

# Bootstrapping Pseudo - $R^2$ Measures for Binary Response Variable Model

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## To cite this article:

Zakariya Yahya Algamal, Haithem Taha Mohammad Ali. Bootstrapping Pseudo- $R^2$  Measures for Binary Response Variable Model.

*Biomedical Statistics and Informatics*. Vol. 2, No. 3, 2017, pp. 107-110. doi: 10.11648/j.bsi.20170203.13

**Received:** March 7, 2017; **Accepted:** March 16, 2017; **Published:** March 31, 2017

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**Abstract:** Statistical inference is based generally on some estimates that are functions of the data. Bootstrapping procedure offers strategies to estimate or approximate the sampling distribution of a statistic. Logistics regression model with binary response is commonly used. This paper focuses on the behavior of bootstrapping pseudo -  $R^2$  measures in logistic regression model. Simulation and real data results also presented. We conclude and suggest to use either  $R^2_M$  or  $R^2_D$ , since they have convergence in there values.

**Keywords:** Logistic Regression, Pseudo -  $R^2$ , Bootstrap, Logit, Propit

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## 1. Introduction

One of the important methods in statistics is that the regressing a binary response variable on a set of explanatory variables. Binary response variable has two values, typically coded 0 for the event did not occur and 1 for the event did occur [12]. For the standard linear regression model the familiar coefficient of determination,  $R^2$ , is a widely used goodness of fit measure. The term bootstrap which is due to the Efron [5] is an illusion to the expression "pulling on self up by one's bootstraps" meaning doing the impossible [6]. The bootstrap is a method to derive properties like standard error, confidence intervals, of the sampling distribution of estimators. The bootstrap resampling consists of  $n$  elements that are drawn randomly from the  $n$  original data points with replacement [7]. This paper focuses on the behavior of bootstrapping pseudo-  $R^2$  measures. Simulation and real data results also presented. The contents of this paper may be divided into eight sections. In section 2 and 3 we review the binary response variable model and pseudo measures, respectively. In section 4 we introduce bootstrapping pseudo  $R^2$ . The simulation results, real data results, conclusions and references are given in sections 5, 6, 7, and 8, respectively.

## 2. Binary Response Variable Model

Binary response is commonly studies in medical and epidemiologic research, for instance, the presence or absence of a particular disease, death during surgery. Models for mutually exclusive binary outcomes focus on the determinates of the probability  $p$  of the occurrence of one outcome rather than an alternative outcome that occurs with a probability of  $1-p$ . In regression analysis we want to measure how the probability

$p$  varies across individuals as a function of explanatory variables. Binary response variable has two values, typically coded 0 for the event did not occur and 1 for the event did occur [12]. The expected value of a binary variable is the probability that it takes the value 1.

Let  $p(y_i = 1) = \pi_i$  and  $p(y_i = 0) = 1 - \pi_i$ , then

$$E(y_i) = 0 * (1 - \pi_i) + 1 * \pi_i = p(y_i = 1) = \pi_i \quad (1)$$

With explanatory variables,  $x_i$ 's ,

$$E(y_i | x_i) = \pi_i = p(y_i = 1 | x_1, x_2, \dots, x_k) = \beta_0 + \beta_1 x_1 + \dots + \beta_k x_k \quad (2)$$

Since  $\pi_i$  is a probability, it must be between 0 and 1. The linear function given in (2) is not an adequate statistical

model since the equation (2) can lie outside  $[0, 1]$  and does not represent a probability [3]. Binary response models directly describe the response probability that the response variable takes value 1 is modeled as

$$E(y_i | x_i) = p(y_i = 1 | x_1, x_2, \dots, x_k) = F(x_i' \beta) \quad (3)$$

A binary response model is referred to as a probit model if  $F(\cdot)$  is the cumulative normal distribution function. It is called logit model if  $F(\cdot)$  is the cumulative logistic distribution function. The estimation problem is to estimate the unknown parameters  $\beta$ . In practice, the ordinary least squares predictions of the conditional probability can be greater than one or less than zero [9]. The probit model is:

$$E(y_i | x_i) = \varphi(x_i' \beta) = \int_{-\infty}^{x_i' \beta} f(t) dt = \int_{-\infty}^{x_i' \beta} \frac{1}{\sqrt{2\pi}} e^{-\frac{t^2}{2}} dt \quad (4)$$

