# Coefficient of determination

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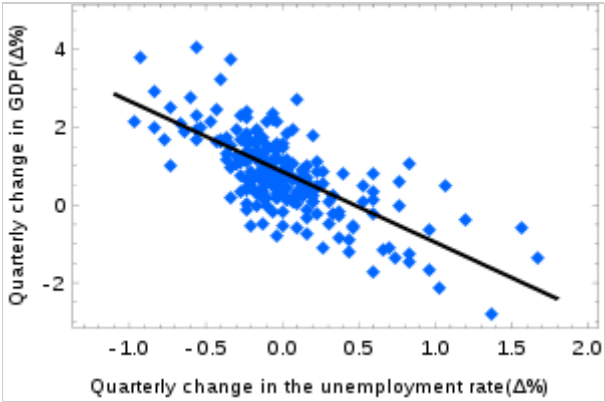
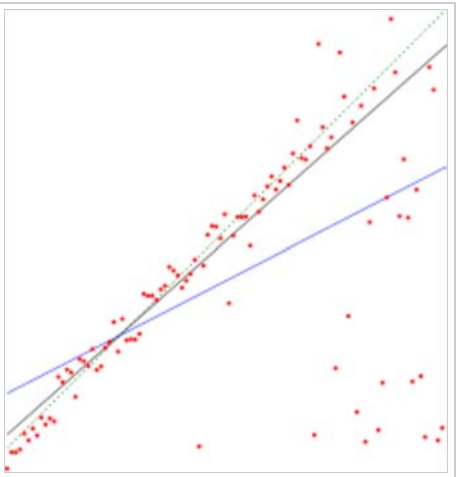
In statistics, the **coefficient of determination**, denoted $R^2$ or $r^2$ and pronounced **R squared**, is a number that indicates how well data fit a statistical model – sometimes simply a line or a curve. An $R^2$ of 1 indicates that the regression line perfectly fits the data, while an $R^2$ of 0 indicates that the line does not fit the data at all. This latter can be because the data is utterly non-linear, or because it is random.




Ordinary least squares regression of Okun's law. Since the regression line does not miss any of the points by very much, the $R^2$ of the regression is relatively high.

It is a statistic used in the context of statistical models whose main purpose is either the prediction of future outcomes or the testing of hypotheses, on the basis of other related information. It provides a measure of how well observed outcomes are replicated by the model, as the proportion of total variation of outcomes explained by the model (pp. 187, 287).[1][2][3]

There are several definitions of $R^2$ that are only sometimes equivalent. One class of such cases includes that of simple linear regression where $r^2$ is used instead of $R^2$. In this case, if an intercept is included, then $r^2$ is simply the square of the sample correlation coefficient (i.e., $r$) between the outcomes and their predicted values. If additional explanators are included, $R^2$ is the square of the coefficient of multiple correlation. In both such cases, the coefficient of determination ranges from 0 to 1.



Comparison of the Theil–Sen estimator (black) and simple linear regression (blue) for a set of points with outliers. Because of the many outliers, neither of the regression lines fits the data well, as measured by the fact that neither gives a very high $R^2$.

Important cases where the computational definition of $R^2$ can yield negative values, depending on the definition used, arise where the predictions that are being compared to the corresponding outcomes have not been derived from a model-fitting procedure using those data, and where linear regression is conducted without including an intercept. Additionally, negative values of $R^2$ may occur when fitting non-linear functions to data.[4] In cases where negative values arise, the mean of the data provides a better fit to the outcomes than do the fitted function values, according to this particular criterion.[5]

