

Monte Carlo estimates of model comparisons.

Let \mathbf{y} denote $n \times 1$ vector of responses generated by the true model and \mathbf{X} be $n \times p$ matrix of predictors, where p is the number of parameters in the fitted model. Under the Gauss-Markov assumptions $\mathbb{E}(\epsilon_i) = 0$, $Var(\epsilon_i) = \sigma^2$, $Cov(\epsilon_i, \epsilon_j)$ for all i, j we denote the vector of joint maximum likelihood estimates for the regression coefficients by $\hat{\boldsymbol{\beta}}$. By definition of Schwarz Criterion

$$S(M) = 2p \log(n) - 2 \log \mathbb{P}(\mathbf{y}|\mathbf{X}, \hat{\boldsymbol{\beta}}).$$

If Akaike's Information Criterion is used, $2p$ replaces $2p \log(n)$. The loglikelihood in the second term is equal to n times the log of the residual sums of squares and it can be written as

$$\log \mathbb{P}(\mathbf{y}|\mathbf{X}, \hat{\boldsymbol{\beta}}) = n \log(\mathbf{y}'\mathbf{y} - \mathbf{y}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}) + C,$$

where C is a term dependent only on M_T . For transition probabilities, we are interested in $\mathbb{P}(S(M_i) < S(M_j))$. We have

$$\begin{aligned} S(M_i) - S(M_j) &= (p_i - p_j) \log(n) + n \log(\mathbf{y}'\mathbf{X}_i(\mathbf{X}'_i\mathbf{X}_i)^{-1}\mathbf{X}'_i\mathbf{y}) \\ &\quad - n \log(\mathbf{y}'\mathbf{X}_j(\mathbf{X}'_j\mathbf{X}_j)^{-1}\mathbf{X}'_j\mathbf{y}), \end{aligned} \quad (1)$$

where subscripts i, j now denote quantities that depend on model M_i and M_j . The random variable $\mathbf{I}_{\{S(M_i) - S(M_j) < 0 | M_T\}}$ is Bernoulli distributed with probability of success $\mathbb{P}(S(M_i) - S(M_j) < 0)$ which is equal to its expectation $\mathbb{E}(\mathbf{I}_{\{S(M_i) - S(M_j) < 0 | M_T\}})$ whose Monte Carlo estimate is given by

$$\widehat{\mathbb{E}}(\mathbf{I}_{\{S(M_i) - S(M_j) < 0 | M_T\}}) = \frac{1}{V} \sum_{v=1}^V \mathbf{I}_{\{S(M_i) - S(M_j) < 0 | \mathbf{y}_v\}}. \quad (2)$$

An estimate of $\mathbb{P}(S(M_i) - S(M_j) < 0)$ is obtained using Eq. (2) conditional on true model M_T and its predictors X_T as follows. First, generate the set of k predictor variables and build \mathbf{X}_i and \mathbf{X}_j for M_i and M_j respectively. Then generate $\boldsymbol{\beta}_{T_v}$, $v = 1, 2, \dots, V$ independently of each other. Finally, simulate $\mathbf{y}_v | \mathbf{X}_T, \boldsymbol{\beta}_{T_v}$ from the normal distribution with expected value $\mathbb{E}(\mathbf{y}_v) = \mathbf{X}_T \boldsymbol{\beta}_{T_v}$ and variance σ^2 . Each realization $(\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_v)$ is used in Eq. (1) to assess $S(M_i) - S(M_j) < 0$ and the estimate is obtained using the mean in Eq. (2).