

# Northumbria Research Link

Citation: Ogundimu, Emmanuel (2019) Prediction of default probability by using statistical models for rare events. *Journal of the Royal Statistical Society: Series A (Statistics in Society)*, 182 (4). pp. 1143-1162. ISSN 0964-1998

Published by: Wiley-Blackwell

URL: <https://doi.org/10.1111/rssa.12467> <<https://doi.org/10.1111/rssa.12467>>

This version was downloaded from Northumbria Research Link:  
<http://nrl.northumbria.ac.uk/id/eprint/39072/>

Northumbria University has developed Northumbria Research Link (NRL) to enable users to access the University's research output. Copyright © and moral rights for items on NRL are retained by the individual author(s) and/or other copyright owners. Single copies of full items can be reproduced, displayed or performed, and given to third parties in any format or medium for personal research or study, educational, or not-for-profit purposes without prior permission or charge, provided the authors, title and full bibliographic details are given, as well as a hyperlink and/or URL to the original metadata page. The content must not be changed in any way. Full items must not be sold commercially in any format or medium without formal permission of the copyright holder. The full policy is available online: <http://nrl.northumbria.ac.uk/policies.html>

This document may differ from the final, published version of the research and has been made available online in accordance with publisher policies. To read and/or cite from the published version of the research, please visit the publisher's website (a subscription may be required.)



**Northumbria  
University**  
NEWCASTLE



**UniversityLibrary**

# Prediction of default probability by using statistical models for rare events

Emmanuel O. Ogundimu

*Department of Mathematics, Physics and Electrical Engineering, Northumbria University, UK*

## Abstract

Prediction models in credit scoring usually involve the use of data sets with highly imbalanced distribution of the event of interest (default). Logistic regression, which is widely used to estimate probability of default ( $PD$ ), often suffers from the problem of separation when the event of interest is rare and consequently poor predictive performance of the minority class in small sample. A common solution is to discard majority-class examples, duplicate minority-class examples, or use combination of both to balance the data. These methods may overfit data. It is unclear how penalized regression models such as the Firth (1993) estimator, which reduces bias and mean square-error relative to classical logistic regression performs in modelling  $PD$ . We review some methods for class imbalanced data and compare them in a simulation study using the Taiwan credit card data. We emphasized the impact of events per variable (EPV) for developing accurate model- an often neglected concept in  $PD$  modelling. The data balancing technique considered are ROSE (Random Over-Sampling Examples) and SMOTE (Synthetic Minority Over-Sampling Technique) methods. The results indicate that SMOTE improved predictive accuracy of  $PD$  regardless of sample size. Among the penalized regression models analyzed, the log-F prior and ridge regression methods are preferred.

Keywords: *Credit scoring; Default probability; Firth method; Imbalanced data; Rare event; SMOTE technique*

## 1 Introduction

Prediction models for credit risk forecasting, often referred to as credit scoring models, are widely used in finance and banking. This is because bank regulations required banks to develop

a systematic approach to evaluating and controlling risks based on timely data and their analysis and interpretations (Basel Committee on Banking Supervision (June, 2004)). Basel II accord emphasized the importance of the interface between statistical modelling (credit scoring) and application of these models for internal ratings of credit worthiness of a loan applicant.

Credit scoring is a set of decision models that aid lenders in the granting of consumer credit (Thomas et al. (2002)). Its ultimate aim is to predict risk and not explain it. The scoring system are based on the past performance of consumers who are similar to those who will be assessed under the system. In other words, a number of particular loan applicant attributes are used to assign a score. These scores are used to determine credit worthiness of the applicant. In practice, the credit scores are transformed into probability of default ( $PD$ ).  $PD$  is the expected probability that a borrower will default on the debt before its maturity.

Durand (1941) was the first to propose the use of discriminant analysis to distinguish bad loans from good ones. The approach was popularized by Altman (1968), who used discriminant analysis to model credit risk. Several authors have proposed methods for modelling  $PD$ . Two streams of literature are distinguished- literature that relies on the machine learning techniques and classical methods that involves the use of statistical models. The former placed emphasis on predictions and not development of explanation, while the latter prioritized the interpretation of covariate effects (Berk & Bleich (2013)) over predictions. Some research that compared these techniques concluded that the machine learning techniques for credit scoring, such as neural networks and fuzzy algorithms are better than the classical methods. Others such as Ghotra et al. (2015) ranked the performance of random forest and logistic regression above learners such as support vector machine, decision trees and Naive Bayes. The implication of the discordant viewpoints is that there is generally no overall best statistical technique that can be recommended for developing credit scoring models (Hand & Henley (1997)). Thus, the choice of models should be guided by factors such as data structure (Courvoisier et al. (2011)), the degree of balance in categorical predictors (Ogundimu et al. (2016)) and the purpose for which the model is being developed (Harrell et al. (1996)). A resounding problem in the use of logistic regression for modelling  $PD$  is the rarity of the event of interest (default). As noted by King & Zeng (2001), the model underestimates the probability of rare events because they tend to be biased towards the majority class, which is the less important class. This has led to the proposal of skew models for predictions in class imbalanced data.

In a series of research papers, Raffaella Calabrese and co-authors proposed the use of generalized extreme value (GEV) regression for modelling  $PD$ . Calabrese & Osmetti (2011) and Calabrese & Osmetti (2013) evaluated the use of logistic regression and GEV regression in modelling rare events using data from bankruptcy in Italian SMEs (Small and medium-sized

enterprizes). The authors justified the use of the model on the skewness induced in the data as a consequence of class imbalance in the binary outcome. Indeed, when the probability of a given binary response approaches zero at a different rate than it approaches one, the symmetric link such as the logit or probit is inappropriate (Czado & Santner 1992, Chen 2004). Whilst the argument for skewness is generally true, the issue of imbalance in this framework can also be construed as a small sample problem. It is unclear whether models such as the GEV model should be preferred over models that can attenuate the effect of separation due to rarity of the event of interest. Separation occurs when one or more model covariates perfectly predict the outcome of interest. In logistic regression, the probability of separation depends on sample size, the number of dichotomous risk factors, the magnitude of the odds ratios associated with them and on the degree of balance in their distribution (Heinze & Schemper (2002)). Weiss (2004) identified two classes of problems associated with rare events and imbalanced data: *absolute rarity*, where the number of examples associated with the minority class is small in absolute sense. This is essentially a small sample problem and as common in logistic regression, maximum likelihood estimator (MLE) breaks down due to potential separation problem (Heinze & Schemper 2002, Zorn 2005, Rainey 2016). The second is *relative rarity*, where minority class (usually the class of interest) are rare relative to the other class. This constitutes a challenge for classification algorithms. It is unclear whether the benefit of the additional parameter estimated in the GEV model outweighs its cost (Taylor et al. (1996)).

Recent developments in the statistical literature have seen the emergence of newer methods for circumventing the estimation challenges posed by rare events when using logistic regression in the frequentist framework (Mansournia et al. (2018)). A method based on the penalization of likelihood function using the information matrix was proposed by Firth (1993). The original motivation for the method is the reduction of bias and mean square-error relative to the MLE. It has been adapted to mitigate the effect of separation and monotone likelihood in binary and survival models respectively (Heinze & Schemper 2002, Heinze & Schempe 2001). An intuitive explanation of complete separation and application of the Firth method is as follows. Consider the case of 10 observations with a single predictor  $X$  (positive values denoted as 1 and negative values denoted as 0) and a binary response  $Y$ , where  $y_i = 0$  whenever  $x_i$  is negative and 1 otherwise,  $i = 1, \dots, 10$  (see Table 1a). The implied two way table is given in Table 1b. Clearly, the odds ratio is infinite using maximum likelihood (ML) on this data. Firth's penalization however, is equivalent to ML estimation after augmentation of the cell counts by 0.5 (see Table 1c). This amended estimator has been described elsewhere (see (Agresti 2002, p. 70-71)). In this case, the odds ratio is finite and thus have merits in modelling  $PD$  where probability of separation is high. Figure 1 shows the plots of the fitted probabilities from standard and Firth logistic regression models using the data. The Firth method showed better predictions than the unrealistic heaviside function produced by the logistic regression model.

The concept and importance of events per variable (EPV) requirements for developing accurate prediction model has been underemphasized in the literature on credit scoring. EPV is the simple ratio of the number of the less frequent outcome and the number of estimated regression coefficients, and thus useful for quantifying the amount of information in the data relative to model complexity. The aim of this paper is therefore to evaluate the performance of statistical approaches for rare events and EPV requirements for accurate predictions in credit scoring. Since statistical models for rare events are rarely used in this framework, we compared Firth (1993) method (Firth), modification of Firth logistic regression called Firth’s logistic regression with added covariate (FLAC- proposed by Puhr et al. (2017)) and logistic regression penalized by log-F prior (LF22- by Greenland & Mansournia (2015)) with methods such as linear discriminant analysis (LDA), Ridge regression (Ridge), GEV model and logistic regression (logit). In particular, we “balanced” the data using ROSE (Random Over-Sampling Examples, by Menardi & Torelli (2014) and Lunardon et al. (2014)) and SMOTE (Synthetic Minority Over-Sampling Technique, by Chawla et al. (2002)) methods for various EPV values and develop prediction models using logistic regression. Since the main reason for modelling *PD* is to predict loan applicants who have the tendency to default, we focus on model evaluation criteria for predictions in the context of regression analysis rather than classification. This is to ensure that the predictive performance measures are not threshold dependent. We also corrected the performance measures for overfitting both in the simulation study and data analysis. The approach we adopted for model validation is based on the bootstrap internal validation method which has been recommended for the validation of prediction models in small sample (Smith et al. (2014)).

The rest of the paper is organized as follows. In Section 2, we describe the data used in the study. The models and methods are reviewed in Section 3. We also provided brief explanations of the model evaluation criteria. In Section 4, we described the simulation study and the two methods of data balancing considered in the article. The results from the simulation study are also analysed. Results from the real data example is presented in Section 5 and conclusions are given in Section 6. We present results of apparent performance of the models and sample codes in the Appendix.

## 2 Data set

We used the Taiwan credit card data set (Yeh & Lien (2009)) in this study. The data is used in the simulation study to evaluate sample size requirements for adequate predictions when the number of variables and prevalence (event rate) are taken into account.

