

# Confidence intervals for $R^2$

Andrey Konovalov

MIPT

April 14, 2014

# Coefficient of Determination

Given a data set  $\{y_i, x_{1i}, \dots, x_{ki}\}_{i=1}^n$

$$TSS = \sum_{i=1}^n (y_i - \bar{y})^2 \quad \text{Total Sum of Squares}$$

$$ESS = \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 \quad \text{Explained Sum of Squares}$$

$$RSS = \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad \text{Residual Sum of Squares}$$

Coefficient of Determination:

$$R^2 = \frac{ESS}{TSS} = 1 - \frac{RSS}{TSS}$$

## Coefficient of Determination (cont'd)

- $R^2$  takes on values between 0 and 1.
- The higher the  $R^2$ , the more useful the model.
- Interpretation:  $R^2$  tells us how much better we do by using the regression equation rather than just the mean  $\bar{y}$  to predict  $y$ .
- Despite the interpretation the value of  $R^2$  doesn't mean much by itself.
- The value of  $R^2$  can be small, but your regression is perhaps still better than doing nothing.
- $R^2$  might be interesting in some rare cases, like comparing two models on the same dataset.

# Pearson's correlation coefficient

For a population:

$$\rho_{x_1 x_2} = \frac{\text{cov}(x_1, x_2)}{\sigma_1 \sigma_2} = \frac{E[(x_1 - \mu_1)(x_2 - \mu_2)]}{\sigma_1 \sigma_2}$$

$$\rho_{x_1(x_2 \dots x_k)} = 1 - \frac{|\hat{R}|}{\hat{R}_{11}}, \quad \hat{R} = |\rho_{x_i x_j}|, \quad \hat{R}_{11} \text{ is cofactor of } \rho_{x_1 x_1}$$

For a sample:

$$r_{x_1 x_2} = \frac{\sum_{i=1}^n (x_{1i} - \bar{x}_1)(x_{2i} - \bar{x}_2)}{\sqrt{\sum_{i=1}^n (x_{1i} - \bar{x}_1)^2 \sum_{i=1}^n (x_{2i} - \bar{x}_2)^2}}$$

$$r_{x_1(x_2 \dots x_k)} = 1 - \frac{|\hat{R}|}{\hat{R}_{11}}, \quad \hat{R} = |r_{x_i x_j}|, \quad \hat{R}_{11} \text{ is cofactor of } r_{x_1 x_1}$$

Turns out  $R^2 = r_{y(x_1 \dots x_k)}^2$

## Olkin and Finn models

- Model A: Determining whether an additional variable provides an improvement in predicting the criterion:  $\rho_{0(12)}^2 - \rho_{01}^2$ . This comparison shows whether an additional variable  $x_2$  provides an improvement over  $x_1$  alone in predicting  $y = x_0$ .
- Model B: Deciding which of two variables adds more to the prediction of the criterion:  $\rho_{0(12)}^2 - \rho_{0(13)}^2$ . This comparison shows whether the pair of predictors  $x_1, x_2$  or the pair  $x_1, x_3$  is more effective in predicting criterion  $y = x_0$ .
- Model E: Deciding if a given set of predictors performs equally well in two separate populations:  $\rho_I^2 - \rho_{II}^2$ . This comparison shows whether a given set of predictors  $(x_1, x_2, \dots, x_k)$  performs equally well in two independent samples of data.

## General procedure form

- $r_A$  and  $r_B$  - two sample correlations to be compared
- $\rho_A$  and  $\rho_B$  - their corresponding population values

The large sample distribution for the comparison:

$$\begin{aligned} [(r_A - r_B) - (\rho_A - \rho_B)] &\sim N(0, \sigma_\infty^2) \\ \sigma_\infty^2 &= \text{var}(r_A) + \text{var}(r_B) - 2\text{cov}(r_A, r_B) \end{aligned}$$

A  $100(1 - \alpha)\%$  confidence interval:

$$r_A - r_B \pm c\hat{\sigma}_\infty$$

where

- $c$  is the standard normal deviate  $z_{\alpha/2}$
- $\hat{\sigma}_\infty$  is an estimate of  $\sigma_\infty$  in which sample values replace population values

## General procedure form (cont'd)

The general form of variance of function of a set of correlations:

$$\begin{aligned}\text{var}_{\infty} f(r_{12}, r_{13}, r_{23}) &= \mathbf{a}\Phi\mathbf{a}' \\ \mathbf{a} &= \left( \frac{\partial f}{\partial r_{12}}, \frac{\partial f}{\partial r_{13}}, \frac{\partial f}{\partial r_{23}} \right) \\ \Phi &= \begin{pmatrix} \text{var}(r_{12}) & \text{cov}(r_{12}, r_{13}) & \text{cov}(r_{12}, r_{23}) \\ & \text{var}(r_{13}) & \text{cov}(r_{13}, r_{23}) \\ & & \text{var}(r_{23}) \end{pmatrix}\end{aligned}$$

