

Mean Absolute Error(MAE)

MAE is a very simple metric which calculates the absolute difference between actual and predicted values. Mean Absolute Error(MAE) is similar to Mean Square Error(MSE). However, instead of the sum of square of error in MSE, MAE is taking the sum of the absolute value of error.

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

The diagram shows the MAE formula: $MAE = \frac{1}{N} \sum |Y - \hat{Y}|$. Annotations include: 'Divide by total Number of Data Points' pointing to $\frac{1}{N}$; 'Actual Output' pointing to Y and 'Predicted Output' pointing to \hat{Y} ; 'Sum Of' pointing to the summation symbol \sum ; and 'Absolute Value of residual' pointing to the absolute value bars $|Y - \hat{Y}|$.

Mean Absolute Error formula

Compare to MSE or RMSE, MAE is a more direct representation of sum of error terms. **MSE gives larger penalization to big prediction error by square it while MAE treats all errors the same.**

Advantages of MAE

- The MAE you get is in the same unit as the output variable.
- It is most Robust to outliers.

Disadvantages of MAE

- The graph of MAE is not differentiable so we have to apply various optimizers like Gradient descent which can be differentiable.

Mean Square Error(MSE)/Root Mean Square Error(RMSE)

While R Square is a relative measure of how well the model fits dependent variables, Mean Square Error is an absolute measure of the goodness for the fit.

$$MSE = \frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2$$
$$MSE = \frac{1}{n} \sum \underbrace{\left(y - \hat{y} \right)}_{\substack{\text{The square of the difference} \\ \text{between actual and} \\ \text{predicted}}}^2$$

Mean Square Error formula

MSE is calculated by the sum of square of prediction error which is real output minus predicted output and then divide by the number of data points. It gives you an absolute number on how much your predicted results deviate from the actual number. You cannot interpret many insights from one single result but it gives you a real number to compare against other model results and help you select the best regression model.

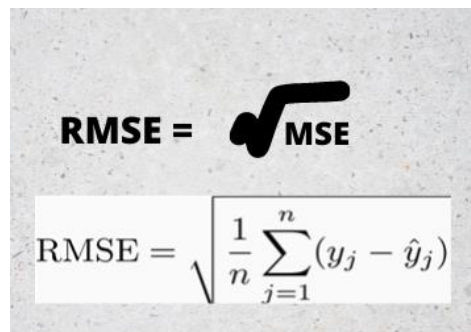
Advantages of MSE

- The graph of MSE is differentiable, so you can easily use it as a loss function.

Disadvantages of MSE

- The value you get after calculating MSE is a squared unit of output. for example, the output variable is in meter(m) then after calculating MSE the output we get is in meter squared.
- If you have outliers in the dataset then it penalizes the outliers most and the calculated MSE is bigger. So, in short, It is not Robust to outliers which were an advantage in MAE.

Root Mean Square Error(RMSE) is the square root of MSE. It is used more commonly than MSE because firstly sometimes MSE value can be too big to compare easily. Secondly, MSE is calculated by the square of error, and thus square root brings it back to the same level of prediction error and makes it easier for interpretation.



The image shows a hand-drawn diagram on a textured background. At the top, it says 'RMSE = √ MSE'. Below this, a white rectangular box contains the mathematical formula for RMSE:
$$RMSE = \sqrt{\frac{1}{n} \sum_{j=1}^n (y_j - \hat{y}_j)^2}$$

Advantages of RMSE

- The output value you get is in the same unit as the required output variable which makes interpretation of loss easy.

Disadvantages of RMSE

- It is not that robust to outliers as compared to MAE.
- for performing RMSE we have to NumPy square root function over MSE.

Root Mean Squared Log Error(RMSLE)

Taking the log of the RMSE metric slows down the scale of error. The metric is very helpful when you are developing a model without calling the inputs. In that case, the output will vary on a large scale. To control this situation of RMSE we take the log of calculated RMSE error and resultant we get as RMSLE.

To perform RMSLE we have to use the NumPy log function over RMSE. It is a very simple metric that is used by most of the datasets hosted for Machine Learning competitions.