Table 1: Example of complete separation and Firth correction in a  $2 \times 2$  contingency table

(a) Artificial data with separation										
$i$	1	2	3	4	5	6	7	8	9	10
$x_i$	-5	-4	-3	-2	-1	1	2	3	4	5
$y_i$	0	0	0	0	0	1	1	1	1	1

(b) Corresponding $2 \times 2$ contingency table					
		x			
		0	1		
y	0	5	0		
	1	0	5		

(c) Augmented table by Firth's penalization					
		x			
		0	1		
y	0	5.5	0.5		
	1	0.5	5.5		

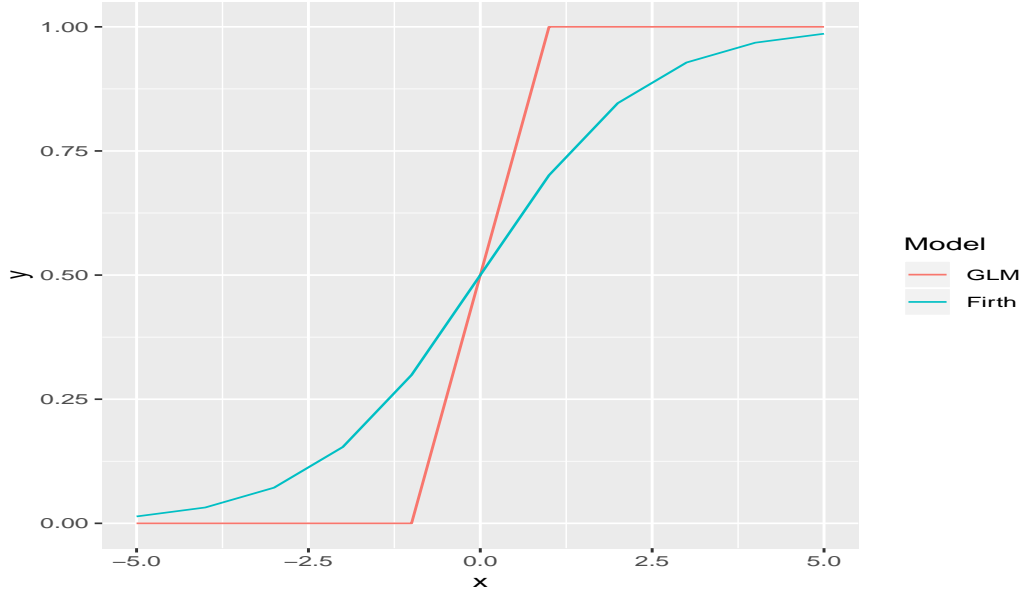


Figure 1: Predicted probabilities from classical logistic regression and logistic model using Firth method

## 2.1 Taiwan Credit Card data

The data set is from credit card clients from a bank in Taiwan, who is a cash and credit card issuer. The data is available within the University of California Irvine (UCI) machine learning repository. There are 30,000 observations in the data with 6636 (22.12%) defaulters. The outcome of interest is default payment (Yes = 1, No = 0). In the same vein as Yeh & Lien (2009), we used the following 23 variables in the models.

- (a) **Limit\_bal**: Given credit amount (NT dollar). This include both the individual applicant credit and his/her family (supplementary) credit
- (b) **Sex**: 1 = male; 2 = female

- (c) **Education:** 1 = graduate school; 2 = undergraduate; 3 = high school; 4 = others. We combined both groups 3 and 4 for this study
- (d) **Marital Status:** 1 = married; 2 = single; 3 = others. The “others” category is small so, we combined groups 2 and 3
- (e) **Age** (year)
- (f) **Pay\_0 - Pay\_6:** History of past payment. Past monthly payment records tracked from April to September 2005 as follows: **Pay\_0** = repayment status in September, 2005; **Pay\_2** = repayment status in August, 2005; ...; **Pay\_6** = repayment status in April, 2005. The measurement scale for the repayment status is -1 = pay duly; 1 = payment delay for one month; 2 = payment delay for two months; ...; 8 = payment delay for eight months; 9 = payment delay for nine months and above. We take this as ordinal variable.
- (g) **Bill\_Amt1 - Bill\_Amt6:** Amount of bill statement (NT dollar). **Bill\_Amt1** = amount of bill statement in September, 2005; **Bill\_Amt2** = amount of bill statement in August, 2005; ...; **Bill\_Amt6** = amount of bill statement in April, 2005
- (h) **Pay\_Amt1 - Pay\_Amt6:** Amount of previous payment (NT dollar). **Pay\_Amt1** = amount paid in September, 2005; **Pay\_Amt2** = amount paid in August, 2005; ...; **Pay\_Amt6** = amount paid in April, 2005.

The continuous variables in the data are log-transformed to cushion the effect of skewness.

## 3 Models and Predictive accuracy measures

### 3.1 Models

The main criteria for the choice of models considered in this section is to assess the performance of newer statistical methods for rare events in the framework of modelling *PD*. The newer methods evaluated are Firth, FLAC and LF22 models, and are evaluated alongside LDA, GEV model and Ridge regression.

We assume there are  $n$  loan applicants with two possible events- default or non-default which is governed by a Bernoulli random variable  $Y_i \in \{0, 1\}, i = 1, \dots, n$ . The event of interest is  $Y = 1$ , the positive event of defaults, with associated *PD*,  $\pi = P(Y = 1|X = x)$ . The  $p$ -dimensional applicants attributes,  $X$  (covariates) include personal details, past credit history and behavioral data. The statistical problem is to estimate  $\pi = P(Y = 1|X = x)$  and a commonly used method is the logistic regression.

### 3.1.1 Logistic Regression

Logistic regression assumes that the probability of default,  $\pi$  is a linear function of the observed covariates. That is,

$$\pi = P(Y = 1|X = x) = \exp(\beta'x) / (1 + \exp(\beta'x)),$$

where  $x = (1, x_1, \dots, x_p)$  is the design matrix and  $\beta = (\beta_0, \beta_1, \dots, \beta_p)$  is the  $(p+1)$  dimensional vector of regression parameters. The decision boundary is linear via the linear predictor,  $lp = \beta'x$ . Thus,  $lp > 0$  (equivalently  $\{x : \hat{\pi} > 0.5\}$ , where  $\hat{\pi}$  is the fitted probability) is classified as 1 and zero otherwise. In addition to its instability in modelling rare event data and well separated classes, it does not work well with non-linear effects of the covariates. The log-likelihood function for  $n$  subjects, which is not optimized for predictions, is given by

$$l(\beta) = \sum_{i=1}^n \left[ y_i (\beta'x_i) - \log (1 + \exp(\beta'x_i)) \right]. \quad (1)$$

We evaluated the performance of logistic regression on the probability scale as a model for *PD* rather than as a classifier.

### 3.1.2 Firth (1993) Method

Firth's penalized log-likelihood function for logistic regression can be written as

$$l(\beta^{Firth}) = l(\beta) + 1/2 \log |I(\beta)|,$$

where  $l(\beta)$  is the log-likelihood function in equation (1) and  $|I(\beta)|$  is the determinant of the Fisher information matrix. Alternatively, parameter estimates can be obtained by solving the modified score equation:

$$\sum_{i=1}^n \left\{ y_i - \pi_i + h_i \left( \frac{1}{2} - \pi_i \right) \right\} x_{ir} = 0; \quad r = 0, \dots, p, \quad (2)$$

where  $h_i$  is the  $i$ -th diagonal elements of the hat matrix  $H = \mathbf{W}^{1/2} \mathbf{X} (\mathbf{X}' \mathbf{W} \mathbf{X})^{-1} \mathbf{X} \mathbf{W}^{1/2}$ ,  $\mathbf{W}$  is the diagonal matrix  $\text{diag}\{\pi_i(1 - \pi_i)\}$  and  $p$  is the dimension of the covariates. Consequently, the Fisher information matrix,  $I(\beta) = \mathbf{X}' \mathbf{W} \mathbf{X}$ . The estimator prevents bias in the MLEs and produce useful standard errors. This is because the penalizing factor contains information on



the curvature of the likelihood function and thus contains information on the variation of the coefficient estimates. The penalty term is asymptotically negligible in large data sets, and thus coefficient estimates from the Firth estimator coincides with the ML. A major disadvantage of using Firth estimator for prediction in rare events setting is that it introduces bias in predicted probabilities towards  $\pi = 0.5$  (Puhr et al. (2017)). This is because the determinant of the Fisher information matrix is maximized for  $\pi = 0.5$  and thus push the predicted probabilities towards 0.5 compared with the MLE.

### 3.1.3 Firth's Logistic regression with Added Covariate (FLAC)

Puhr et al. (2017) proposed the FLAC approach to overcome the bias problem in average predicted probabilities of the Firth estimator. The method involves the following steps:

1. Apply Firth's logistic regression and calculate the diagonal elements  $h_i$  of the hat matrix.
2. Construct an augmented data set by stacking:
  - (i) the original observations weighted by 1,
  - (ii) the original observations weighted by  $h_i/2$  and
  - (iii) the original observations weighted by  $h_i/2$  but with reversed values of the binary outcome variable ( $y_i$  replaced by  $1 - y_i$ ).
3. Define an indicator variable  $g$  on this augmented data set, where for (i)  $g = 0$  and for (ii) and (iii)  $g = 1$ .
4. The FLAC estimates are then obtained by ML estimation on the augmented data set adding  $g$  as covariate.

Following from equation (2), the FLAC method has a modified score equation given as

$$\underbrace{\sum_{i=1}^n (y_i - \pi_i) x_{ir}}_{\text{Original data}} + \underbrace{\sum_{i=1}^n \frac{h_i}{2} (y_i - \pi_i) x_{ir}}_{\text{Original data, weighted by } h_i/2} + \underbrace{\sum_{i=1}^n \frac{h_i}{2} (1 - y_i - \pi_i) x_{ir}}_{\text{Data with reversed outcome}} = 0.$$

$g = 0$ 
 $g = 1$ 
(indicator variable)

Pseudo data

The FLAC method, like the Firth method, circumvents the problem of separation in low EPV settings.

### 3.1.4 log-F Prior Penalty

The Firth penalty is data dependent since it is proportional to  $\exp(1/2 \ln |I(\beta)|)$  and  $I(\beta)$  is composed of the design matrix of the observed covariates. Consequently, the covariates can induce correlations in the penalty term as well as in the coefficient estimates. These artifactual prior correlations lead to a serious practical defect of the Firth penalty. In order to circumvent this problem, Greenland & Mansournia (2015) proposed a class of penalty functions which is not data dependent. The method is developed in the Bayesian framework but can be easily implemented in any logistic regression package by translating each desired coefficient penalty into a pseudo record data. For example, let  $\beta_1$  be an element of  $\beta$ , with  $x_1$  as the corresponding element of  $x$ . Because a log-F( $m, m$ ) density is proportional to  $e^{m\beta_1/2}/(1 + e^{\beta_1})^m$ , penalization of  $\beta$  by a log-F( $m, m$ ) prior can be performed by adding a data record with  $m/2$  successes on  $m$  trials. In general, the prior degrees of freedom  $m$  in a log-F prior is exactly the number of observations added by the prior. Penalization by log-F( $m, m$ ) priors is in general equivalent to multiplying the likelihood function corresponding to equation (1) by  $e^{m\beta/2}/(1 + e^\beta)^m$ . The log-likelihood function is therefore

$$l(\beta^{LF22}) = l(\beta) + m\beta/2 - m \log(1 + e^\beta).$$

When  $m = 0$ , the function reduces to the log-likelihood function in equation (1). Greenland et al. (2016) suggested the use of log-F prior as a default prior for the general sparse-data settings. We consider  $m = 2$  (denoted as LF22 method) for this study.