## Contents

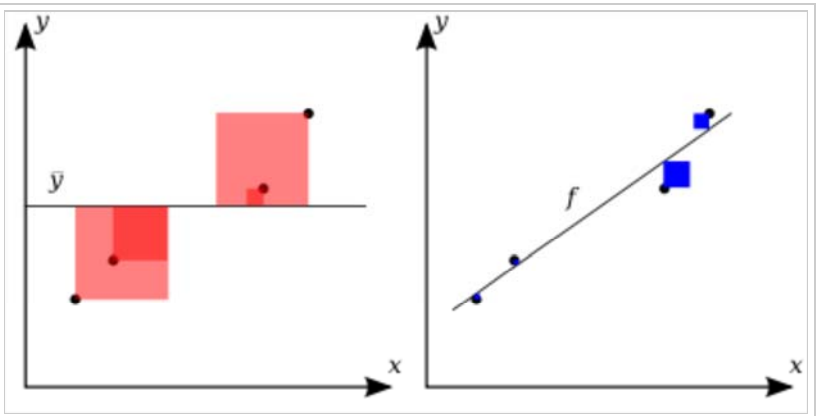
# Definitions

A data set has $n$ values marked $y_1...y_n$ (collectively known as $y_i$), each associated with a predicted (or modeled) value $f_1...f_n$ (known as $f_i$, or sometimes $\hat{y}_i$).

If $\bar{y}$ is the mean of the observed data:

$$\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$$

then the variability of the data set can be measured using three sums of squares formulas:




$$R^2 = 1 - \frac{SS_{\text{res}}}{SS_{\text{tot}}}$$

The better the linear regression (on the right) fits the data in comparison to the simple average (on the left graph), the closer the value of $R^2$ is to 1. The areas of the blue squares represent the squared residuals with respect to the linear regression. The areas of the red squares represent the squared residuals with respect to the average value.

- The total sum of squares (proportional to the variance of the data):

$$SS_{\text{tot}} = \sum_i (y_i - \bar{y})^2,$$

- The regression sum of squares, also called the explained sum of squares:

$$SS_{\text{reg}} = \sum_i (f_i - \bar{y})^2,$$

- The sum of squares of residuals, also called the residual sum of squares:

$$SS_{\text{res}} = \sum_i (y_i - f_i)^2$$

The notations $SS_R$ and $SS_E$ should be avoided, since in some texts their meaning is reversed to **R**esidual sum of squares and **E**xplained sum of squares, respectively.

The most general definition of the coefficient of determination is

$$R^2 \equiv 1 - \frac{SS_{\text{res}}}{SS_{\text{tot}}}.$$

## Relation to unexplained variance

In a general form, $R^2$ can be seen to be related to the unexplained variance, since the second term compares the unexplained variance (variance of the model's errors) with the total variance (of the data). See fraction of variance unexplained.

## As explained variance

Suppose r=0.7 then r^2= 0.49 and it implies that 49% of the variability between the two variables have been accounted for and the remaining 51% of the variability is still unaccounted for. In some cases the total sum of squares equals the sum of the two other sums of squares defined above,

$$SS_{\text{res}} + SS_{\text{reg}} = SS_{\text{tot}}.$$

See partitioning in the general OLS model for a derivation of this result for one case where the relation holds. When this relation does hold, the above definition of $R^2$ is equivalent to

$$R^2 = \frac{SS_{\text{reg}}}{SS_{\text{tot}}} = \frac{SS_{\text{reg}}/n}{SS_{\text{tot}}/n}.$$

In this form $R^2$ is expressed as the ratio of the explained variance (variance of the model's predictions, which is $SS_{\text{reg}} / n$) to the total variance (sample variance of the dependent variable, which is $SS_{\text{tot}} / n$).

This partition of the sum of squares holds for instance when the model values $f_i$ have been obtained by linear regression. A milder sufficient condition reads as follows: The model has the form

$$f_i = \alpha + \beta q_i$$

where the $q_i$ are arbitrary values that may or may not depend on $i$ or on other free parameters (the common choice $q_i = x_i$ is just one special case), and the coefficients α and β are obtained by minimizing the residual sum of squares.

This set of conditions is an important one and it has a number of implications for the properties of the fitted residuals and the modelled values. In particular, under these conditions:

$$\bar{f} = \bar{y}.$$

## As squared correlation coefficient

In linear least squares regression with an estimated intercept term, $R^2$ equals the square of the Pearson correlation coefficient between the observed and modeled (predicted) data values of the dependent variable. Specifically, $R^2$ equals the squared Pearson correlation coefficient of the dependent and explanatory variable in an univariate linear least squares regression.

