



R²: Coefficient of Determination

A measure that efficiently summarizes how well the Xs can be used to predict Y is R² (called R-squared or the coefficient of determination):

$$R^2 = 1 - SSE/SST$$

where

SSE =
$$\sum_{i=1}^{n} \hat{\varepsilon}_i^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$
$$SST = \sum_{i=1}^{n} (y_i - \bar{y})^2$$

R² is interpreted as the proportion of total variability in Y that can be explained by the linear regression model.

Georgia Tech

3

R²: Notation and Terminology

SSE, **SST**, and **SSR** refer to *sum of squared errors*, *sum of squares total*, and *sum of squares for regression*. Unfortunately, the field of statistics abounds in inconsistent terminology and notation.

- SSE: sometimes denoted SS_{error} or SS_{err}, is also known as RSS (residual sum of squares) and SS_{res} (sum of squared residuals, sometimes SSR).
- SST: sometimes written as SS_{total} or SS_{tot}. It is also called total sum of squares and written as TSS.
- SSR: also called the sum of squares due to regression, and it is sometimes written as SS_{reg}. It's also called explained sum of squares (ESS). Don't confuse ESS with SSE, and, for R², remember that SSR is SS regression, not SS residuals!



Model Evaluation

- F-test for overall regression
 - H_0 : $\beta_1 = \beta_1 = \cdots = \beta_p = 0$
 - $F_0 = MSR/MSE \sim F(p, n-p-1)$
 - MSR = SSR/p
 - SSR = $\sum_{i=1}^{n} (\hat{y}_i \bar{y})^2$
 - MSE = SSE/(n-p-1)
- · Coefficient of determination
 - $R^2 = 1 SSE/SST = SSR/SST$
 - R² increases when additional predictors are added to a model
 - Such increase might not indicate increased explanatory power
- Adjusted coefficient of determination
 - Penalizes for more predictors
 - adjusted $R^2 = 1 (n-1)(1-R^2)/(n-p-1)$



5

Correlation Coefficient

A statistic that efficiently summarizes how well one of the Xs is *linearly* related to Y (or to another X) is ρ , the (Pearson) correlation coefficient:

$$\rho_{X_j,Y} = \operatorname{cor}(X_j,Y) = \frac{\sum_{i=1}^n (x_{i,j} - \bar{x}) (y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_{i,j} - \bar{x}_j)^2} \sqrt{\sum_{i=1}^n (y_i - \bar{y})^2}}$$

- Can be used to evaluate the *linear* relationship between the response variable and any of the predicting variables, X_i
 - Useful when looking for transformations of predicting variables
- · Can also be used to evaluate correlation between predicting variables
 - Can help detect near linear dependence (multicollinearity)



Multicollinearity

Recall that finding the ordinary least squares estimator of $\widehat{\boldsymbol{\beta}}$

$$\widehat{\boldsymbol{\beta}} = (\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X})^{-1}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{Y}$$

depends on X^TX being invertible (nonsingular or nondegenerate). From linear algebra, a square matrix is invertible if and only if its columns are linearly independent (i.e., no column is a linear combination of the others).

If that doesn't hold, the ordinary least squares estimator of $\hat{\beta}$ doesn't exist. That's probably due to a specification error where one or more predictors should be eliminated as redundant (e.g., if years and number of rings were included in a model for trees).

Even if the columns of X^TX are linearly independent, some problems might arise if the value of one predictor can be closely estimated from the other predictors. We call this condition *multicollinearity* or *near collinearity*.

7

Multicollinearity

- Indications that near collinearity is present:
 - The estimated coefficients $\hat{\beta}$ are unstable: When the value of one predictor changes slightly, the fitted regression coefficients change dramatically
 - The standard error of $\widehat{\pmb{\beta}}$ is artificially large
 - The overall F statistic is significant, but individual t-statistics are not
- Prediction may be affected
 - The relationship to the response may change widely
- · Some computational algorithms are sensitive to multicollinearity
- But no inflation or deflation in R2

Georgia Tech

Multicollinearity Diagnosis

Compute the variance inflation factor (VIF_j) for each predicting variable X_j

$$VIF_j = \frac{1}{1 - R_j^2}$$

where R_j^2 is the coefficient of determination for the regression of X_j against all other predicting variables.

What is an acceptable VIF (i.e., multicollinearity is not problematic)?

- VIF < $max(10, 1/(1 R_{model}^2))$
 - \bullet $\ R^2_{model}$ is the coefficient of determination for the original model
 - · Rule of thumb only



a

Multicollinearity Diagnosis

Steps:

- 1. For j = 1,...,p, regress X_j against all other X_i , i = 1,...,p, $i \neq j$ (i.e., $X_i \sim X_1,...,X_{j-1},X_{j+1},...,X_p$).
- 2. For each regression run, compute R^2 for that regression (i.e., compute R_i^2 for j = 1, ..., p).
- 3. For each regression run, compute VIF_j based on the computed R_j^2 for that regression.
- 4. If any $\widetilde{VIF}_j \ge 10$ and it is also $\ge 1/(1-R_{\mathrm{model}}^2)$, where R_{model}^2 is the coefficient of determination for the original model, the test is positive for multicollinearity.

High multicollinearity is not detected if each $VIF_j < max(10, \frac{1}{1-R_{model}^2})$.



Multicollinearity Interpretation

VIF measures the proportional increase in the variance of $\hat{\beta}_i$ compared to what it would have been if the predicting variables had been completely uncorrelated.

- VIF of 1 (the minimum possible VIF) means the tested predictor is not correlated with the other predictors
- The higher the VIF:
 - The more correlated a predictor is with the other predictors
 - The more the standard error is inflated
 - The larger the confidence interval
 - The less likely it is that a coefficient will be evaluated as statistically significant



11