### 3.1.5 Ridge Regression

The ridge method minimizes the mean squared error of predictions by introducing some bias to the estimates of the regression coefficients. The log-likelihood function in equation (1) can be reconstructed as a constrained likelihood problem, where  $l(\beta)$  is maximized subject to  $\sum_{j=1}^p \beta_j^2 \leq t$ ;  $t \geq 0$ , where  $t$  is a scalar chosen by the investigator. Equivalently, the ridge penalized likelihood function can be written as

$$l(\beta^{Ridge}) = l(\beta) - \lambda \sum_{j=1}^p \beta_j^2, \quad (3)$$

where  $\lambda \geq 0$  has a one-to-one correspondence with  $t$ , and it is referred to as the regularization parameter,  $\beta^{Ridge}$  are the parameter estimates from the ridge regression. The larger the value of  $\lambda$ , the further the parameter estimates are shrunk towards zero. In particular, the standard logistic regression is recovered when  $\lambda = 0$  in (3). The ridge estimator is a convex optimization

problem and it is sometimes referred to as an  $L_2$ -type regularization procedure (Verweij & Van Houwelingen (1994)). Except for cases of complete separation, the ridge estimator will converge.

### 3.1.6 Linear Discriminant Analysis (LDA)

LDA, also known as Fisher's LDA (Fisher (1936)), is a widely used method aimed at finding linear combinations of observed attributes,  $X$  which best separate two or more classes of events. For credit scoring, LDA assumes that there is a prior probability,  $P(Y = 1) = \pi^*$ , of default and that the conditional distribution of  $P(X = x|Y = j) \sim N(\mu_j, \Sigma)$ ,  $j = \{0, 1\}$ , a multivariate normal with  $\mu_j$  and covariance matrix  $\Sigma$ . Using Baye's theorem,

$$P(Y = 1|X = x) = \frac{\pi^* \exp(-\frac{1}{2}d_1(x))}{\pi^* \exp(-\frac{1}{2}d_1(x)) + (1 - \pi^*) \exp(-\frac{1}{2}d_0(x))},$$

where  $d_j = (x - \mu_j)' \Sigma^{-1} (x - \mu_j)$  is the Mahalanobis distance from  $x$  to  $\mu_j$ . Since the decision boundary is linear, the log-odds can be computed as

$$\begin{aligned} \log \frac{P(Y = 1|X = x)}{P(Y = 0|X = x)} &= \log \frac{\pi^*}{1 - \pi^*} - \frac{1}{2}(\mu_1 + \mu_0)' \Sigma^{-1} (\mu_1 - \mu_0) + x' \Sigma^{-1} (\mu_1 - \mu_0) \\ &= \beta' x. \end{aligned}$$

The predicted probabilities using the linear predictor are available in all major statistical software.

### 3.1.7 Generalized Extreme Value (GEV) regression model

The GEV model has been used to estimate and predict extreme events in many applications such as environment, engineering, economics and finance. Calabrese & Osmetti (2013) proposed its use for modelling  $PD$ . The cumulative distribution function is given by

$$F(x) = \exp \left\{ - \left[ 1 + \xi \left( \frac{x - \mu}{\sigma} \right) \right]^{-1/\xi} \right\} \quad -\infty < \xi < \infty, \quad -\infty < \mu < \infty, \quad \sigma > 0,$$

defined on the support  $S = \{x : 1 + \xi((x - \mu)/\sigma) > 0\}$ . The parameter  $\xi$  is the shape parameter,  $\mu$  and  $\sigma$  are the location and scale parameters respectively. The probability of default is  $\pi(x_i) = \exp\{-[1 + \xi(\beta' x_i)]^{-1/\xi}\}$ . The corresponding linear predictor can be derived as

$$\frac{\{-\ln[\pi(x_i)]\}^{-\xi} - 1}{\xi} = \beta' x_i.$$

We fitted this model using the GJRM (Generalised Joint Regression Modelling) package in R statistical software (Marra & Radice (2017)).

### 3.2 Criteria for predictive performance

**Brier score (BS):** It is a measure of agreement between the observed binary outcome (i.e., default vs. non-default) and the predicted *PD* (Brier (1950)). We used brier score plus (*BS*<sup>+</sup> - brier score computed for only the positive outcome).

**Area under the receiver operating curve (AUROC):** The generalization of the AUROC is the c-index (Harrell et al. (1982)). It is a measure of model performance that separates subjects with the event of interest from subjects without the event (discrimination). It calculates the proportion of pairs in which the predicted event probability is higher for the subject with the event of interest than that of the subject without the event. A model with no discriminatory ability has value around 0.5 whereas a value close to 1 suggests excellent discrimination.

**Area under the Precision-Recall curve (AUPRC):** The Precision-Recall curve shows the relationship between precision ( $P(Y = 1|\hat{Y} = 1)$ ), where  $\hat{Y}_i$  are fitted values, and recall ( $P(\hat{Y} = 1|Y = 1)$ ) for every possible threshold values. It takes into account the prior probability of the outcome of interest. The AUPRC is therefore a summary statistic that reflects the ability of a classifier to identify the minority group. Unlike the AUROC, it values ranges from 0 to 1. Its value approaches zero as the prior probability of the outcome decreases. Davis & Goadrich (2006) recommended its use over AUROC in rare event and class imbalance data settings.

**Calibration slope (CS):** The slope is used to check the agreements between the observed and predicted probabilities. We regressed the binary outcome on the linear predictors obtained from the models using logistic regression (except for the GEV regression model where the regression was done using the GEV model). The resulting slope in this regression is the calibration slope. A slope of one suggests perfect calibration (Cox (1958)).

## 4 Simulation based on the Taiwan credit card data set

### 4.1 Simulation settings

We used the Taiwan credit card data as the basis for the simulation and varied the prevalence and EPV. Let  $Y_i$  (outcome) and  $x_i$  (covariates) be defined as in Section 3.1. The assumed regression model for the data (suppressing index,  $i$ ) is of the form  $\text{logit}(E(Y)) = \beta'x$ . We simulated the training data sets using the steps in Pavlou et al. (2016) as follows.

1. Fit a logistic regression model to the original data set to obtain  $\hat{\beta}' = (\hat{\beta}_0, \hat{\beta}_1)$  where  $\hat{\beta}_0$  is the estimate of the intercept term and  $\hat{\beta}_1$  is the estimate of the vector of regression coefficients for the covariates.
2. Choose the required prevalence ( $prev$ ) and replace  $\hat{\beta}_0$  by the value  $\hat{\beta}_0^*$  that makes the average fitted probability equal to  $prev$ . Define  $\beta^{*'} = (\hat{\beta}_0^*, \hat{\beta}_1)$ .
3. To create the data, choose the EPV and  $prev$ , and calculate sample size for each EPV given the number of covariates  $p$ . The sample size is given by  $n = \frac{EPV \times p}{prev}$ . Sample with replacement  $n$  values of the covariates in the true model from the original data and generate a new outcome  $Y_{sim} \sim \text{Bernoulli}(\text{logit}^{-1}(\beta^{*'}x))$ . The resulting data set of size  $n$  is  $(Y_{sim}, x)$  and the process is repeated to produce 500 training data sets (number of replication).

We considered prevalence of 5%, 10% and 20% (22.12% is the prevalence of the entire data set). The models are evaluated on  $EPV = \{2, 3, 5, 7, 10\}$ , with EPV of 10 recommended for model accuracy (Peduzzi et al. (1996)). Each of the models developed in the training samples are validated using the bootstrap validation method (Harrell et al. (1996)). The steps for the model validation are as follows.

- (a) Simulate the data set based on the required EPV. Fit the models using the methods in section 3.1 and compute *Apparent* predictive performance based on the performance measure of interest, say  $AUROC_{app}$ .
- (b) Take  $B$  bootstrap samples from the simulated data set, where  $b = 1 \dots B$ . Fit the models and compute  $AUROC_{boot}^{(b)}$ . This is the bootstrap performance.
- (c) Test the performance of each of the  $B$  models on the original simulated data by computing  $AUROC_{orig}^{(b)}$ . This is the test performance.

(d) Optimism in model fit for each of the bootstrap sample is  $Opt^{(b)} = AUROC_{boot}^{(b)} - AUROC_{orig}^{(b)}$ .

The average optimism is

$$Opt = \frac{\sum_{b=1}^B Opt^{(b)}}{B}.$$

(e) Optimism corrected measures for the original model is  $AUROC_{correct} = AUROC_{app} - Opt$ .

We take  $B = 150$  for this study.

## 4.2 SMOTE and ROSE techniques for data balancing

In addition to the models examined in Section 3.1, we evaluated the use of SMOTE and ROSE methods for data balancing.

**SMOTE:** The technique generates randomly new examples or instances of the minority class from the nearest neighbours of line joining the minority class sample to increase the number of instances. These instances are created based on the features of the original data set so that they are similar to the original instances of the minority class (Chawla (2005)).

The SMOTE algorithm can be constructed as follows.

For each minority class instance  $\mathbf{x}$ :

1. Compute its nearest neighbours, say  $k = 5$  neighbours.
2. Randomly choose one of the neighbours, say  $\mathbf{x}^*$ .
3. Create a synthetic new minority sample,  $\mathbf{x}_{new}$  using  $\mathbf{x}'s$  feature vector and the feature vector's difference of  $\mathbf{x}^*$  and  $\mathbf{x}$  multiplied by a random number from the uniform distribution.

That is,

$$\mathbf{x}_{new} = \mathbf{x} + u \cdot (\mathbf{x}^* - \mathbf{x}),$$

where  $u \sim U(0, 1)$ . We kept the proportion  $r = |m|/|M|$  to 0.75, where  $r$  is the ratio of the number of examples in the minority class ( $m$ ) to the number in the majority class ( $M$ ).

**ROSE:** The method is based on the generation of new artificial data according to a smoothed bootstrap approach. The method is as follows.

Let  $P(\mathbf{x}) = f(\mathbf{x})$  be the probability density function on  $X$ . Let  $n_j < n$  be the size of  $Y_j$ ,  $j = 0, 1$ . A new sample is generated using the following three steps:

1. select  $y = Y_j$ ,  $j \in \{0, 1\}$ , with probability  $1/2$ .
2. select  $(\mathbf{x}_i, y_i)$  in the sample such that  $y_i = y$  with probability  $p_i = 1/n_j$ .
3. sample the vector of covariates  $\mathbf{x}$  from the kernel probability distribution  $K_{\mathbf{H}_j}(\cdot, \mathbf{x}_i)$  centered on  $\mathbf{x}_i$  and depending on the matrix of smoothing parameters  $\mathbf{H}_j$ .