Under more general modeling conditions, where the predicted values might be generated from a model different from linear least squares regression, an $R^2$ value can be calculated as the square of the correlation coefficient between the original and modeled data values. In this case, the value is not directly a measure of how good the modeled values are, but rather a measure of how good a predictor might be constructed from the modeled values (by creating a revised predictor of the form $\alpha + \beta f_i$). According to Everitt (p. 78),[6] this usage is specifically the definition of the term "coefficient of determination": the square of the correlation between two (general) variables.

# Interpretation

$R^2$ is a statistic that will give some information about the goodness of fit of a model. In regression, the $R^2$ coefficient of determination is a statistical measure of how well the regression line approximates the real data points. An $R^2$ of 1 indicates that the regression line perfectly fits the data.

Values of $R^2$ outside the range 0 to 1 can occur where it is used to measure the agreement between observed and modeled values and where the "modeled" values are not obtained by linear regression and depending on which formulation of $R^2$ is used. If the first formula above is used, values can be less than zero. If the second expression is used, values can be greater than one. Neither formula is defined for the case where $y_1 = \ldots = y_n = \bar{y}$.

In all instances where $R^2$ is used, the predictors are calculated by ordinary least-squares regression: that is, by minimizing $SS_{\text{res}}$. In this case $R^2$ increases as we increase the number of variables in the model ($R^2$ is monotone increasing with the number of variables included—i.e., it will never decrease). This illustrates a drawback to one possible use of $R^2$, where one might keep adding variables (Kitchen sink regression) to increase the $R^2$ value. For example, if one is trying to predict the sales of a model of car from the car's gas mileage, price, and engine power, one can include such irrelevant factors as the first letter of the model's name or the height of the lead engineer designing the car because the $R^2$ will never decrease as variables are added and will probably experience an increase due to chance alone.

This leads to the alternative approach of looking at the adjusted $R^2$. The explanation of this statistic is almost the same as $R^2$ but it penalizes the statistic as extra variables are included in the model. For cases other than fitting by ordinary least squares, the $R^2$ statistic can be calculated as above and may still be a useful measure. If fitting is by weighted least squares or generalized least squares, alternative versions of $R^2$ can be calculated appropriate to those statistical frameworks, while the "raw" $R^2$ may still be useful if it is more easily interpreted. Values for $R^2$ can be calculated for any type of predictive model, which need not have a statistical basis.

## In a non-simple linear model

Consider a linear model with more than a single explanatory variable, of the form

$$Y_i = \beta_0 + \sum_{j=1}^{p} \beta_j X_{i,j} + \varepsilon_i,$$

where, for the *i*th case, $Y_i$ is the response variable, $X_{i,1}, \ldots, X_{i,p}$ are *p* regressors, and $\varepsilon_i$ is a mean zero error term. The quantities $\beta_0, \ldots, \beta_p$ are unknown coefficients, whose values are estimated by least squares. The coefficient of determination $R^2$ is a measure of the global fit of the model. Specifically, $R^2$ is an element of [0, 1] and represents the proportion of variability in $Y_i$ that may be attributed to some linear combination of the regressors (explanatory variables) in *X*.

$R^2$ is often interpreted as the proportion of response variation "explained" by the regressors in the model. Thus, $R^2 = 1$ indicates that the fitted model explains all variability in $y$, while $R^2 = 0$ indicates no 'linear' relationship (for straight line regression, this means that the straight line model is a constant line (slope = 0, intercept = $\bar{y}$) between the response variable and regressors). An interior value such as $R^2 = 0.7$ may be interpreted as follows: "Seventy percent of the variance in the response variable can be explained by the explanatory variables. The remaining thirty percent can be attributed to unknown, lurking variables or inherent variability."

A caution that applies to $R^2$, as to other statistical descriptions of correlation and association is that "correlation does not imply causation." In other words, while correlations may provide valuable clues regarding causal relationships among variables, a high correlation between two variables does not represent adequate evidence that changing one variable has resulted, or may result, from changes of other variables.

