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RESEARCH ARTICLE

Decoding Predictive Power: A Simulation Study on Information Criteria vs. Internal Performance Measures

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KEYWORDS
Simulation study, Information criteria, Internal performance measures, Predictive power, Model selection

1 | INTRODUCTION

In public health, prediction models have the ability to target preventive interventions to persons at high risk of having or developing a disease (prognosis and diagnosis). In clinical practice, prediction models may inform patients and their doctors on the probability of a diagnosis or prognostic outcome[1]. Identification of patients at high risk can be based on a combination of risk factors, risk indicators or other predictors (e.g. a particular patient characteristic, bio-marker or test result). The performance of these prediction models impacts public health and clinical practice, thus making correct modelling choices crucial[2].

2 | BACKGROUND

The traditional approach to medical prediction models uses logistic regression[3]. For model selection, two methodologies are often employed. Information Criteria (IC) -or model selection methods- estimate the information loss when the probability distribution of the true model is approximated by the probability distribution of a candidate model. By minimizing this discrepancy (Kullback-Leibler divergence[4]) between these distributions, the goal is to select the model that represents the data generating mechanism. The second methodology is the procedure of using internal model performance measures for estimating the out-of-sample performance of the proposed candidate models. Model performance includes discriminatory ability, calibration and overall accuracy. Commonly used techniques are Area under the Receiver Operated Curve (AUROC) and R^2, based on which the best performing proposed model can be selected.

Information criteria, like the Akaike's information criterion (AIC[5]) and the Bayesian information criterion (BIC[6]), are both commonly used for model selection in health studies. The AIC and BIC share the same goodness-of-fit term, but the penalty terms differ based on the manner in which the dimension k (number of parameters) and n (sample size) is incorporated: BIC employs a complexity penalization of $k \log n$ as opposed to $2k$ of the AIC. Consequently, BIC tends to choose fitted models that are more parsimonious than those favored by AIC[7]. Conversely, the AIC favours more complex models in large sample setting. Information criteria only provide information about the relative quality between models using the same likelihood function and data set[8].

Several internal performance measures are available for an estimate of out-of-sample model performance. The AUROC analysis is developed for predictive model selection[9] and is widely adopted in clinical science to assess the model sensitivity and specificity trade-off[10]. Bootstrapping is a preferred technique for assessing prediction models using performance measures such as AUROC[11,12], since using the cases from the original analysis sample results in an overly optimistic performance estimate[13]. The AUROC is also criticized for being a semi-proper scoring rule[14], which means that the best performance can be attained by a misspecified model. Another performance measure of prediction models is the R^2. In ordinary least-squares regression it is interpretable as the proportion of outcome variation, which can be explained by the predictors. Pseudo R^2 indices have been developed for logistic regression, such as methods of Cox and Snell[15], Nagelkerke[16], and McFadden[17]. Import to note is that R^2 measures increase monotonically with increasing number of covariates even if they have no prognostic value at all[18].

Concluding, ICs and internal performance measures intend to approximate the data generating model and have the best out-of-sample performance, aiming for the highest predictive power in the total population. We are interested in their ability to choose the correct model when the data generating mechanism is known. Testing the IC success rate and performance measures (AUROC and R^2) for choosing the correct model in different simulation contexts, such as sample size and data quality, may yield information for future prediction modelling choices. The according research question will be: How successful are Information Criteria and internal performance measures in choosing the correct prediction model in different simulated contexts? We expect a difference in these factors and a specific use and integration of the techniques in real life application. We will follow a mini-thesis structure that only look at one simple data generating mechanism. The results of this study will be used to inform the design of the thesis.

3 | METHODS

In this study, we focus on prediction models designed for dichotomous risk prediction, such as disease occurence. To investigate the succes rate of IC and internal performance measures, we simulated a population dataset and sampled from this dataset. The simulations, analyses and visualizations were performed in R-studio[19].