That is, an observation belonging to one of the two classes is drawn from the training set with the same probability. A new sample is then generated in its neighborhood of width governed by  $\mathbf{H}_j$ . Further details on how to select the smoothing matrix  $\mathbf{H}_j$  can be found in Menardi & Torelli (2014) and Lunardon et al. (2014).

We used similar bootstrap steps in section 4.1 to correct for overfitting in the models. Here, the training data sets are first “balanced” using either SMOTE or ROSE techniques. The balanced data is then used in the bootstrap steps to develop models for *PD* using logistic regression. The original imbalanced data (test data) is used to test predictive accuracy of the developed models in the bootstrap samples.

## Simulation results

Figures 2-4 shows the predictive performance of the methods for different values of prevalence. When the prevalence is 5% (Figure 2), ROSE data balancing method outperforms the other methods on discrimination as shown by AUROC and AUPRC. The SMOTE method, another data balancing technique, shows the second best discriminatory ability on AUROC but performs poorly on AUPRC. Of the three Firth-type penalization methods, the LF22 is superior to Firth and FLAC methods on AUROC. Although GEV model performs well on AUROC, its estimates are not generally stable at  $EPV=2$ , resulting in AUROC estimates for  $EPV=2$  being greater than  $EPV = 3$ . The FLAC method is practically indistinguishable from the logit. However, both methods show better discrimination than the Firth method at  $EPV \leq 5$ . This is in line with the submission in Pühr et al. (2017), where the authors opined that Firth method introduces bias in predicted probabilities. Ridge on the other hand does not perform well at  $EPV=2$  when AUROC is used to evaluate discrimination. However, it exhibits gradual improvement until it surpasses the other methods (except ROSE and SMOTE) at  $EPV \geq 7$ . Again, Ridge performs well on AUPRC, where it is outperformed only by ROSE.

In terms of calibration, the Ridge is the best performing method as shown by the calibration slope (value of 1 indicates perfect calibration). The slope is better calibrated for FLAC than Firth and LF22 models. The GEV model and logit are indistinguishable on this performance measure. However, LDA is poorly calibrated. This may be due, in part, to the use of logistic model for the computation of the calibration slope as described in Section 3.2. Figure 2 (bottom

left) shows the  $BS^+$  computed on the defaulters. Overall, ROSE has the least error followed by SMOTE. Among the Firth-type method, Firth method is the best. This is not surprising as the method is generally known to have low mean square error. Although Ridge outperforms Firth when the standard Brier score is used (result not shown), its performance is the worst on  $BS^+$ .

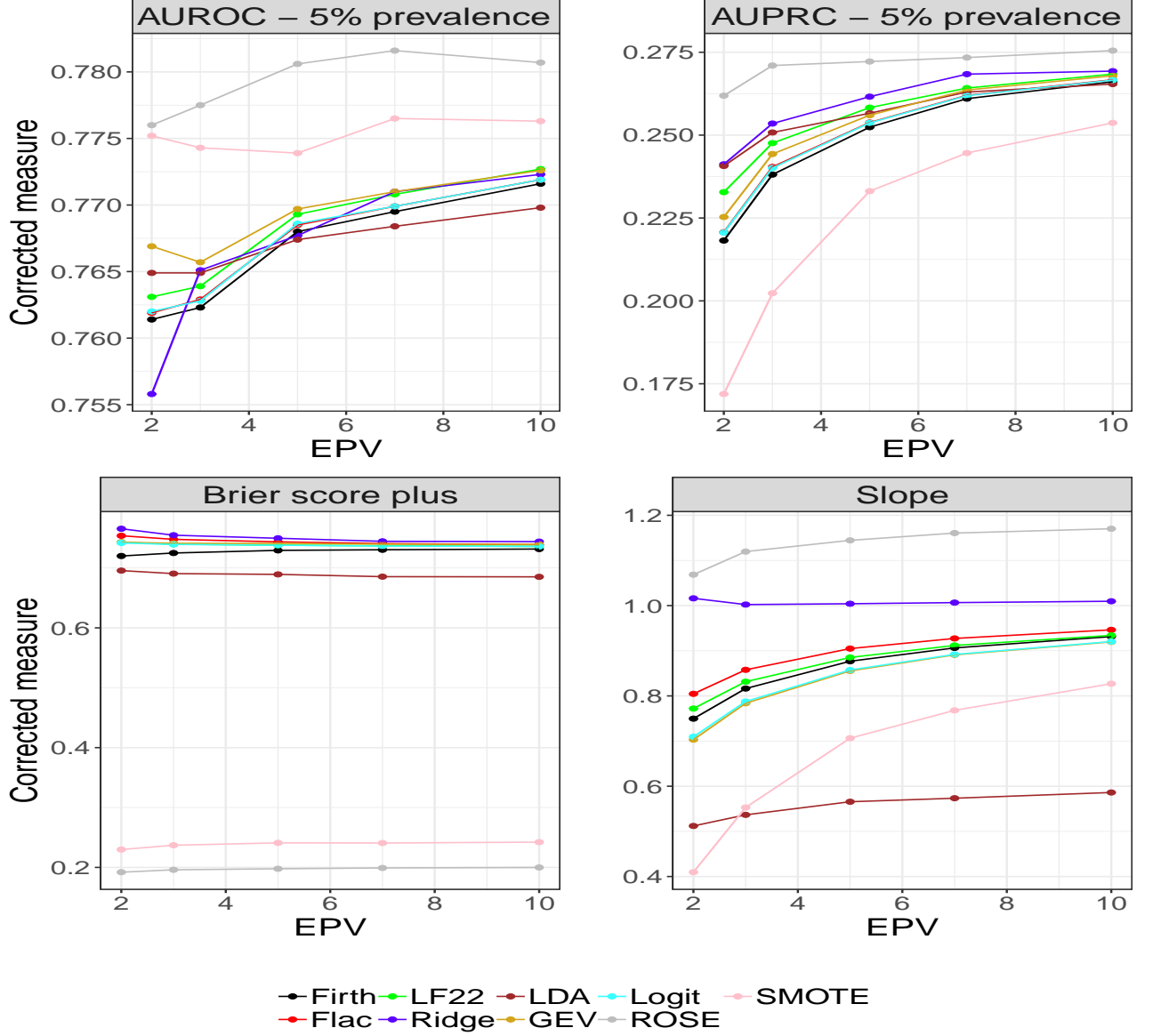


Figure 2: Optimism corrected predictive accuracy measures for prevalence of 5%

Some of the methods compared improved as prevalence of the outcome variable increases. from 5% to 10% (see Figure 3). Again, both ROSE and SMOTE perform well on AUROC, but the SMOTE technique is superior. Similar to the results in Figure 2, Ridge becomes increasingly better from  $EPV = 2$  and outperforms other methods (except ROSE and SMOTE) at  $EPV > 5$  when AUROC is the performance measure of interest. The more stable AUPRC



ranked ROSE and Ridge as the best among the methods. The performance of SMOTE improved from prevalence of 5% to 10%. The performance of the methods on calibration slope and  $BS^+$  follow the same pattern as shown in Figure 2 for the prevalence of 5%.

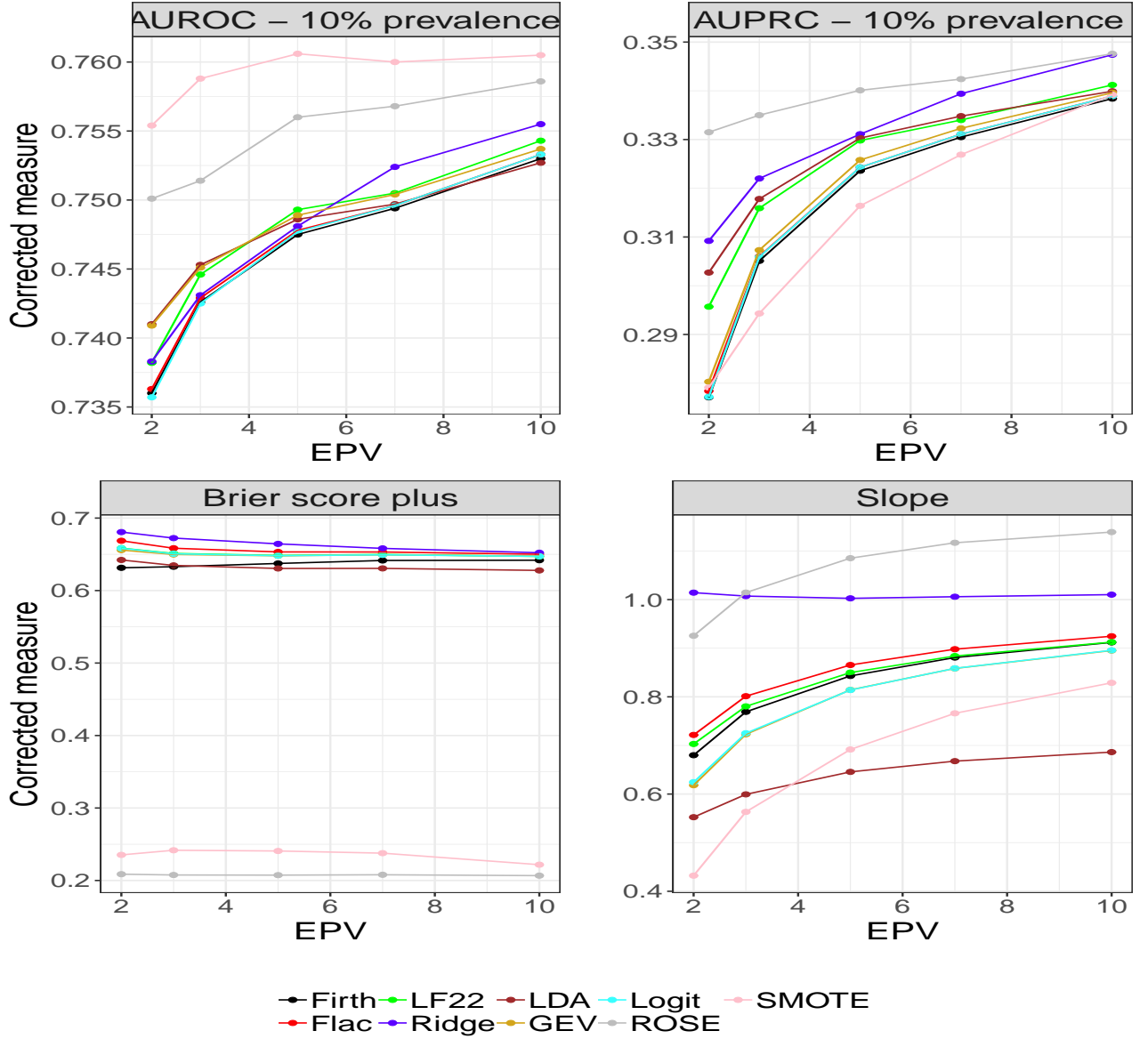


Figure 3: Optimism corrected predictive accuracy measures for prevalence of 10%

The results of model performance at prevalence of 20% are shown in Figure 4. SMOTE maintained a strong discriminatory ability on AUROC but ROSE deteriorated. Its performance on AUROC is consistent across the three event rates. On the other hand, ROSE and Ridge perform consistently well across the three levels of prevalence and EPV values considered for AUPRC (Figure 5). The LF22 model performs consistently better than the Firth, FLAC, GEV model and logit on AUROC and AUPRC. Again, the performance of the methods on calibration slope and  $BS^+$  follow the same pattern as seen in Figures 2 and 3. While the slope

for Ridge get closer to 1 as EPV approaches 6, it approaches 1 as EPV increases for SMOTE.