In case of a single regressor, fitted by least squares, $R^2$ is the square of the Pearson product-moment correlation coefficient relating the regressor and the response variable. More generally, $R^2$ is the square of the correlation between the constructed predictor and the response variable. With more than one regressor, the $R^2$ can be referred to as the coefficient of multiple determination.

### Inflation of $R^2$

In least squares regression, $R^2$ is weakly increasing with increases in the number of regressors in the model. Because increases in the number of regressors increase the value of $R^2$, $R^2$ alone cannot be used as a meaningful comparison of models with very different numbers of independent variables. For a meaningful comparison between two models, an F-test can be performed on the residual sum of squares, similar to the F-tests in Granger causality, though this is not always appropriate. As a reminder of this, some authors denote $R^2$ by $R_p{}^2$, where $p$ is the number of columns in $X$ (the number of explanators including the constant).

To demonstrate this property, first recall that the objective of least squares linear regression is:

$$\min_b SS_{\text{res}}(b) \Rightarrow \min_b \sum_i (y_i - X_i b)^2$$

The optimal value of the objective is weakly smaller as additional columns of $X$ are added, by the fact that less constrained minimization leads to an optimal cost which is weakly smaller than more constrained minimization does. Given the previous conclusion and noting that $SS_{tot}$ depends only on $y$, the non-decreasing property of $R^2$ follows directly from the definition above.

The intuitive reason that using an additional explanatory variable cannot lower the $R^2$ is this: Minimizing $SS_{\text{res}}$ is equivalent to maximizing $R^2$. When the extra variable is included, the data always have the option of giving it an estimated coefficient of zero, leaving the predicted values and the $R^2$ unchanged. The only way that the optimization problem will give a non-zero coefficient is if doing so improves the $R^2$.

### Notes on interpreting $R^2$

$R^2$ does not indicate whether:

- the independent variables are a cause of the changes in the dependent variable;
- omitted-variable bias exists;
- the correct regression was used;
- the most appropriate set of independent variables has been chosen;
- there is collinearity present in the data on the explanatory variables;
- the model might be improved by using transformed versions of the existing set of independent variables;
- there are enough data points to make a solid conclusion.

## Adjusted $R^2$

The use of an adjusted $R^2$ (often written as $\bar{R}^2$ and pronounced "R bar squared") is an attempt to take

account of the phenomenon of the $R^2$ automatically and spuriously increasing when extra explanatory variables are added to the model. It is a modification due to Theil[7] of $R^2$ that adjusts for the number of explanatory terms in a model relative to the number of data points. The adjusted $R^2$ can be negative, and its value will always be less than or equal to that of $R^2$. Unlike $R^2$, the adjusted $R^2$ increases only when the increase in $R^2$ (due to the inclusion of a new explanatory variable) is more than one would expect to see by chance. If a set of explanatory variables with a predetermined hierarchy of importance are introduced into a regression one at a time, with the adjusted $R^2$ computed each time, the level at which adjusted $R^2$ reaches a maximum, and decreases afterward, would be the regression with the ideal combination of having the best fit without excess/unnecessary terms. The adjusted $R^2$ is defined as

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

where $p$ is the total number of explanatory variables in the model (not including the constant term), and $n$ is the sample size.

Adjusted $R^2$ can also be written as

$$\bar{R}^2 = 1 - \frac{SS_{\text{res}}/df_e}{SS_{\text{tot}}/df_t}$$

where $df_t$ is the degrees of freedom $n$– 1 of the estimate of the population variance of the dependent variable, and $df_e$ is the degrees of freedom $n - p - 1$ of the estimate of the underlying population error variance.

