Out of sample R-squared.

Assume data are normalized so that the mean is subtracted off.

y = actual vector

 = predicted vector

u=y- residual vector

Formula 1:



Formula 2:



Formula 3:



These formulae are the same only when the residuals are ordinary least squares residuals.

Theorem: If u are the ordinary least squares residuals and the ordinary least squares predicted values, then all three formulae are the same.

Proof:



but  and since ordinary least squares residuals and predicted values are orthogonal,  so or



So formula 1 and formula 2 are the same. Similarly,  . For formula 3



 where again we use  So

 , which is formula 1.

What made this work was the orthogonality of the in-sample ordinary least squares residuals and in-sample ordinary least squares predicted values.

None of these formulae are the same without orthogonality. However, formulae 1 and 3 are both meaningful. But of these I think formula 3 is most meaningful: squared correlation of actual and fitted values. This will always be between zero and 1 and if the actual and fitted are close will be close to 1 and if not close to zero. Neither formula 1 nor 2 have this property, 2 can be negative. Though it has more meaning as the fraction of variation explained, Formula 1 can give  greater than 1, so it explains more variation than there is. You might want to prove or demonstrate both (a simple example of each does it.)