Jeffreys-prior penalty, finiteness and shrinkage in binomial-response generalized linear models

Ioannis Kosmidis
ioannis.kosmidis@warwick.ac.uk
and
David Firth
d.firth@warwick.ac.uk

Department of Statistics, University of Warwick
Coventry CV4 7AL, UK
and
The Alan Turing Institute
British Library, London NW1 2DB, UK

August 15, 2019

Abstract

This paper studies the finiteness properties of the reduced-bias estimator for logistic regression that results from penalization of the likelihood by Jeffreys’ invariant prior; and it provides geometric insights on the shrinkage towards equiprobability that the penalty induces. Some implications of finiteness and shrinkage for inference are discussed, particularly when inference is based on Wald-type procedures. We show how the finiteness and shrinkage properties continue to hold for link functions other than the logistic, and also when the Jeffreys-prior penalty is raised to a positive power. In that more general context, we show how maximum penalized likelihood estimates can be obtained by using repeated maximum likelihood fits on iteratively adjusted binomial responses and totals, and we provide a general algorithm for maximum penalized likelihood estimation. These theoretical results and methods underpin the increasingly widespread use of reduced-bias and similarly penalized logistic regression models in many applied fields. We illustrate the results here through one specific example, a Bradley-Terry model to estimate the relative strengths of NBA basketball teams.

Keywords: logit; probit; bias reduction; penalized likelihood; data separation; infinite estimate; working weight; Bradley-Terry model

1 Introduction

Logistic regression (see, for example, McCullagh and Nelder, 1989, Chapter 4) is one of the most frequently applied generalized linear models in statistical practice, both for inference about covariate effects on binomial probabilities, and for prediction.

Consider realizations $y_1, \ldots, y_n$ of independent binomial random variables $Y_1, \ldots, Y_n$ with probabilities of success $\pi_1, \ldots, \pi_n$ and totals $m_1, \ldots, m_n$, respectively. Furthermore, suppose that each $y_i$ is accompanied by a $p$-dimensional covariate vector $x_i$ and that the model matrix
X with rows \( x_1, \ldots, x_n \) has full rank. A logistic regression model has

\[
\pi_i = G \circ \eta_i(\beta) \quad \text{with} \quad G(\eta) = \frac{e^{\eta}}{1 + e^{\eta}} \quad \text{and} \quad \eta_i(\beta) = \sum_{t=1}^{p} \beta_t x_{it} \quad (i = 1, \ldots, n), \quad (1)
\]

where \( \beta = (\beta_1, \ldots, \beta_p)^T \) is the \( p \)-dimensional parameter vector, and \( x_{it} \) is the \( t \)th element of \( x_i \) \( (i = 1, \ldots, n) \); if an intercept parameter is present in the model then the first column of \( X \) is a vector of ones.

The maximum likelihood estimator \( \hat{\beta} \) of \( \beta \) in (1) results from the maximization of the log-likelihood function

\[
l(\beta) = \sum_{i=1}^{n} y_i \eta_i(\beta) - \sum_{i=1}^{n} m_i \log \left\{ 1 + e^{\eta_i(\beta)} \right\} . \quad (2)
\]

Albert and Anderson (1984) categorized the possible settings for the sample points \((y_1, x_1^T)^T, \ldots, (y_n, x_n^T)^T\) into complete separation, quasi-complete separation and overlap. Specifically, if there exists a vector \( \omega \in \mathbb{R}^p \) such that \( \omega^T x_i > 0 \) for all \( i \) with \( y_i > 0 \) and \( \omega^T x_i < 0 \) for all \( i \) with \( y_i = 0 \), then there is complete separation in the sample points; if there exists a vector \( \omega \in \mathbb{R}^p \) such that \( \omega^T x_i \geq 0 \) for all \( i \) with \( y_i > 0 \) and \( \omega^T x_i \leq 0 \) for all \( i \) with \( y_i = 0 \), then there is quasi-complete separation in the sample points; and if neither complete nor quasi-complete separation is present, then the sample points overlap. Albert and Anderson (1984) showed that separation is a necessary and sufficient condition for the maximum likelihood estimate to have at least one infinite-valued component. A parallel result is found in Silvapulle (1981), where it is shown that if \( G(\eta) \) in (1) is any distribution function that is strictly increasing such that \(-\log G(\eta)\) and \(\log(1 - G(\eta))\) are convex, and \(x_{i1} = 1 \ (i = 1, \ldots, n)\), then the maximum likelihood estimate has all components finite if and only if there is overlap.