3.1 | Data generating mechanism

To generate our population dataset, we simulated a population of 2,000,000 individuals, each characterized by three covariates (X1, X2, and X3). These covariates were independently derived from standard normal distributions. The mean vector (μ) and the covariance matrix (Σ) for these distributions were defined as follows:

$$\boldsymbol{\mu} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \boldsymbol{\Sigma} = \begin{bmatrix} 1 & 0.2 & 0.2 \\ 0.2 & 1 & 0.2 \\ 0.2 & 0.2 & 1 \end{bmatrix}$$

The probability of each individual belonging to the outcome group was determined based on their covariate values. This was done using a logistic regression model, which defined the probability of the outcome $Y = 1$ as a function of the covariates X_1, X_2, X_3:

$$P(Y = 1|X_1, X_2, X_3) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3)}} \tag{1}$$

In our model, the coefficients were set as $\beta_0 = 0, \beta_1 = 0.8, \beta_2 = 0.8, \beta_3 = 0.4$. The outcome for each individual was then generated following a Bernoulli distribution, with the probability $P(Y = 1|X_1, X_2, X_3)$ and a cutoff value of 0.5. This simulation approach results in a true C-statistic or AUROC (Area Under the Receiver Operating Characteristic curve) of 0.80, reflecting the model's true discriminative ability.

3.2 | Analysis

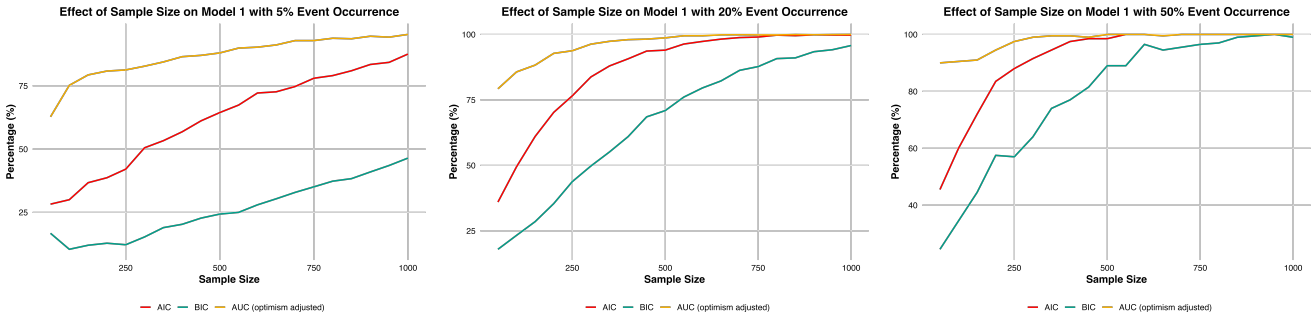
In this study, we analyzed the success rate by comparing the true model, which was the one used to generate the data, with the models identified by IC and internal performance measures. The true model was defined as the model that generated the data. For each potential model, we calculated both the ICs and internal performance measures. The success rate was quantified as the proportion of instances where the true model $(X_1, X_2, X3)$ was correctly chosen as the best performing model, opposed to the model with only X_1 and X_2 as covariates (X_1, X_2).

For our internal performance evaluation, we specifically used the AUC, calculated by using the pROC package[20]. To correct for the optimism in the apparent AUC in the sample, we bootstrap the sample and calculate the optimism-corrected AUC. The optimism-corrected AUC is calculated by subtracting the average bootstrapped optimism from the apparent AUC. The optimism is calculated by taking the difference between the AUC in the bootstrap sample and the AUC in the test sample[21].For this purpose, a bootstrap with 80 resamples was performed in each iteration.

This analysis procedure was repeated for three different event rates (5%, 20%, and 50%). Per event rate, we calculated the success rate for three different ICs (AIC, BIC, and AICc) for a sample size ranging from 50 to 1,000 with intervals of 50. Per sample size, 2,500 iterations were performed. The success rate was calculated for each combination of event rate and sample size.

4 | RESULTS

For all sample sizes, the success rate was calculated. This is shown in plot 1.



(a) 5% disease.

(b) 20% disease.

(c) 50% disease.

FIGURE 1 Creating subfigures in LaTeX.

5 | DISCUSSION

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6 | CONCLUSIONS

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