Machine Learning in Python Supervised Learning - Regression and Evaluation

Cristian A. Marocico, A. Emin Tatar

Center for Information Technology University of Groningen

Wednesday, July 2nd 2025

Outline

Introduction to Regression

- Simple Linear Regression
- State

 Evaluation Metrics for Regression

Marocico, Tatar (CIT) Machine Learning in Python Jul 2nd 2025

Introduction to Regression

Regression Definition

Marocico, Tatar (CIT) Machine Learning in Python Jul 2nd 2025

Introduction to Regression

Regression

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

Jul 2nd 2025

Simple Linear Regression Definition

Marocico, Tatar (CIT) Machine Learning in Python Jul 2nd 2025

Definition

Simple Linear Regression is a method to model the relationship between two variables by fitting a linear equation to observed data.

Simple Linear Regression

Definition

Simple Linear Regression is a method to model the relationship between two variables by fitting a linear equation to observed data. Mathematically:

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

where:

- y is the dependent variable (response).
- x is the independent variable (predictor).
- β_0 is the y-intercept (constant term).
- β_1 is the slope of the line (coefficient).
- \bullet ϵ is the error term (residuals).

Marocico, Tatar (CIT) Machine Learning in Python Jul 2nd 2025 4/12

A Simple Linear Regression Machine Learning model will learn the coefficients β_0 and β_1 from the training data to minimize the difference between the predicted values and the actual values.

• Linearity: The relationship between the independent and dependent variable is linear.

Jul 2nd 2025

- Linearity: The relationship between the independent and dependent variable is linear.
- Independence: Observations are independent of each other.

- Linearity: The relationship between the independent and dependent variable is linear.
- Independence: Observations are independent of each other.
- Homoscedasticity: Constant variance of the error terms.

- Linearity: The relationship between the independent and dependent variable is linear.
- Independence: Observations are independent of each other.
- Homoscedasticity: Constant variance of the error terms.
- Normality: The residuals (errors) of the model are normally distributed.

Jul 2nd 2025

Evaluation Metrics for Regression

Common Metrics for Regression

Definition

Common Metrics for Regression

Definition

7/12

Common metrics to evaluate regression models include:

- Mean Absolute Error (MAE)
- Mean Squared Error (MSE)
- Root Mean Squared Error (RMSE)
- R-squared (R²)
- Adjusted R-squared

Mean Absolute Error (MAE) Definition

Mean Absolute Error (MAE)

Definition

8 / 12

Mean Absolute Error (MAE) is the average of the absolute differences between the predicted and the actual values:

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

Definition

Mean Absolute Error (MAE) is the average of the absolute differences between the predicted and the actual values:

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

where:

- *n* is the number of observations.
- y_i is the actual value.
- \hat{y}_i is the predicted value.

Mean Absolute Error (MAE)

Definition

Mean Absolute Error (MAE) is the average of the absolute differences between the predicted and the actual values:

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

where:

- *n* is the number of observations.
- y_i is the actual value.
- \hat{y}_i is the predicted value.

MAE is a linear score, which can be used when all errors are equally important; it is also less sensitive to outliers compared to MSE.

Marocico, Tatar (CIT) Machine Learning in Python Jul 2nd 2025 8/12

Mean Squared Error (MSE)

Definition

Marocico, Tatar (CIT) Machine Learning in Python Jul 2nd 2025

Mean Squared Error (MSE)

Definition

9/12

Mean Squared Error (MSE) is the average of the squared differences between the predicted and the actual values:

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

Marocico, Tatar (CIT) Machine Learning in Python Jul 2nd 2025

Definition

Mean Squared Error (MSE) is the average of the squared differences between the predicted and the actual values:

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

where:

- *n* is the number of observations.
- y_i is the actual value.
- \hat{y}_i is the predicted value.

Definition

Mean Squared Error (MSE) is the average of the squared differences between the predicted and the actual values:

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

where:

- *n* is the number of observations.
- y_i is the actual value.
- \hat{y}_i is the predicted value.