When data separation occurs, standard maximum-likelihood estimation procedures, such as iteratively reweighted least squares (Green, 1984), can be subject to numerical instabilities mainly due to the occurrence of large, in absolute value, parameter values as the procedures attempt to maximize (2). In addition, inferential procedures that directly depend on the estimates and the estimated standard errors, such as Wald tests, can give misleading results. For a recent review of such problems and some solutions, see Mansournia et al. (2018).

Firth (1993) showed that if one penalizes the logistic regression likelihood by Jeffrey’s invariant prior, then the resulting maximum penalized likelihood estimators have bias of smaller asymptotic order than that of the maximum likelihood estimator. Specifically, for logistic regressions the reduced-bias estimator \( \tilde{\beta} \) of Firth (1993) results from the maximization of

\[
\tilde{l}(\beta) = l(\beta) + \frac{1}{2} \log \left| X^T W(\beta) X \right| , \quad (3)
\]

with \( W(\beta) = \text{diag}\{w_1(\beta), \ldots, w_n(\beta)\} \), and where \( w_i(\beta) = m_i \omega \circ \eta_i(\beta) \) is the working weight for the \( i \)th observation with \( \omega \circ \eta_i(\beta) = \omega(\eta_i(\beta)) \) and \( \omega(\eta) = e^{\eta}/(1 + e^{\eta})^2 \ (i = 1, \ldots, n) \).

Heinze and Schm{"{a}}per (2002), in extensive numerical studies, observed that the reduced-bias estimates have finite values even in cases where the maximum likelihood estimates have infinite components. Based on an argument about parameter-dependent adjustments to \( y_1, \ldots, y_n \) and \( m_1, \ldots, m_n \) stemming from the form of the gradient of (3), Heinze and Schm{"{a}}per (2002) conjectured that the finiteness of the reduced-bias estimates holds for every combination of data and logistic regression model. Heinze and Schm{"{a}}per (2002) also observed that the reduced-bias estimates are typically smaller in absolute value than the corresponding maximum likelihood estimates, when the latter are finite. These observations are in agreement with the asymptotic bias of the maximum likelihood estimator in logistic regressions being approximately collinear with the parameter vector (see, for example, Copas, 1988; Cordeiro and McCullagh, 1991).
Example 1 illustrates the finiteness and shrinkage properties of the maximum penalized likelihood estimator in the context of estimating the abilities of NBA basketball teams using a Bradley-Terry model (Bradley and Terry, 1952).

**Example 1:** Suppose that \( y_{ij} = 1 \) when team \( i \) beats team \( j \), and \( y_{ij} = 0 \), otherwise. The Bradley-Terry model assumes that the contest outcome \( y_{ij} \) is the realization of a Bernoulli random variable with probability \( \pi_{ij} = \exp(\beta_i - \beta_j) / \{1 + \exp(\beta_i - \beta_j)\} \), and that the outcomes for the available contests are independent. The Bradley-Terry model is a logistic regression with probabilities as in (1), for the particular \( X \) matrix whose rows are indexed by contest identifiers \((i,j)\) and whose general element is

\[
x_{ij,t} = \delta_{it} - \delta_{jt} \quad (t = 1, \ldots, p).
\]

Here \( \delta_{it} \) is the Kronecker delta, equal to 1 when \( t = i \) and zero otherwise. The parameter \( \beta_t \) can be thought as measuring the ability or strength of team \( t \) \((t = 1, \ldots, p)\). Only ability contrasts are estimable, and an identifiable parameterization can be achieved by simply setting one of the abilities to zero. See, for example, Agresti (2012), section 11.6, for a general discussion of the model.

We use the Bradley-Terry model to estimate the ability of NBA teams using game outcomes from the regular season of the 2014–2015 NBA conference. For illustrative purposes, we have considered only the 262 games in the conference before 3 December 2014. The latter date is when Philadelphia 76ers made their first win against Minnesota Timberwolves, after 17 consecutive losses. The data was retrieved from [www.basketball-reference.com](http://www.basketball-reference.com) and is also available as part of the supplementary material. The ability of the San Antonio Spurs, the champion team of the 2013–2014 conference, is set to zero, so that \( \beta_i \) is the contrast of the ability of team \( i \) with San Antonio Spurs. The model is estimated using the iteratively reweighted least squares procedure (Green, 1984), as implemented in the `glm` R function with default settings for the optimization. No warning or error was returned during the fitting process.