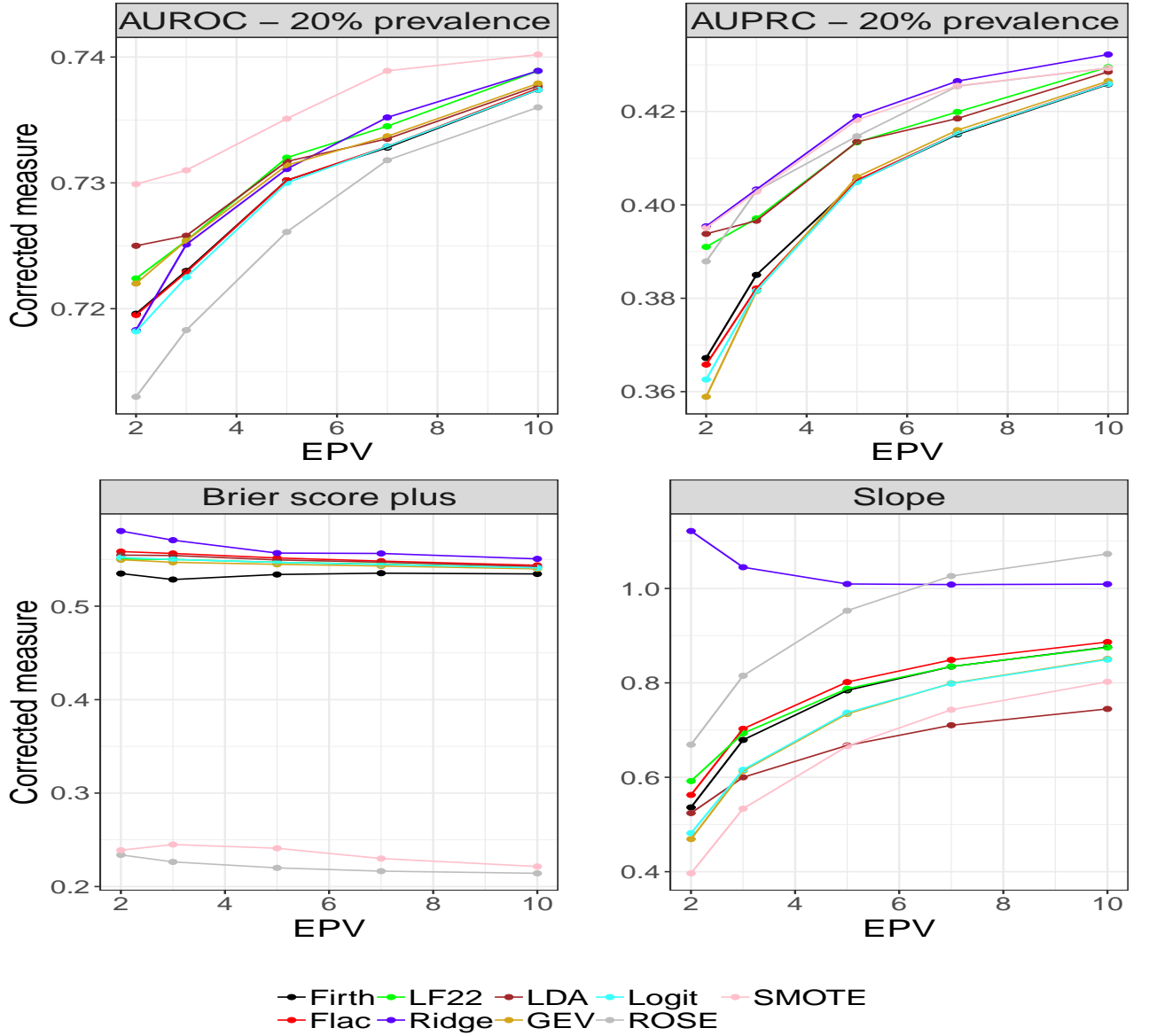


Figure 4: Optimism corrected predictive accuracy measures for prevalence of 20%

Figures 6- 8 (Appendix A) shows the results of apparent performance measures from the simulation study. All the Figures show high degree of overfitting especially at low EPV. In particular, Figures 6- 8 (top, left) shows that Ridge does not perform well when the model is not adjusted for optimism. In principle, this model is the least susceptible to overfitting. Also, there is severe overfitting in models developed with ROSE and SMOTE on AUPRC across the event rates. This corroborates the importance of internal validation of predictive models.

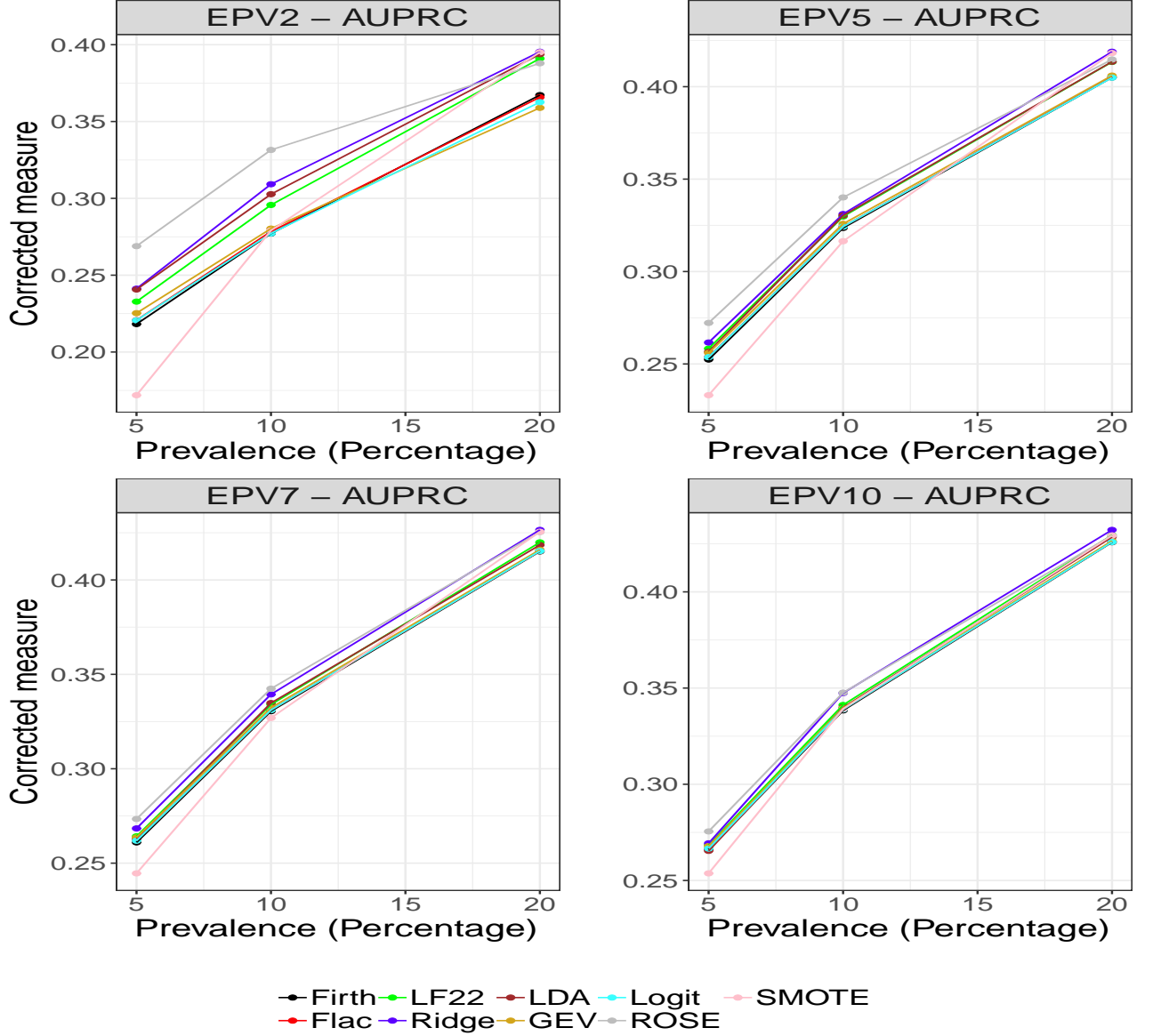


Figure 5: Comparison of predictive performance on AUPRC across prevalence

## 5 Data Analysis

We used the Taiwan credit card data described in section 2 to evaluate the performance of our models. In the data, the higher the amount of credit given, the higher the probability of default. In particular, all applicants older than 50 years of age borrowed 620,000 Taiwanese dollars or more, and they are defaulters. Age does not affect the chance of paying back amount borrowed that is less than 500,000 dollars.

The results from fitting the models are summarized in Table 2. Logistic regression with data balancing technique using SMOTE slightly outperforms the other methods on three out of the

four measures of predictive accuracy (AUROC,  $BS^+$  and Calibration slope). The performance of Firth, FLAC and the LF22 methods (Firth-type penalization) are essentially the same. This is expected since the sample size is now large ( $EPV = 289$ ). The GEV model outperforms the logit on AUROC and  $BS^+$ , which is in line with previous observation (Calabrese & Osmetti (2013)). It should be noted that the performance of SMOTE using AUROC is in concord with our observation from the simulation study. That is, the method is very good when AUROC is used for discrimination regardless of prevalence and corresponding EPV values. One noticeable result is the performance of SMOTE on calibration slope. Again, this follows from the simulation study, whereby AUROC value approaches 1 as EPV increases.