And the logit model is

$$E(y_i | x_i) = \frac{e^{x_i' \beta}}{1 + e^{x_i' \beta}} \quad (5)$$

The probit and logit models are typically estimated by maximum likelihood (ML) method. Assuming independence across observations, the likelihood function is:

$$L = \prod_{i|y_i=0}^n p(y_i = 0 | x_i) \prod_{i|y_i=1}^n p(y_i = 1 | x_i) \quad (6)$$

$$= \prod_{i=1}^n [1 - F(w_i)]^{1-y_i} F(w_i)^{y_i} \quad (7)$$

Where  $p(y_i = 1 | x_i) = F(w_i) = \varphi(w_i)$  in the probit model and  $p(y_i = 1 | x_i) = F(w_i) = \frac{e^{x_i' \beta}}{1 + e^{x_i' \beta}}$  in the logit model. The corresponding Log likelihood function is:

$$\log L = \sum_{i=1}^n [y_i \log F(w_i) + (1 - y_i) \log(1 - F(w_i))] \quad (8)$$

The first derivative of (8) is

$$\frac{\partial \log L}{\partial \beta} = \sum_{i=1}^n \left[ y_i \frac{f(w_i)}{F(w_i)} + (1 - y_i) \frac{-f(w_i)}{F(w_i)} \right] x_i' = 0 \quad (9)$$

Solving (9) using an iterative method one can get the maximum likelihood estimation of  $\beta$  [8].

### 3. Pseudo - $R^2$ Measures

For the standard linear regression model the familiar coefficient of determination,  $R^2$ , is a widely used goodness of fit measure. Application of this measure to binary response variable model such as logit and probit has no universal definition. A number of measures can be proposed. Pseudo-

$R^2$  usually have the property that, on specialization to the linear model, the coincide with an interpretation of the linear model  $R^2$  [1]. Many different Pseudo-  $R^2$  measures have been proposed in the past four decades [11].

#### 3.1. McFadden's Pseudo - $R^2$

McFadden's [13] defines the pseudo-  $R^2$  based on the maximum log likelihood, it is:

$$R^2_M = 1 - \left[ \frac{\log L(\text{Full model})}{\log L(\text{Null model})} \right] \quad (10)$$

Where the Full model is the model with all variables in the model, whereas the null model is the model with intercept only. Theoretically the range of this coefficient is between 0 and 1.

#### 3.2. Cragg and Uhler Pseudo - $R^2$

Cragg and Uhler [4] introduced a normal version of the transformation of the likelihood ratio, it is defined as:

$$R^2_{cu} = \left[ \frac{\exp(\log L(\text{Full model}))^{2/n} - \exp(\log L(\text{Null model}))^{2/n}}{1 - \exp(\log L(\text{Null model}))^{2/n}} \right] \quad (11)$$

#### 3.3. Deviance Pseudo - $R^2$

Mittlbick and Heinzl [14] proposed pseudo  $R^2$  measure for generalized linear models based on the concept of deviance. This measure,  $R^2_D$ , is defined as:

$$R^2_D = 1 - \frac{D(\text{Full model})}{D(\text{Null model})} \quad (12)$$

Where D (Full model) is the deviance of the full model, and D (Null model) is the deviance of the null model. It cannot become negative and increases monotonically with increasing number of explanatory variables.

## 4. Bootstrap Pseudo - $R^2$

The term bootstrap which is due to the Efron [5] is an illusion to the expression "pulling on self up by one's bootstraps" meaning doing the impossible [6]. The bootstrap is a method to derive properties like standard error, confidence intervals, of the sampling distribution of estimators. The bootstrap resampling consists of  $n$  elements that are drawn randomly from the  $n$  original data points with replacement [7]. In the term of regression analysis, we have two kind of bootstrapping, residual bootstrapping and paired bootstrapping. Consider a sample with  $n$  independent observations of the response variable  $y$  and  $k+1$  explanatory variables  $x$ . A paired bootstrap sample is obtained by independently drawing rows with replacement from the pairs  $(y_i, x_i)$ . The bootstrap sample has the same number of observations, however some observations appear several time and others never. The bootstrap involves drawing a large number  $B$  of bootstrap samples. An

individual bootstrap sample is denoted  $(y_b^*, x_b^*)$  [2]

$$R^{2(\text{boot})}_{\text{pseudo}} = \frac{\sum_{b=1}^B R^{2(b)}_{\text{pseudo}}}{B} \tag{13}$$

