_1 x_1 + \dots + \beta_n x_n.$$

• Logistic: Applies the sigmoid function to a linear combination:

$$p=rac{1}{1+e^{-(eta_0+eta_1x_1+\cdots+eta_nx_n)}}.$$

Output is bounded between 0 and 1 (probability).

Differences Between Linear and Logistic Regression (contd.)

3. Loss Function or Cost Function:

- **Linear Regression**: Mean Squared Error (MSE) is used as the loss function.
- **Logistic Regression**: Uses Log-Loss or Cross-Entropy as the loss function.

4. Output:

- Linear: Predicts a continuous value, which can range from negative to positive infinity.
- Logistic: Predicts the probability of belonging to a class (e.g., $p \ge 0.5 \rightarrow Class 1$).

Logistic Regression as a Classification Model

- Logistic regression is used for binary classification problems, where the outcome is one of two possible classes.
- It models the probability that a given input point belongs to a particular class, typically denoted as 1 (positive class) or 0 (negative class).
- Converts predicted probabilities into discrete classes using a decision boundary (default: 0.5).

Sigmoid Function and Probability Interpretation

• The **sigmoid function** is used to convert the linear combination of inputs into a probability. The function has the form:

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

where
$$z = \beta_0 + \beta_1 x_1 + \cdots + \beta_n x_n$$
.

• Squashes z into [0, 1], interpreted as P(y=1|x).

Relationship Between Log-Odds and Coefficients

 In logistic regression, the output is the log-odds of the event occurring. The relationship between the input features and the log-odds is:

log-odds is: $\ln\left(rac{p}{1-p}
ight)=eta_0+eta_1x_1+\cdots+eta_nx_n.$

- **Log-Odds**: The log of the odds is the logarithm of the ratio of the probability of the event happening to the probability of the event not happening.
- Coefficients: The coefficients $\beta_1,...,\beta_n$ represent the change in the log-odds for a one-unit change in the corresponding feature x_i .

Case studies using regression models in domains such as healthcare, finance, and marketing.

Mini Projects and Presentations (Lab)

Interpretation of Coefficients

Interpretation of Coefficients

• The coefficients (βi) in logistic regression represent the change in the logodds for a one-unit increase in the corresponding feature, holding all other features constant.

• Example:

Suppose θ 1=0.5.

- A one-unit increase in x1 increases the log-odds by 0.5.
- The odds increase by a factor of $e^{0.5} \approx 1.65$.
- Interpretation: The odds of the event occurring increase by 65% for each one-unit increase in x1.

Log loss (cross-entropy loss):

$$ext{Loss} = -rac{1}{N}\sum_{i=1}^N \left[y_i\log(p_i) + (1-y_i)\log(1-p_i)
ight]$$

Chapter 7

7.1 Ethical Considerations in Data Science

- **Bias and Fairness:** Ensure that data models are developed in a way that prevents the reinforcement of biases or discriminatory practices based on race, gender, or other characteristics..
- **Transparency:** Models and algorithms should be explainable and interpretable.
- Accountability: Data scientists must take responsibility for the consequences of their models and decisions.
- Consent: Always seek user consent when collecting and processing personal data.
- Security: Protect data against breaches and unauthorized access.

7.2 Data Privacy Regulations

- General Data Protection Regulation (GDPR): European regulation that governs data collection, processing, and protection.
- California Consumer Privacy Act (CCPA): US law giving consumers rights over their data.
- Personal Data Protection Bill (India): Proposed legislation focused on protecting personal data in India.
- Key Principles:
 - Consent and transparency
 - Data minimization
 - Right to be forgotten
 - Data portability

7.3 Responsible Data Usage

- Best Practices:
 - Anonymization: To protect identities.
 - Data Minimization: Collect only essential data.
 - Security Measures: Encryption, access controls, and regular audits.
 - **Ethical Sharing**: Guidelines for collaborative research (e.g., federated learning).
- **Data Governance:** Role of Data Stewards and Ethics Boards to oversee compliance and ethical alignment.

7.4 The Five Cs

A framework often used in data management and analysis:

- 1. Correctness: Data must be accurate and error-free.
- 2. Completeness: All necessary data should be collected.
- **3. Consistency:** Ensure data values remain consistent across systems.
- **4. Credibility:** Data should be from reliable and trustworthy sources.
- 5. Context: Data should be relevant and aligned with its purpose.

7.5 Future Trends

Technological Shifts:

- Al Ethics Tools: Automated bias detection and fairness metrics.
- Decentralized Data: Blockchain for transparent consent management.

Regulatory Trends:

- Global harmonization of privacy laws and stricter penalties.
- Rise of "Ethical AI Certification" standards.

Organizational Changes:

• Growth of Chief Ethics Officers and cross-functional ethics committees.