Table 2: Model performance in predicting default probability in Taiwan credit card data

	AUROC	AUPRC	$BS^+$	Slope
logit	0.7459	0.5036	0.4676	0.9912
Firth	0.7459	0.5036	0.4674	0.9923
Flac	0.7459	0.5036	0.4677	0.9926
LF22	0.7459	<b>0.5037</b>	0.4676	0.9914
Ridge	0.7474	0.5019	0.4727	1.0498
LDA	0.7447	0.5016	0.4726	0.8975
GEV	0.7480	0.4997	0.4756	0.9914
logit-rose	0.7478	0.4996	0.2117	1.1910
logit-smote	<b>0.7482</b>	0.4988	<b>0.2108</b>	<b>0.9939</b>

## 6 Concluding remarks

This paper examined six modifications of the logistic regression (Firth, FLAC, LF22, Ridge, ROSE and SMOTE), linear discriminant analysis (LDA) and binary regression model using generalized extreme value distribution (GEV) in the estimation of probability of default ( $PD$ ). The simulation study is based on the modification of event rate in the Taiwan credit card data. We evaluated measures of model performance identified in the literature for the evaluation of predictive accuracy in class imbalanced data settings. Sample size was taken into account in the evaluation of the methods using events per variable (EPV). Since the design factors (number of predictors and event rate) are kept constant, both EPV and sample size have one-to-one correspondence and the same conclusion is expected.

The key result showed that SMOTE should be preferred when the aim is to obtain optimal discrimination using AUROC in small and large samples. SMOTE exhibited patterns of improved predictive accuracy as EPV increases on three of the measures of performance (AUROC,  $BS^+$  and Slope). In particular, the slope approaches 1 as EPV becomes large. This is further corroborated in the data analysis where EPV equals 289. For optimal performance on AUPRC, we recommend the use of ROSE and ridge regression. Of the statistical methods analyzed, the LF22 and FLAC methods are generally superior to Firth, logit and GEV models. In addition, the two models converge and will generally produce accurate predictions in the presence of sparse data structure (e.g. binary predictors with low prevalence), whereas models such as GEV and logistic regression are likely to fail in such setting. Although the computational time is higher for FLAC and LF22 models than the logit model, improved predictive accuracy in small sample cannot be traded for computational complexity.

The measure of predictive accuracy based on AUPRC appears to be a more realistic measure of discrimination than AUROC in rare event settings. As can be seen from Figure 5, the performance of all the methods increases on this measure from 5% prevalence to 20% as expected. Consider the ridge regression for example, the corrected AUPRC at  $EPV = 2$  for 5% prevalence is 0.2412. This value increases to 0.3092 for 10% prevalence and 0.3954 for 20% prevalence. On the other hand, and at  $EPV = 2$  the AUROC values are 0.7558, 0.7383 and 0.7183 for 5%, 10% and 20% prevalence respectively, indicating consistent decline across prevalence.

A possible criticism of the bootstrap method used for internal validation is the possibilities of model non-convergence within the bootstrap samples for models such as logistic regression and GEV models. As noted by Loughin (1998), separation has significant probability of occurring in resamples when the event of interest is rare. Whilst this argument may be valid in certain cases, the chance of not selecting any member of the minority group is just approximately

1/3. We accommodated the possibility of such divergence/singularity in the resample. We also emphasized the merits of model evaluation in simulation studies using optimism corrected measures (Ogundimu & Collins (2018)).

Although we showed the conditions for preference of SMOTE and LF22 methods on the data, the latter can be improved to cater for various modelling challenges that are often encountered while modelling *PD*. For example, the method can be combined with the ridge method (in a similar way as Shen & Gao (2008) combined Firth and Ridge methods) to optimize predictive accuracy of *PD*. In addition to optimized predictive accuracy, this method will alleviate the effect of multicollinearity- a common problem in credit scoring. We have combined both undersampling of the majority class and oversampling of the minority class to achieve a ratio of 0.75 for data balancing using SMOTE. This is not necessarily optimal as SMOTE can be used without undersampling. The performance of SMOTE can also be improved by developing sampling strategy such that the amount of oversampling and the nearest neighbours used for a particular data is selected in some optimal way. There are still open questions on variable selection and methods for dealing with incomplete data in credit scoring. SMOTE (and its variants) and LF22 methods have enormous potential in these settings.

## References

- Agresti, A. (2002), *Categorical data analysis*, second edn, John Wiley & Sons Ltd, New York.
- Altman, E. (1968), ‘Financial ratios, discriminant analysis and the prediction of corporate bankruptcy’, *J. Finance*. **23**(4), 589–609.
- Basel Committee on Banking Supervision (June, 2004), *International convergence of Capital Measurement and Capital Standards: A Revised Framework*.
- Berk, R. A. & Bleich, J. (2013), ‘Statistical procedures for forecasting criminal behavior: A comparative assessment’, *Criminol. Public Policy*. **12**(3), 513–544.
- Brier, G. W. (1950), ‘Verification of forecasts expressed in terms of probability’, *Mon. Weather Rev.* **78**, 1–3.
- Calabrese, R. & Osmetti, S. A. (2011), ‘Generalized extreme value regression for binary rare events data: an application to credit defaults’, *Discussion Paper*.
- Calabrese, R. & Osmetti, S. A. (2013), ‘Modelling small and medium enterprise loan defaults as rare events: the generalized extreme value regression model’, *J. Appl. Stat.* **40**(6), 1172–1188.
- Chawla, N. V. (2005), Data mining for imbalanced datasets: An overview, in O. Maimon & L. Rokach, eds, ‘Data mining and knowledge discovery handbook’, Springer, Boston, MA, pp. 853–867.
- Chawla, N. V., Bowyer, K. W., Hall, L. O. & Kegelmeyer, W. P. (2002), ‘SMOTE: Synthetic Minority OverSampling Technique’, *J. Artif. Intell. Res.* **16**, 321–357.
- Chen, M. (2004), Skewed link models for categorical response data, in M. G. Genton, ed., ‘Skew-Elliptical Distributions and Their Applications: A Journey Beyond Normality’, Chapman & Hall, CRC, Boca Raton, Florida, pp. 223–241.
- Courvoisier, D. S., Combescure, C., Agoritsas, T., Gayet-Ageron, A. & Perneger, T. V. (2011), ‘Performance of logistic regression modeling: beyond the number of events per variable, the role of data structure’, *J. Clin. Epidemiol* **64**, 993–1000.
- Cox, D. R. (1958), ‘Two further applications of a model for binary regression’, *Biometrika* **45**, 562–565.
- Czado, C. & Santner, T. J. (1992), ‘The effect of link misspecification on binary regression inference’, *J. Stat. Plan. Inference*. **33**(2), 213–231.

- Davis, J. & Goadrich, M. (2006), The Relationship Between Precision-Recall and ROC Curves, in ‘Proceedings of the 23rd International Conference on Machine Learning’, ICML ’06, ACM, New York, NY, USA, pp. 233–240.
- Durand, D. (1941), ‘Risk elements in consumer installment financing’, *New York: National Bureau of Economic Research* pp. 189–201.
- Firth, D. (1993), ‘Bias reduction of maximum likelihood estimates’, *Biometrika* **80**, 27–38.
- Fisher, R. (1936), ‘The use of multiple measurements in taxonomic problems’, *Ann. Eugen.* **7**(2), 179–188.
- Ghotra, B., McIntosh, S. & Hassan, A. E. (2015), ‘Revisiting the impact of classification techniques on the performance of defect prediction models’, In *37th ICSE-Volume 1. IEEE Press* pp. 789–800.
- Greenland, S. & Mansournia, M. A. (2015), ‘Penalization, bias reduction, and default priors in logistic and related categorical and survival regressions’, *Stat. Med.* **34**, 3133–3143.
- Greenland, S., Mansournia, M. A. & Altman, D. G. (2016), ‘Sparse data bias: a problem hiding in plain sight’, *BMJ.* **352**, i1981.
- Hand, D. J. & Henley, W. E. (1997), ‘Statistical classification methods in consumer credit scoring: A review’, *J. R. Stat. Soc. Series A.* **160**(3), 523–541.
- Harrell, F., Califf, R., Pryor, D., Lee, K. & Rosati, R. (1982), ‘Evaluating the yield of medical tests’, *JAMA* **247**, 2543–2546.
- Harrell, F. E., Lee, K. L. & Mark, D. B. (1996), ‘Tutorial in biostatistics, multivariable prognostic models: Issues in developing models, evaluating assumptions and adequacy, and measuring and reducing errors’, *Stat. Med.* **15**, 361–387.
- Heinze, G. & Schempe, M. (2001), ‘A solution to problem of monotone likelihood in Cox regression’, *Biometrics* **57**, 114–119.
- Heinze, G. & Schemper, M. (2002), ‘A solution to the problem of separation in logistic regression’, *Stat. Med.* **21**, 2409–2419.
- King, G. & Zeng, L. (2001), ‘Logistic regression in rare events data’, *Polit. Anal.* **9**, 137–163.
- Loughin, T. M. (1998), ‘On the bootstrap and monotone likelihood in the Cox proportional hazards regression model’, *Lifetime Data Anal.* **4**(4), 393–403.
- Lunardon, N., Menardi, G. & Torelli, N. (2014), ‘ROSE: a package for Binary Imbalanced Learning’, *R Journal* **6**(1), 79–89.



- Mansournia, M. A., Geroldinger, A., Greenland, S. & Heinze, G. (2018), ‘Separation in logistic regression: causes, consequences, and control’, *Am J Epidemiol.* **187**, 864–870.
- Marra, G. & Radice, R. (2017), ‘A joint regression modeling framework for analyzing bivariate binary data in R’, *Dependence Modeling* **5**(1), 268–294.
- Menardi, G. & Torelli, N. (2014), ‘Training and assessing classification rules with imbalanced data’, *Data Min. Knowl. Discov.* **28**(1), 92–122.
- Ogundimu, E. O., Altman, D. G. & Collins, G. S. (2016), ‘Adequate sample size for developing prediction models is not simply related to events per variable’, *J. Clin. Epidemiol.* **76**, 175–182.
- Ogundimu, E. O. & Collins, G. S. (2018), ‘Predictive performance of penalized beta regression model for continuous bounded outcomes’, *J. Appl. Stat.* **45**(6), 1030–1040.
- Pavlou, M., Ambler, G., Seaman, S., De Iorio, M. & Omar, R. Z. (2016), ‘Review and evaluation of penalised regression methods for risk prediction in low-dimensional data with few events’, *Stat Med.* **180**(7), 1159–1177.
- Peduzzi, P., Concato, J., Kemper, E., Holford, T. R. & Feinstein, A. (1996), ‘A simulation study on the number of events per variable in logistic regression analysis’, *J. Clin. Epidemiol.* **49**, 1373–1379.
- Puhr, R., Heinze, G., Nold, M., Lusa, L. & Geroldinger, A. (2017), ‘Firth’s logistic regression with rare events: accurate effect estimates and predictions?’, *Stat. Med.* **36**(14), 2302–2317.
- Rainey, C. (2016), ‘Dealing with separation in logistic regression models’, *Polit. Anal.* **24**(3), 339–355.
- Shen, J. & Gao, S. (2008), ‘A solution to separation and multicollinearity in multiple logistic regression’, *J. Data Sci.* **6**(4), 515–531.
- Smith, G. C., Seaman, S. R., Wood, A. M., Royston, P. & White, I. R. (2014), ‘Correcting for optimistic prediction in small data sets’, *Am. J. Epidemiol.* **180**(3), 318–324.
- Taylor, J. M. G., Siqueira, A. L. & Weiss, R. E. (1996), ‘The cost of adding parameters to a model’, *J. R. Statist. Soc. B.* **58**(3), 593–607.
- Thomas, L. C., Edelman, D. B. & Crook, J. N. (2002), *Credit scoring and its applications*, Society for Industrial and Applied Mathematics, Philadelphia.
- Verweij, P. J. M. & Van Houwelingen, H. C. (1994), ‘Penalized likelihood in Cox regression’, *Stat Med.* **13**, 2427–2436.