The principle behind the adjusted $R^2$ statistic can be seen by rewriting the ordinary $R^2$ as

$$R^2 = 1 - \frac{VAR_{\text{res}}}{VAR_{\text{tot}}}$$

where $VAR_{\text{res}} = SS_{\text{res}}/n$ and $VAR_{\text{tot}} = SS_{\text{tot}}/n$ are the sample variances of the estimated residuals and the dependent variable respectively, which can be seen as biased estimates of the population variances of the errors and of the dependent variable. These estimates are replaced by statistically unbiased versions: $VAR_{\text{res}} = SS_{\text{res}}/(n-p-1)$ and $VAR_{\text{tot}} = SS_{\text{tot}}/(n-1)$.

Adjusted $R^2$ does not have the same interpretation as $R^2$—while $R^2$ is a measure of fit, adjusted $R^2$ is instead a comparative measure of suitability of alternative nested sets of explanators. As such, care must be taken in interpreting and reporting this statistic. Adjusted $R^2$ is particularly useful in the feature selection stage of model building.

# Coefficient of partial determination

The coefficient of partial determination can be defined as the proportion of variation that cannot be explained in a reduced model, but can be explained by the predictors specified in a full(er) model.[8][9][10] This coefficient is used to provide insight into whether or not one or more additional predictors may be useful in a more fully specified regression model.

The calculation for the partial $r^2$ is relatively straight forward after estimating two models and generating the ANOVA tables for them. The calculation for the partial $r^2$ is:

(SSEreduced - SSEfull) / SSEreduced

which is analogous to the usual coefficient of determination

(SST - SSE) / SST.

# Generalized $R^2$

The generalized $R^2$ was originally proposed by Cox & Snell,[11] and independently by Magee:[12]

$$R^2 = 1 - \left(\frac{L(0)}{L(\hat{\theta})}\right)^{2/n}$$

where $L(0)$ is the likelihood of the model with only the intercept, $L(\hat{\theta})$ is the likelihood of the estimated model (i.e., the model with a given set of parameter estimates) and $n$ is the sample size.

Nagelkerke[13] noted that it had the following properties:

1. It's consistent with the classical coefficient of determination when both can be computed;
2. Its value is maximised by the maximum likelihood estimation of a model;
3. It is asymptotically independent of the sample size;
4. The interpretation is the proportion of the variation explained by the model;
5. The values are between 0 and 1, with 0 denoting that model does not explain any variation and 1 denoting that it perfectly explains the observed variation;
6. It does not have any unit.

However, in the case of a logistic model, where $L(\hat{\theta})$ cannot be greater than 1, $R^2$ is between 0 and $R^2_{\max} = 1 - (L(0))^{2/n}$: thus, Nagelkerke suggests the possibility to define a scaled $R^2$ as $R^2/R^2_{\max}$.[14]

# Comparison with norm of residuals

Occasionally the norm of residuals is used for indicating goodness of fit. This term is encountered in MATLAB and is calculated by

$$\text{norm of residuals} = \sqrt{SS_{\text{res}}}$$

Both $R^2$ and the norm of residuals have their relative merits. For least squares analysis $R^2$ varies between 0 and 1, with larger numbers indicating better fits and 1 represents a perfect fit. Norm of residuals varies from 0 to infinity with smaller numbers indicating better fits and zero indicating a perfect fit. One advantage and disadvantage of $R^2$ is the $SS_{\text{tot}}$ term acts to normalize the value. If the $y_i$ values are all multiplied by a constant, the norm of residuals will also change by that constant but $R^2$ will stay the same. As a basic example, for the linear least squares fit to the set of data:

$$x = 1,\ 2,\ 3,\ 4,\ 5$$
$$y = 1.9,\ 3.7,\ 5.8,\ 8.0,\ 9.6$$

$R^2 = 0.998$, and norm of residuals = 0.302. If all values of y are multiplied by 1000 (for example, in an SI prefix change), then $R^2$ remains the same, but norm of residuals = 302.

# See also

- Fraction of variance unexplained
- Goodness of fit
- Nash–Sutcliffe model efficiency coefficient (hydrological applications)
- Pearson product-moment correlation coefficient
- Proportional reduction in loss
- Regression model validation
- Root mean square deviation
- t-test of $H_0$: $R^2 = 0$.

# Notes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