The top panel in the left plot of Figure 1 shows the maximum likelihood estimates of the contrasts, along with their corresponding nominally 95% individual Wald-type confidence intervals. The contrast for Philadelphia 76ers is the one standing out in the output from `glm` with a value of \(-19.24\) and a corresponding estimated standard error of 84.97. These values are in fact representations of \(-\infty\) and \(\infty\), respectively, as confirmed by the `detect_separation` method of the `brglm2` (Kosmidis, 2018) R package, which implements separation-detection algorithms from a 2007 University of Oxford Department of Statistics PhD thesis by K. Konis (Konis, 2007). The data is separated, with the maximum likelihood estimates for all teams being finite except that for Philadelphia 76ers, which is minus infinity. A particularly worrying side-effect of data separation here is that if the computer output is used naively, a Wald test for difference in ability between Philadelphia 76ers and San Antonio Spurs results in no apparent evidence of a difference, which is counter intuitive given that the former had no wins in 17 games and the latter had 13 wins in 17 games. In contrast, the reduced-bias estimates in the bottom panel of the left of Figure 1 all have finite values and finite standard errors. The right plot in Figure 1 illustrates the shrinkage of the reduced-bias estimates towards zero that has also been discussed in a range of different settings, for example in Heinze and Schemper (2002) and Zorn (2005).

The apparent finiteness and shrinkage properties of the reduced-bias estimator, coupled with the fact that the estimator has the same asymptotic distribution that the maximum likelihood estimator has in general, are key reasons for the increasingly widespread and diverse use of Jeffreys-prior penalized logistic regression in applied work. At the time of writing, Google Scholar records approximately 2400 citations of Firth (1993), more than half of which are from 2015 or later. The list of application areas is very diverse, including for example agriculture and fisheries research, animal and plant ecology, criminology, commerce, economics, health sciences, politics, psychology and many more. In political science, the work of Zorn (2005) has been notably
Figure 1: Left: Estimated contrasts with San Antonio Spurs, in ability of NBA teams. The abilities are estimated using a Bradley-Terry model on the outcomes of the 262 games before 03 December 2014 in the regular season of the 2014–2015 NBA conference, using the maximum likelihood (ML, top) and the reduced-bias (RB, bottom) estimator. The vertical segments are nominally 95% Wald-type confidence intervals. Right: reduced-bias estimates of ability contrasts versus maximum likelihood estimates of ability contrasts. The maximum likelihood estimate for Philadelphia 76rs is not plotted. The solid 45° line is displayed for reference.

influential. The strong uptake of the method in health and medical sciences stems largely from the work of Heinze and Schemper (2002) and associated software (Heinze and Ploner, 2003, 2018). In related work, Heinze and Schenper (2001) showed how to extend the reduced-bias estimator to the Cox (1972) proportional-hazards modelling of censored survival data, and this too has contributed to the method’s wide use in medical research. A different extension, to multinomial models (Bull et al., 2002), has also had influence in various applied fields. The reduced-bias estimator has now become part of textbook treatments of logistic regression; see, for example, Agresti (2012) section 7.4, or Hosmer et al. (2013) section 10.3.

However, a definitive theoretical account of those finiteness and shrinkage properties has yet to appear in the literature. Such a formal account is even more imperative in light of recent advances that demonstrate the benefits of the reduced-bias estimator in wider contexts than the ones for which it was originally developed. An example of such an advance is Lunardon (2018), which explores the performance of bias reduction in stratified settings and shows that bias reduction is particularly effective for inference about a low-dimensional parameter of interest in the presence of high-dimensional nuisance parameters. For the estimation of high-dimensional logistic regression models with \( p/n \to \kappa, \kappa \in (0, 1) \), experiments reported in the supplementary information file of Sur and Candès (2019) show that bias reduction performs similarly to their newly proposed method, and markedly better than maximum likelihood. These new theoretical and empirical results justify and motivate the use of the reduced-bias estimator in even more complex applied settings than the one covered by the framework of Firth (1993); in such settings, more involved methods such as modified profile likelihoods (see, for example Sartori, 2003) and approximate message-passing algorithms (see, for example Sur and Candès, 2019) have also been proposed for recovering inferential accuracy.