- Weiss, G. M. (2004), ‘Mining with rarity: a unifying framework’, *SIGKDD Explorations Newsletter* **6**(1), 7–19.
- Yeh, I. & Lien, C. (2009), ‘The comparisons of data mining techniques for the predictive accuracy of probability of default of credit card clients’, *Expert Syst Appl.* **36**, 2473–2480.
- Zorn, C. (2005), ‘A solution to separation in binary response models’, *Polit. Anal.* **13**(2), 157–170.

# Appendix

## A Apparent Predictive Accuracy Measures

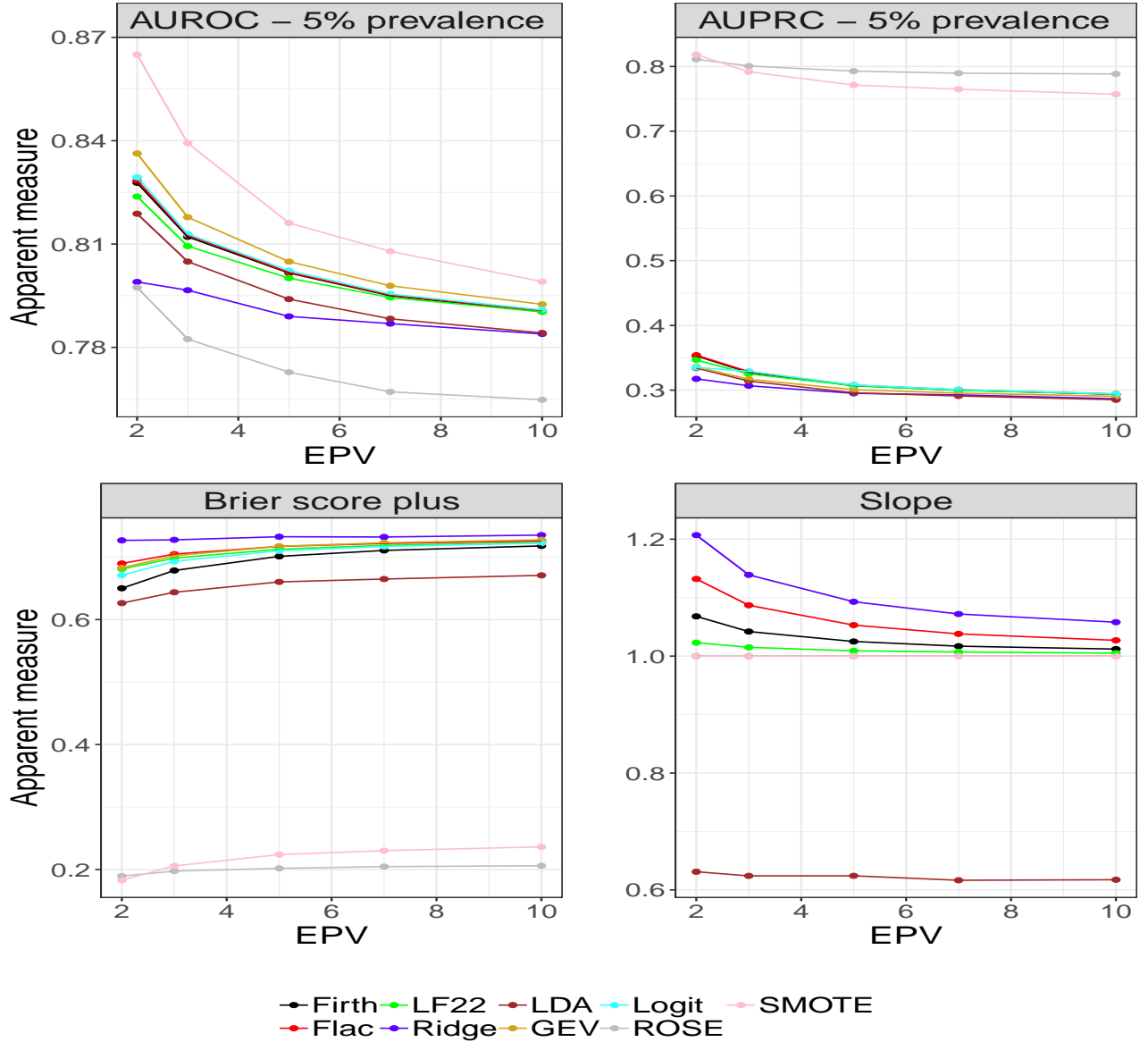


Figure 6: Apparent predictive accuracy measures for prevalence of 5%

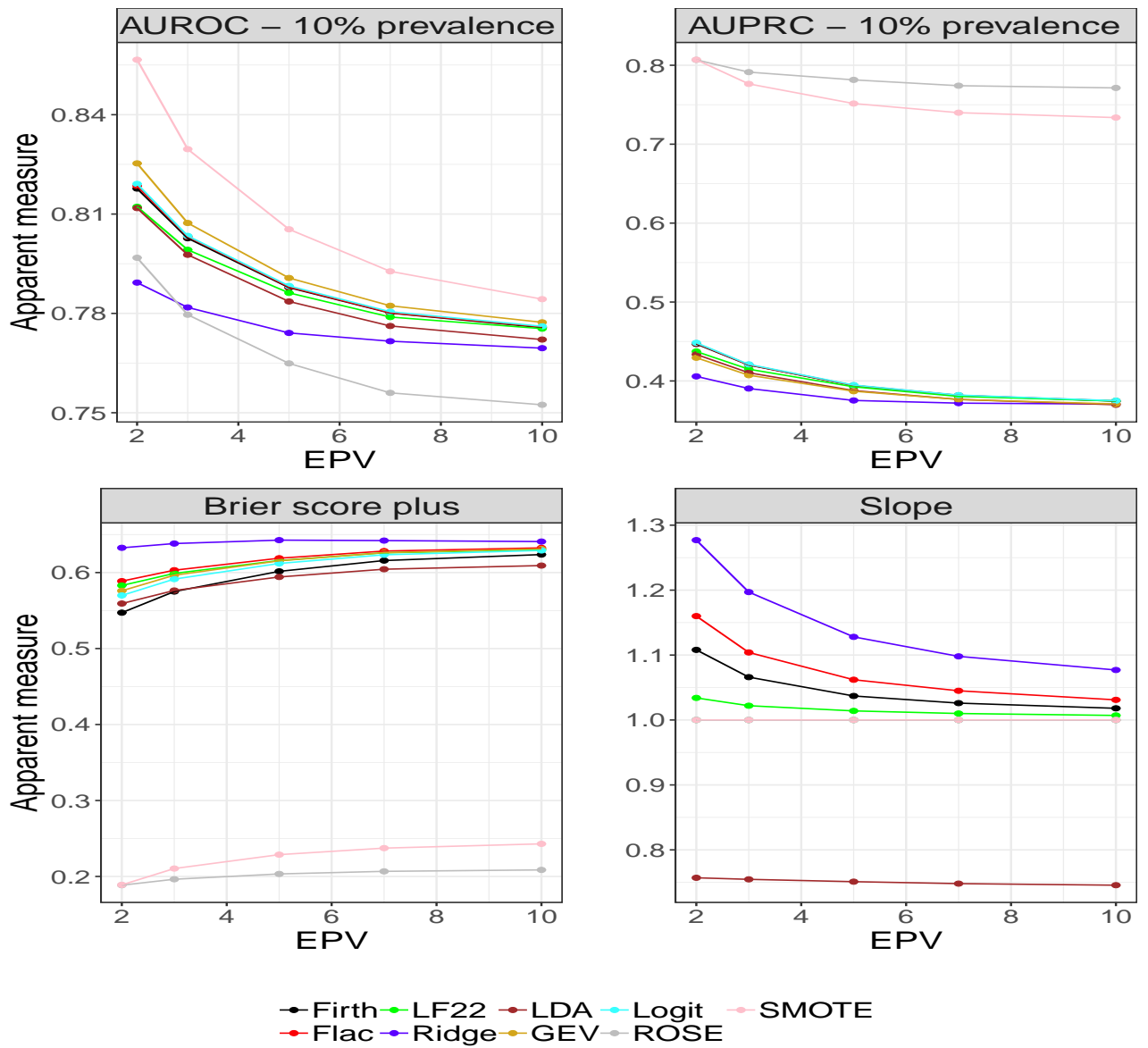


Figure 7: Apparent predictive accuracy measures for prevalence of 10%

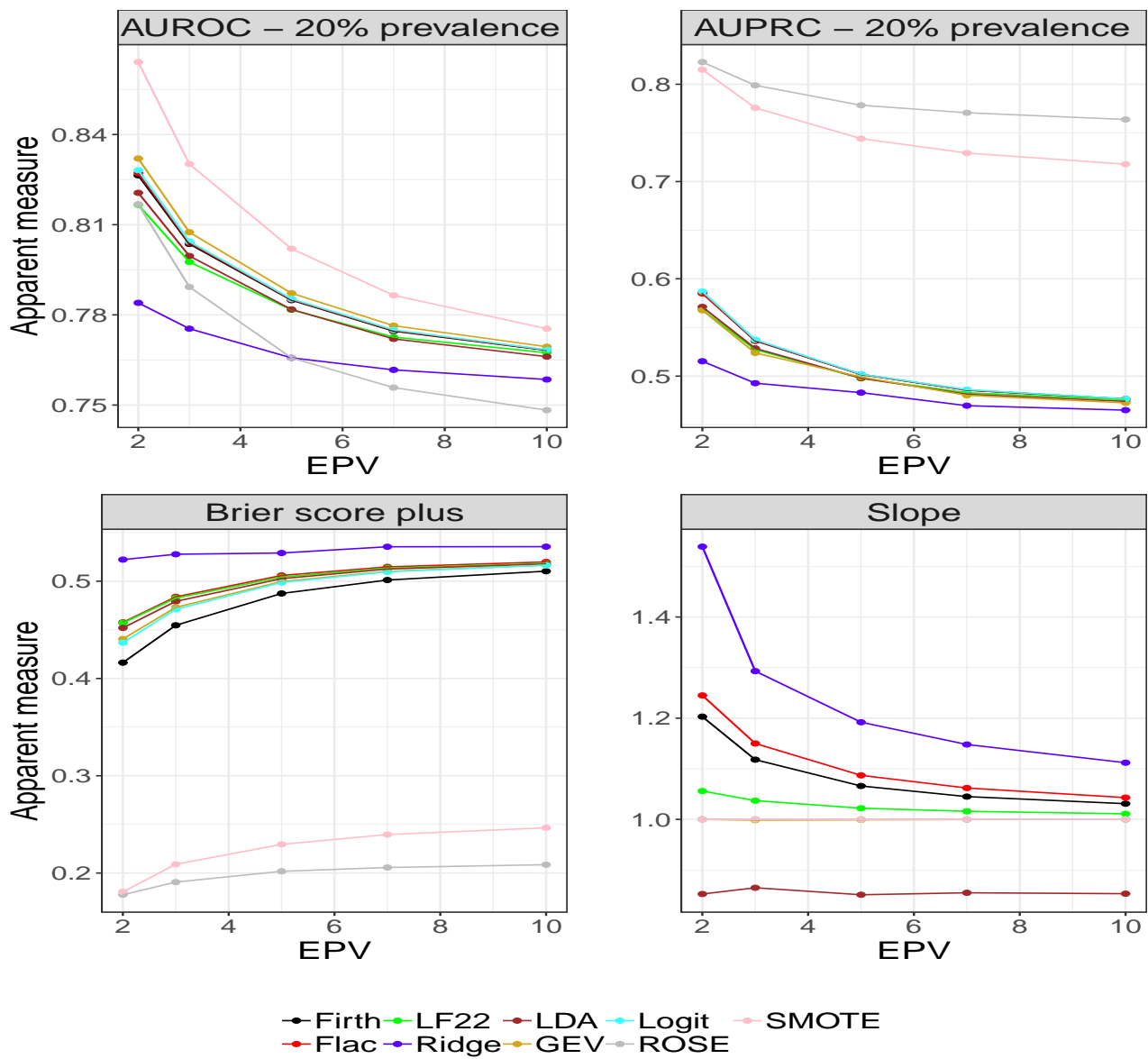


Figure 8: Apparent predictive accuracy measures for prevalence of 20%

## B Sample R code for Internal validation

### Bootstrap validation code for logistic regression

```
logitboot <- function(formula, data, B, seed){
  if (match("MASS",.packages(),0)==0) require(MASS)
  if (match("PRROC",.packages(),0)==0) require(PRROC)
  if (match("ROCR",.packages(),0)==0) require(ROCR)
  set.seed(seed)
  mf <- model.frame(formula, data)
  y <- model.response(mf, "numeric")
  X <- model.matrix(formula, data = data)
  int <- slope <- auc <- pauc1 <- brier <- brierp <- cal <- c()
  intest <- slopetest <- auctest <- pauctest1 <- briertest <- brierpt <- calt <- c()

  # Looping to generate B bootstrap data
  bootdata <- mydat <- list()
  for(i in 1:B){
    iboot <- sample(1:nrow(data), replace=TRUE)
    bootdata[[i]] <- data[iboot,]
  }
  for(i in 1:B){
    options(warn=2)
    dattest <- X
    res <- try(glm(formula, data=bootdata[[i]], family=binomial(link = "logit")))
    if (any(class(res=="try-error"))){
      int[i] <- slope[i] <- auc[i] <- pauc1[i] <- brier[i] <- brierp[i] <- cal[i] <- NA
      intest[i] <- slopetest[i] <- auctest[i] <- pauctest1[i] <- briertest[i] <- NA
      brierpt[i] <- calt[i] <- NA
    } else{

      p <- res$fitted.values
      lp <- res$linear.predictors
      mf2 <- model.frame(formula, bootdata[[i]])
      yboot <- model.response(mf2, "numeric")

      lptest <- dattest%*%coef(res)
      prtest <- plogis(lptest)
      fg <- p[yboot == 1]
      bg <- p[yboot == 0]
```

```

roc <- roc.curve(scores.class0 = fg, scores.class1 = bg)
pr <- pr.curve(scores.class0 = fg, scores.class1 = bg)
ab <- glm(yboot~lp,family = binomial(logit))# usual calibration
pred <- prediction(p, yboot)

int[i] <- ab$coef[1]
slope[i] <- ab$coef[2]
auc[i] <- roc$auc
pauc1[i] <- pr$auc.integral
brier[i] <- mean((p-yboot)^2)
brierp[i] <- mean((p[yboot == 1]-yboot[yboot==1])^2)
cal[i] <- mean(unlist(performance(pred, "cal",window.size=100)@y.values))#sample size >100

# doing the test back in the original data
fgt <- prtest[y == 1]
bgt <- prtest[y == 0]

roct <- roc.curve(scores.class0 = fgt, scores.class1 = bgt)
prt <- pr.curve(scores.class0 = fgt, scores.class1 = bgt)

abt <- glm(y~lpptest,family = binomial(logit))
predt <- prediction(prtest, y)

intest[i] <- abt$coef[1]
slopetest[i] <- abt$coef[2]
auctest[i] <- roct$auc
pauctest1[i] <- prt$auc.integral
briertest[i] <- mean((prtest-y)^2)
brierpt[i] <- mean((prtest[y == 1]-y[y==1])^2)
calt[i] <- mean(unlist(performance(predt, "cal",window.size=100)@y.values))
}}

aaa <- auc
ck <- sum(is.na(aaa))
int <- mean(int, na.rm=T)
slope <- mean(slope,na.rm=T)
auc <- mean(auc,na.rm=T)
pauc1 <- mean(pauc1,na.rm=T)
brier <- mean(brier,na.rm=T)

```

```

brierp <- mean(brierp, na.rm=T)
cal <- mean(cal, na.rm =T)

intt <- mean(intest, na.rm=T)
slopet <- mean(slopetest, na.rm=T)
