

Numerical Model Comparison Criteria

As one searches through myriad possible MLR models potentially describing the relationship between predictors x and a response, y , one generally wants a model with a "small" number of predictors (a simple or parsimonious model), a "large" value of R^2 and a "small" value of s_e . The naive "solution" to the model search problem of just "picking the biggest possible model" is in fact no solution, in light of the potential for "overfitting" a data set (adopting a model with too many "wiggles" that can nicely reproduce the y 's in the data set, but that does a very poor job when used to produce even mild extrapolations or interpolations).

For a given prediction problem (and therefore fixed $SSTot$), R^2 and $s_e = \sqrt{MSE}$ are "equivalent" in the sense that one could be obtained from the other (and $SSTot$). They don't, however, necessarily produce the same ordering of reduced models of some grand MLR model in terms of "best looking" values of the criteria (e.g. the full model has the largest R^2 but may not have the smallest s_e). There are several other functions of SSE that have been suggested as possible statistics for model diagnostics/selection. Among them are Mallows' C_p and Akaike's Information Criterion (the AIC).

Mallows' C_p is based on the fact that the average total squared difference between the n values \hat{y}_i from a MLR fit and their (real) means μ_i can be worked out theoretically. When divided by σ^2 , this is a quantity Γ_p that is

- a) p , when there is a choice of p coefficients β in a $(p - 1)$ -predictor reduced MLR model that produces correct means for all n data points, and
- b) larger than p , when there is no such choice.

Mallows' suggestion for comparing reduced versions of a full (k -predictor) MLR model, is that for a reduced model with $(p - 1) \leq k$ predictors, one compute

$$C_p = \frac{SSE_{Red}}{MSE_{Full}} + 2p - n$$

(an estimate of Γ_p if the full k -variable MLR model is correct) and look for small p and C_p no more than about p . The thinking is that such a reduced model is simpler than the full model and appears to produce predictions comparable to the full model predictions *at the (x_1, x_2, \dots, x_k) vectors in the data set.*

Akaike's Information Criterion is based on considerations beyond the scope of this exposition. For a MLR model with k predictors, it is

$$AIC = n \ln \left(\frac{SSE}{n} \right) + 2(k + 1)$$

and people look for small values of AIC .