And

$$\text{bias} = R^{2(\text{boot})}_{\text{pseudo}} - R^2_{\text{pseudo}} \tag{14}$$

### 5. Simulation Results

In this section, we examine by simulation the performance of the bootstrap procedure based on varies values of B and sample sizes of n of the three pseudo measures in section 3. Three cases of simulation were done; the first set the value of  $\beta_0, \beta_1,$  and  $\beta_2$  as 2, 0.5, and 0.5, respectively. The second case the parameters' values were 2, 1, and 1 respectively. While the third case parameter values were 2, 2, and 2 respectively. The number of bootstrap samples, B, set to be 1000, 10000, and 100000 respectively. We simulate different sample sizes (10, 25, 50, and 100) from uniform distribution with (-1, 1) as explanatory variables and simulate the response variable according to logit model. Tables 1, 2, 3, and 4 show the results.

Table 1. Pseudo -  $R^2$  when  $n = 10$ .

B=1000	$R^2_M (R^2_M)$	$R^2_D (R^2_D)$	$R^2_{cu} (R^2_{cu})$
$\beta_0 \beta_1 \beta_2$	(boot)	(boot)	(boot)
2 0.5 0.5	0.1417 (0.521)	0.1054 (0.505)	0.1417 (0.571)
1 1	0.045 (0.464)	0.0451 (0.417)	0.026 (0.4029)
2 2	0.037 (0.181)	0.038 (0.523)	0.0272 (0.1761)
B=10000			
$\beta_0 \beta_1 \beta_2$			
2 0.5 0.5	0.1417 (0.209)	0.1054 (0.185)	0.1417 (0.21)
1 1	0.045 (0.426)	0.0451 (0.43)	0.0268 (0.39)
2 2	0.037 (0.203)	0.038 (0.193)	0.0272 (0.155)
B=100000			
$\beta_0 \beta_1 \beta_2$			
2 0.5 0.5	0.1417 (0.21)	0.1054 (0.181)	0.1417 (0.209)
1 1	0.045 (0.425)	0.0451 (0.415)	0.0268 (0.394)
2 2	0.037 (0.197)	0.038 (0.228)	0.0272 (0.167)

Table 2. Pseudo -  $R^2$  when  $n = 25$ .

B=1000	$R^2_M (R^2_M)$	$R^2_D (R^2_D)$	$R^2_{cu} (R^2_{cu})$
$\beta_0 \beta_1 \beta_2$	(boot)	(boot)	(boot)
2 0.5 0.5	0.664 (0.843)	0.665 (0.85)	0.548 (0.794)
1 1	0.822 (0.922)	0.821 (0.901)	0.742 (0.903)
2 2	0.253 (0.393)	0.254 (0.464)	0.168 (0.297)
B=10000			
$\beta_0 \beta_1 \beta_2$			
2 0.5 0.5	0.664 (0.836)	0.665 (0.791)	0.548 (0.803)
1 1	0.822 (0.931)	0.821 (0.81)	0.742 (0.85)
2 2	0.253 (0.373)	0.254 (0.45)	0.168 (0.301)
B=100000			
$\beta_0 \beta_1 \beta_2$			
2 0.5 0.5	0.664 (0.838)	0.665 (0.82)	0.548 (0.771)
1 1	0.822 (0.925)	0.821 (0.85)	0.742 (0.82)
2 2	0.253 (0.351)	0.254 (0.395)	0.168 (0.293)

Table 3. Pseudo -  $R^2$  when  $n = 50$ .