auct <- mean(auctest,na.rm=T)
pauct1 <- mean(pauctest1,na.rm=T)
briert <- mean(briertest,na.rm=T)
brierpt <- mean(brierpt, na.rm=T)
calt <- mean(calt, na.rm =T)

# Index measures from the original data set
options(warn=2)
orig <- try(glm(formula, data=data, family=binomial(link = "logit")))
if (any(class(orig)=="try-error")){
  Oint <- Oslope <- Oauc <- Opauc1 <- Obrier <- Obrierp <- Ocal <-999
} else{

  lporig <- orig$linear.predictors
  prorig <- orig$fitted.values
  fgo <- prorig[y == 1]
  bgo <- prorig[y == 0]

  oroc <- roc.curve(scores.class0 = fgo, scores.class1 = bgo)
  opr <- pr.curve(scores.class0 = fgo, scores.class1 = bgo)

  oab <- glm(y~lporig,family = binomial(logit))
  opred <- prediction(prorig, y)

  Oint <- oab$coef[1]
  Oslope <- oab$coef[2]
  Oauc <- oroc$auc
  Opauc1 <- opr$auc.integral
  Obrier <- mean((prorig-y)^2)
  Obrierp <- mean((prorig[y == 1]-y[y==1])^2)
  Ocal <- mean(unlist(performance(opred, "cal",window.size=100)$y.values))
}

index.orig <- c(Oint,Oslope,Oauc,Opauc1,Obrier,Obrierp,Ocal)
training <- c(int,slope,auc,pauc1,brier, brierp,cal )

```



```

test <- c(intt,slopet,auct,pauct1,briert,brierpt,calt)
data.a <- data.frame(index.orig,training,test)
data.a$optimism <- training-test
data.a$index.corrected <- index.orig-data.a$optimism
data.a$n <- rep(B-ck, length(training))
data.a <- round(data.a,digits=4)
xx <- c("int","slope","auc","pauc1","brier", "brierp","cal")
rownames(data.a) <- xx
outt <- list(nonconvergence=ck,resu=data.a)
return(outt)
}

```

This function can be easily extended to other model families as was done in this article. It can also be extended to include other desired measure of predictive accuracy. It gives exactly the same results as for the “validate.lrm” function in the rms package.

```

gendat <- function(n,seed){#data generation
set.seed(seed)
beta = c(0.5, 0.5, 1,1,1,0)
alpha<- -1.8
m <- length(beta)
X <- matrix(runif(n*m), nrow=n, ncol=m)
Xb <- alpha + X%*%beta
pr <- 1/(1+exp(-Xb))
y<- rbinom(n,1,pr)
df <- data.frame(y,X)
return(df)
}

dat <- gendat(1000,1)
formula <- y~X1+X2+X3+X4+X5+X6

res <- logitboot(formula,data=dat,B=10,seed=1)

library(rms)# bootstrap validation in rms package
f <- lrm(y~X1+X2+X3+X4+X5+X6, x=TRUE, y=TRUE, data=dat)
p <- predict(f,type="fitted",data =dat)
set.seed(1)
res.lrm <- validate(f, B=10)

```

```

res
      index.orig training  test optimism index.corrected  n
int      0.0000   0.0000 0.0235  -0.0235           0.0235 10
slope    1.0000   1.0000 0.8715   0.1285           0.8715 10
auc       0.6467   0.6645 0.6433   0.0213           0.6254 10
pauc1     0.6493   0.6618 0.6455   0.0163           0.6330 10
brier     0.2327   0.2283 0.2345  -0.0062           0.2389 10
brierp    0.2287   0.2283 0.2361  -0.0078           0.2365 10
cal       0.0373   0.0491 0.0422   0.0069           0.0304 10

```

```

res.lrm
      index.orig training  test optimism index.corrected  n
Dxy      0.2933   0.3291 0.2865   0.0426           0.2507 10
R2        0.0924   0.1151 0.0876   0.0275           0.0649 10
Intercept 0.0000   0.0000 0.0235  -0.0235           0.0235 10
Slope     1.0000   1.0000 0.8715   0.1285           0.8715 10
Emax      0.0000   0.0000 0.0345   0.0345           0.0345 10
D         0.0708   0.0894 0.0670   0.0224           0.0484 10
U        -0.0020  -0.0020 0.0019  -0.0039           0.0019 10
Q         0.0728   0.0914 0.0651   0.0263           0.0465 10
B         0.2327   0.2283 0.2345  -0.0062           0.2389 10
g         0.6392   0.7247 0.6203   0.1044           0.5347 10
gp        0.1506   0.1681 0.1467   0.0214           0.1292 10

```