R Squared (R2)

It determines how much of the total variation in Y (dependent variable) is explained by the variation in X (independent variable). Mathematically, it can be written as:

$$R - Square = 1 - \frac{\sum(Y_{actual} - Y_{predicted})^2}{\sum(Y_{actual} - Y_{mean})^2}$$

$$R^2 = 1 - \frac{SS_{Regression}}{SS_{Total}} = 1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i (y_i - \bar{y})^2}$$

$$R^2 \text{ Squared} = 1 - \frac{SSr}{SSm}$$

SSr = Squared sum error of regression line

SSm = Squared sum error of mean line

- R Square measures how much variability in dependent variable can be explained by the model. It is the square of the Correlation Coefficient(R) and that is why it is called R Square.
- The value of R-square is always between 0 and 1, where 0 means that the model does not model explain any variability in the target variable (Y) and 1 meaning it explains full variability in the target variable.
- R Square is calculated by the sum of squared of prediction error divided by the total sum of the square which replaces the calculated prediction with mean. R Square value is between 0 to 1 and a bigger value indicates a better fit between prediction and actual value.
- R Square is a good measure to determine how well the model fits the dependent variables. **However, it does not take into consideration of overfitting problem.** If your regression model has many independent variables, because the model is too complicated, it may fit very well to the training data but performs badly for testing data. That is why Adjusted R Square is introduced because it will penalize additional independent variables added to the model and adjust the metric to prevent overfitting issues.

R2 score is a metric that tells the performance of your model, not the loss in an absolute sense that how many wells did your model perform.

In contrast, MAE and MSE depend on the context as we have seen whereas the R2 score is independent of context.

So, with help of R squared we have a baseline model to compare a model which none of the other metrics provides. The same we have in classification problems which we call a threshold which is fixed at 0.5. So basically R2 squared calculates how must regression line is better than a mean line.

Hence, R2 squared is also known as Coefficient of Determination or sometimes also known as Goodness of fit.

R2 Squared

Now, how will you interpret the R2 score? suppose If the R2 score is zero then the above regression line by mean line is equal means 1 so 1-1 is zero. So, in this case, both lines are overlapping means model performance is worst, It is not capable to take advantage of the output column.

Now the second case is when the R2 score is 1, it means when the division term is zero and it will happen when the regression line does not make any mistake, it is perfect. In the real world, it is not possible.

So we can conclude that as our regression line moves towards perfection, R2 score move towards one. And the model performance improves.

The normal case is when the R2 score is between zero and one like 0.8 which means your model is capable to explain 80 per cent of the variance of data.

Adjusted R-square

The only drawback of R^2 is that if new predictors (X) are added to our model, R^2 only increases or remains constant but it never decreases. We can not judge that by increasing complexity of our model, are we making it more accurate?

That is why, we use "Adjusted R-Square".

The Adjusted R-Square is the modified form of R-Square that has been adjusted for the number of predictors in the model. It incorporates model's degree of freedom. The adjusted R-Square only increases if the new term improves the model accuracy.

$$R_a^2 = 1 - \left[\left(\frac{n-1}{n-k-1} \right) \times (1 - R^2) \right]$$

where:

n = number of observations

k = number of independent variables

R_a^2 = adjusted R^2

$$R^2_{\text{adjusted}} = 1 - \frac{(1 - R^2)(N - 1)}{N - p - 1}$$

where

R^2 = Sample R square

p = Number of predictors

N = total sample size

The disadvantage of the R^2 score is while adding new features in data the R^2 score starts increasing or remains constant but it never decreases because it assumes that while adding more data variance of data increases. But the problem is when we add an irrelevant feature in the dataset then at that time R^2 sometimes starts increasing which is incorrect. Hence, To control this situation Adjusted R^2 Squared came into existence.

Now as K increases by adding some features so the denominator will decrease, n-1 will remain constant. R^2 score will remain constant or will increase slightly so the complete answer will increase and when we subtract this from one then the resultant score will decrease. so this is the case when we add an irrelevant feature in the dataset.

And if we add a relevant feature then the R^2 score will increase and $1 - R^2$ will decrease heavily and the denominator will also decrease so the complete term decreases, and on subtracting from one the score increases. Hence, this metric becomes one of the most important metrics to use during the evaluation of the model.

Conclusion

R Square/Adjusted R Square is better used to explain the model to other people because you can explain the number as a percentage of the output variability. MSE, RMSE, or MAE are better be used to compare performance between different regression models. Personally, I would prefer using RMSE and I think Kaggle also uses it to assess the submission. However, it makes total sense to use MSE if the value is not too big and MAE if you do not want to penalize large prediction errors.

Adjusted R square is the only metric here that considers the overfitting problem. R Square has a direct library in Python to calculate but I did not find a direct library to calculate Adjusted R square except using the statsmodel results. If you really want to calculate Adjusted R Square, you can use statsmodel or use its mathematic formula directly.