B=1000	$R^2_M (R^2_M)$	$R^2_D (R^2_D)$	$R^2_{cu} (R^2_{cu})$
$\beta_0 \beta_1 \beta_2$	(boot)	(boot)	(boot)
2 0.5 0.5	0.0732 (0.14)	0.073 (0.141)	0.0489 (0.157)
1 1	0.22 (0.258)	0.221 (0.263)	0.1316 (0.1677)
2 2	0.592 (0.642)	0.593 (0.641)	0.458 (0.524)
B=10000			
$\beta_0 \beta_1 \beta_2$			
2 0.5 0.5	0.0732 (0.143)	0.073 (0.132)	0.0489 (0.155)
1 1	0.22 (0.256)	0.221 (0.26)	0.1316 (0.162)
2 2	0.592 (0.632)	0.593 (0.634)	0.458 (0.519)
B=100000			
$\beta_0 \beta_1 \beta_2$			
2 0.5 0.5	0.0732 (0.135)	0.073 (0.13)	0.0489 (0.143)
1 1	0.22 (0.24)	0.221 (0.252)	0.1316 (0.159)
2 2	0.592 (0.613)	0.593 (0.62)	0.458 (0.48)

Table 4. Pseudo -  $R^2$  when  $n = 100$ .

B=1000	$R^2_M (R^2_M)$	$R^2_D (R^2_D)$	$R^2_{cu} (R^2_{cu})$
$\beta_0 \beta_1 \beta_2$	(boot)	(boot)	(boot)
2 0.5 0.5	0.0129 (0.0425)	0.013 (0.045)	0.009 (0.0307)
1 1	0.15 (0.173)	0.151 (0.177)	0.1038 (0.1258)
2 2	0.375 (0.397)	0.3751 (0.39)	0.248 (0.27)
B=10000			
$\beta_0 \beta_1 \beta_2$			
2 0.5 0.5	0.0129 (0.0422)	0.013 (0.042)	0.009 (0.0302)
1 1	0.15 (0.171)	0.151 (0.175)	0.1038 (0.1248)
2 2	0.375 (0.389)	0.3751 (0.39)	0.248 (0.255)
B=100000			
$\beta_0 \beta_1 \beta_2$			
2 0.5 0.5	0.0129 (0.041)	0.013 (0.041)	0.009 (0.0299)
1 1	0.15 (0.17)	0.151 (0.171)	0.1038 (0.122)
2 2	0.375 (0.385)	0.3751 (0.38)	0.248 (0.25)

From Tables 1, 2, 3, and 4 we observe that the value of the pseudo  $R^2_M, R^2_D,$  and  $R^2_{cu}$  be larger than the original pseudo values and we see the convergency of the pseudo  $R^2_M$  and  $R^2_D$  values.

### 6. Real Data Results

We will use a sample of 30 person from Ibn-Alattheer hospital. The response variable be binary with (1 if the person diagnostic to has Thalassemia and 0 if not). Nine variables have been studied as an explanatory variables, they are, sex (1 for male and 0 for female), age, body mass index, HB, PCV, ferritin, IL-6, TNF, and uric acid. The results are shown in Table 5.

Table 5. Pseudo -  $R^2$  for the real data.

	$R^2_M$	$R^2_D$	$R^2_{cu}$
	( $R^2_M$ (boot))	( $R^2_D$ (boot))	( $R^2_{cu}$ (boot))
B=1000	0.584 (0.578)	0.582 (0.614)	0.448 (0.581)
B=10000	0.584 (0.611)	0.582 (0.5725)	0.448 (0.484)
B=100000	0.584 (0.602)	0.582 (0.5713)	0.448 (0.450)

### 7. Conclusions

In this paper, we have shown from Table 1 when the sample size is 10 and for all values of B, the values of

bootstrapped pseudo measures greatly difference from the original values of the pseudo measures, that is the bias is so large. This bias gradually be small when the sample size change from 25 to 50 and to 100. Furthermore, from Tables (1-5) we conclude and suggest to use either  $R^2_M$  or  $R^2_D$ , since they have convergence in there values. Moreover, we recommended that the bootstrap procedures may be not good to verify the asymptotic normal theory since we will get constant bootstrap samples contain only 1 or 0. But asymptotically of normal theory be met when the sample size is more than 50, the results for the real data in Table 5 support our conclusion.

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