This paper formally derives the finiteness and shrinkage properties of reduced-bias estimators for logistic regressions only under the condition that model matrix \( X \) has full rank. We also provide geometric insights on how the penalized likelihood estimators shrink towards zero in
relation to the maximum likelihood estimator, and extensive discussions about the implications of finiteness and shrinkage in inference, especially in hypothesis tests and confidence regions using Wald-type procedures.

We also show how the results extend in a direct way to other commonly-used link functions, such as the probit, log-log, complementary log-log and cauchit whenever the Jeffreys prior is used as a likelihood penalty. The work presented here thus complements earlier work of Ibrahim and Laud (1991) and especially Chen et al. (2008), which studies the same models from a Bayesian perspective. Here we study the behaviour of the posterior mode and thereby derive results that add to those earlier findings, whose focus was instead on important Bayesian aspects such as propriety and moments of the posterior distribution.

The proofs in this paper also readily extend to situations where penalized log-likelihoods of the form

\[ l^\dagger(\beta; a) = l(\beta) + a \log \mid X^T W(\beta(s)) X \mid (a > 0), \]

are used, with \( a \) allowed to take values other than \( 1/2 \). Such penalized log-likelihoods have proved useful in prediction contexts, where one can tune \( a \) in order to deliver better estimates of the binomial probabilities; and they are the subject of ongoing research (see, for example, Elgmati et al., 2015; Puhr et al., 2017).

Finally we derive and discuss an algorithm that provides easy implementation for the maximization of \( l^\dagger(\beta; a) \) for general binomial-response generalized linear models, when \( a \) is fixed. The algorithm leverages readily available implementations of maximum likelihood to perform repeated maximum-likelihood fits on appropriately adjusted binomial responses and totals. Such implementations include the \texttt{glm} function in R (R Core Team, 2018) and the various implementations in Python modules \texttt{statsmodels} (Seabold and Perktold, 2010) and \texttt{scikit-learn} (Pedregosa et al., 2011).

2 Finiteness of reduced-bias estimators in logistic regression

Let \( \beta(s), s \in \mathbb{R} \) be a path in \( \mathbb{R}^p \) such that \( \beta(s) \to \beta_0 \) as \( s \to \infty \), where \( \beta_0 \) has at least one infinite component. Theorem 1 below describes the limiting behaviour of the determinant of the expected information matrix \( X^T W(\beta(s)) X \) as \( s \) diverges to infinity, only under the assumption that \( X \) is of full rank. An important implication of Theorem 1 is Corollary 1 which shows that the reduced-bias estimators for logistic regressions are always finite. These new results formalize an argument made in Firth (1993, § 3.3) and provide the platform for generalization to other link functions in Section 4.

\textbf{Theorem 1:} Suppose that \( X \) has full rank. Then \( \lim_{s \to \infty} |X^T W(\beta(s)) X| = 0 \).

The proof of Theorem 1 is given in the Appendix.

\textbf{Corollary 1.} Suppose that \( X \) has full rank. The vector \( \hat{\beta} \) that maximizes \( l^\dagger(\beta) \) has all of its components finite.

\textit{Proof.} The binomial log-likelihood \( l(\beta) \) in (2) is bounded above by zero. Hence, according to Theorem 1 and expression (3), \( l(\beta(s)) \to -\infty \) as \( \beta(s) \to \beta_0 \). Such a setting for \( \beta \) is always dominated, by a choice \( b \) with finite components for which \( l(b) \) takes a finite value. Hence, the maximizer of \( l^\dagger(\beta) \) must have finite components. \( \square \)

Corollary 1 also holds for any fixed \( a > 0 \) in (4). As a result, the penalized likelihood estimators from the maximization of \( l^\dagger(\beta; a) \) in (4) have always finite components, for any \( a > 0 \).