MSE is more sensitive to outliers than MAE because it squares the errors, which can disproportionately affect the metric if there are large errors; however, it is useful when larger errors are more significant.

Marocico, Tatar (CIT) Machine Learning in Python Jul 2nd 2025 9 / 12

Root Mean Squared Error (RMSE)

Definition

10 / 12

Marocico, Tatar (CIT) Machine Learning in Python Jul 2nd 2025

Definition

10 / 12

Root Mean Squared Error (RMSE) is the square root of the average of the squared differences between the predicted and the actual values:

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

Marocico, Tatar (CIT) Machine Learning in Python Jul 2nd 2025

Root Mean Squared Error (RMSE)

Definition

10 / 12

Root Mean Squared Error (RMSE) is the square root of the average of the squared differences between the predicted and the actual values:

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

where:

- *n* is the number of observations.
- y_i is the actual value.
- \hat{y}_i is the predicted value.

Marocico, Tatar (CIT)

Machine Learning in Python

Jul 2nd 2025

Root Mean Squared Error (RMSE)

Definition

10 / 12

Jul 2nd 2025

Root Mean Squared Error (RMSE) is the square root of the average of the squared differences between the predicted and the actual values:

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

where:

- *n* is the number of observations.
- y_i is the actual value.
- \hat{y}_i is the predicted value.

RMSE is in the same units as the dependent variable, making it interpretable; it is also sensitive to outliers, similar to MSE.

Marocico, Tatar (CIT) Machine Learning in Python

R-squared (R^2)

R-squared (R^2) Definition

Marocico, Tatar (CIT) Machine Learning in Python Jul 2nd 2025

R-squared (R^2) Definition

R-squared (R^2) is a statistical measure that represents the proportion of the variance for a dependent variable that's explained by an independent variable or variables in a regression model:

$$R^2 = 1 - rac{\mathsf{SS}_{\mathsf{res}}}{\mathsf{SS}_{\mathsf{tot}}}$$

where:

- SS_{res} is the sum of squares of residuals (errors).
- SS_{tot} is the total sum of squares (variance of the dependent variable).

Marocico, Tatar (CIT) Machine Learning in Python Jul 2nd 2025

R-squared (R^2) Definition

R-squared (R^2) is a statistical measure that represents the proportion of the variance for a dependent variable that's explained by an independent variable or variables in a regression model:

$$R^2 = 1 - rac{\mathsf{SS}_{\mathsf{res}}}{\mathsf{SS}_{\mathsf{tot}}}$$

where:

- SS_{res} is the sum of squares of residuals (errors).
- SS_{tot} is the total sum of squares (variance of the dependent variable).

 R^2 values range from 0 to 1, where:

- 0 indicates that the model does not explain any of the variability of the response data around its mean.
- 1 indicates that the model explains all the variability of the response data around its mean.

Marocico, Tatar (CIT) Machine Learning in Python Jul 2nd 2025 11/12

Adjusted R-squared

Adjusted R-squared Definition

Jul 2nd 2025

Adjusted R-squared

Adjusted R-squared

Definition

Adjusted R-squared adjusts the R^2 value for the number of predictors in the model, providing a more accurate measure when comparing models with different numbers of predictors:

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

where:

- n is the number of observations.
- p is the number of predictors in the model.

Adjusted R-squared

Definition

Adjusted R-squared adjusts the R^2 value for the number of predictors in the model, providing a more accurate measure when comparing models with different numbers of predictors:

Adjusted
$$R^2 = 1 - (1 - R^2) \frac{n-1}{n-p-1}$$

where:

- n is the number of observations.
- p is the number of predictors in the model.

Adjusted R^2 can be negative, which indicates that the model is worse than a horizontal line (mean of the dependent variable); it is useful for comparing models with different numbers of predictors.

Marocico, Tatar (CIT)

Machine Learning in Python

Jul 2nd 2025

12 / 12