The variances and covariances of correlations:

$$\begin{aligned}\text{var}(r_{ij}) &= ((1 - \rho_{ij}^2)^2)/n \\ \text{cov}(r_{ij}, r_{jk}) &= ((2\rho_{jk} - \rho_{ij}\rho_{ik})(1 - \rho_{ij}^2 - \rho_{ik}^2 - \rho_{jk}^2)/2 + \rho_{jk}^3)/n \\ \text{cov}(r_{ij}, r_{kl}) &= [\rho_{ij}\rho_{kl}(\rho_{ik}^2 + \rho_{il}^2 + \rho_{jk}^2 + \rho_{jl}^2)/2 + \rho_{ik}\rho_{jl} + \rho_{il}\rho_{jk} \\ &\quad - (\rho_{ij}\rho_{ik}\rho_{il} + \rho_{ji}\rho_{jk}\rho_{jl} + \rho_{ki}\rho_{kj}\rho_{kl} + \rho_{li}\rho_{lj}\rho_{lk})]/n\end{aligned}$$

## Data: A Study of Teenage Use of Abusable Substances

- The data were collected as part of a study of the use of alcohol, cigarettes, and marijuana among urban school children.
- An abusable substance score (USE, ranging from 0 to 3) was created by summing the number of substances (cigarettes, alcohol, or marijuana) that the individual had tried.
- Perceived friends' use (FRIENDS, ranging from 0 to 12) was assessed by questions that asked students to indicate the number of friends, who were using alcohol, cigarettes, or marijuana.
- Perceived family use (FAMILY) is the number of abusable substances, out of three, that were used by any member of the student's family.



## Model A illustration

- Determining whether an additional variable provides an improvement in predicting the criterion.
- The variables are  $x_0 = \text{USE}$ ,  $x_1 = \text{FRIENDS}$ ,  $x_2 = \text{FAMILY}$ .
- The procedure compares  $\rho_{0(12)}^2$  with  $\rho_{01}^2$  using estimates  $r_{0(12)}^2$ ,  $r_{01}^2$  and  $\hat{\sigma}_\infty^2 = \text{var}(r_{0(12)}^2 - r_{01}^2)$

## Model A illustration (cont'd)

Following the procedure,

$$\text{var}(f(r_{01}, r_{02}, r_{12})) = \text{var}(r_{0(12)}^2 - r_{01}^2) = \mathbf{a}\Phi\mathbf{a}'$$

$$\mathbf{a} = \left( \frac{\partial f}{\partial r_{01}}, \frac{\partial f}{\partial r_{02}}, \frac{\partial f}{\partial r_{12}} \right) = (a_1, a_2, a_3)$$

$$a_1 = \frac{2\rho_{12}}{1 - \rho_{12}^2}(\rho_{01}\rho_{12} - \rho_{02}), \quad a_2 = \frac{2}{1 - \rho_{12}^2}(\rho_{02} - \rho_{01}\rho_{12})$$

$$a_3 = \frac{2}{(1 - \rho_{12}^2)^2}(\rho_{12}\rho_{01}^2 + \rho_{12}\rho_{02}^2 - \rho_{01}\rho_{02} - \rho_{01}\rho_{02}\rho_{12}^2)$$

$$\Phi = \begin{pmatrix} \text{var}(r_{01}) & \text{cov}(r_{01}, r_{02}) & \text{cov}(r_{01}, r_{12}) \\ & \text{var}(r_{02}) & \text{cov}(r_{02}, r_{12}) \\ & & \text{var}(r_{12}) \end{pmatrix}$$

## Model A illustration (cont'd)

The sample correlation matrix (obtained from the data):

$$R = \begin{pmatrix} r_{00} & r_{01} & r_{02} \\ & r_{11} & r_{12} \\ & & r_{22} \end{pmatrix} = \begin{pmatrix} 1.000 & 0.433 & 0.199 \\ & 1.000 & 0.178 \\ & & 1.000 \end{pmatrix}$$

The estimate of  $\rho_{01}^2$  is  $r_{01}^2 = 0.188$ . The estimate of  $\rho_{0(12)}^2$  is

$$r_{0(12)}^2 = \frac{r_{01}^2 + r_{02}^2 - 2r_{01}r_{02}r_{12}}{1 - r_{12}^2} = 0.203$$

The difference is  $r_{0(12)}^2 - r_{01}^2 = 0.015$

## Model A illustration (cont'd)

The sample values in  $R$  are substituted in the expressions for  $a_1$ ,  $a_2$  and  $a_3$ :

$$\hat{\mathbf{a}} = (-0.447, 0.2511, -0.1032)$$

The variance-covariance matrix:

$$\hat{\Phi} = \frac{1}{1.415} \begin{pmatrix} 0.6598 & 0.1056 & 0.1265 \\ & 0.9226 & 0.3893 \\ & & 0.9377 \end{pmatrix}$$

Consequently,

$$\hat{\sigma}_\infty = \sqrt{\hat{\mathbf{a}}\hat{\Phi}\hat{\mathbf{a}}'} = \sqrt{\frac{0.0481}{1.415}} = 0.0058$$
$$r_{0(12)}^2 - r_{01}^2 \pm c\hat{\sigma}_\infty = 0.015 \pm (1.96)(0.0058) = [0.004, 0.027]$$

The family's use of abusable substances contributes to explaining use in school, above and beyond the effects of friends.

# References

- Olkin, I., & Finn, J. D. (1995). Correlations Redux.
- `java.dzone.com/articles/damn-r-squared`
- `en.wikipedia.org/wiki/Coefficient_of_determination`
- `en.wikipedia.org/wiki/Pearson_product-moment_correlation_coefficient`