Despite its practical utility, the finiteness of the reduced-bias estimator results in some notable, and perhaps undesirable, side-effects on Wald-type inferences based on the reduced-bias
Table 1: Common link functions and the corresponding forms for $G(\eta)$ and $\omega(\eta)$. For all the displayed link functions, $\omega(\eta)$ vanishes as $\eta$ diverges.

| Link function | $G(\eta)$                                      | $\omega(\eta)$                   |
|---------------|-----------------------------------------------|-----------------------------------|
| logit         | $\frac{e^\eta}{1 + e^\eta}$                  | $\frac{e^\eta}{(1 + e^\eta)^2}$  |
| probit        | $\Phi(\eta)$                                  | $\frac{\{\phi(\eta)\}^2}{\Phi(\eta)\{1 - \Phi(\eta)\}}$ |
| c-log-log     | $1 - e^{-e^{\eta}}$                           | $e^{e^\eta} - 1$                  |
| log-log       | $e^{-e^{-\eta}}$                              | $\frac{1}{e^{-2\eta}}$           |
| cauchit       | $\frac{1}{2} + \frac{\arctan(\eta)}{\pi}$   | $\frac{1}{(1 + \eta^2)^2 \left[ \frac{\eta^2}{4} - \{\tan^{-1}(\eta)\}^2 \right]}$ |

The finiteness of $\hat{\beta}$ implies that the estimated standard errors $s_t(\hat{\beta})$ ($t = 1, \ldots, p$), calculated as the square roots of the diagonal elements of the inverse of $X^\top W(\hat{\beta})X$, are also always finite. Since $y_1, \ldots, y_n$ are realizations of binomial random variables, there is always only a finite number of values that the estimator $\hat{\beta}$ can take for any given $x_1, \ldots, x_n$. Hence, there will always be a parameter vector with large enough components that the usual Wald-type confidence intervals $\hat{\beta}_t \pm z_{1-\alpha/2} s_t(\hat{\beta})$, or confidence regions in general, will fail to cover regardless of the nominal level $\alpha$ that is used. This has also been observed in the complete enumerations of Kosmidis (2014) for proportional odds models which are extensions of logistic regression to ordinal responses; and it is also true when the penalized likelihood is profiled for the construction of confidence intervals, as is proposed, for example, in Heinze and Schemper (2002), and in Bull et al. (2007) for multinomial regression models.

3 Shrinkage of reduced-bias estimators in logistic regression

The following theorem is key when exploring the shrinkage properties of the reduced-bias estimator that have been illustrated in Example 1.

**Theorem 2:** Suppose that $X$ has full rank. Then

i) The function $|X^\top W(\beta)X|$ is globally maximized at $\beta = 0$.

ii) If $\bar{W}(\pi) = \text{diag}\{m_1\pi_1(1 - \pi_1), \ldots, m_n\pi_n(1 - \pi_n)\}$, then $|X^\top \bar{W}(\pi)X|$ is log-concave on $\pi$.

A complete proof of Theorem 2 is in the Appendix. Part i) also follows directly from Chen et al. (2008, Theorem 1).

Consider estimation by maximization of the penalized log-likelihood $l^p(\beta; a)$ in (4) for $a = a_1$ and $a = a_2$ with $a_1 > a_2 \geq 0$. Let $\beta^{(a_1)}$ and $\beta^{(a_2)}$ be the maximizers of $l^p(\beta; a_1)$ and $l^p(\beta; a_2)$, respectively and $\pi^{(a_1)}$ and $\pi^{(a_2)}$ the corresponding estimated $n$-vectors of probabilities. Then, by the concavity of $\log |X^\top \bar{W}(\pi)X|$, the vector $\pi^{(a_1)}$ is closer to $(1/2, \ldots, 1/2)^\top$ than is $\pi^{(a_2)}$, in the sense that $\pi^{(a_1)}$ lies within the hull of that convex contour of $\log |X^\top \bar{W}(\pi)X|$ containing $\pi^{(a_2)}$. With the specific values $a_1 = 1/2$ and $a_2 = 0$ the last result refers to maximization of the likelihood penalized by Jeffreys’ invariant prior and to maximization of the un-penalized likelihood, respectively. Hence, use of reduced-bias estimators for logistic regressions has the effect of shrinking towards the equiprobability model, relative to maximum likelihood. Shrinkage
here is according to a metric based on the expected information matrix rather than to Euclidean distance. Hence, the reduced-bias estimates are only typically, rather than always, smaller in absolute value than the corresponding maximum likelihood estimates.

If the determinant of the inverse of the expected information matrix is considered as a generalized measure of the asymptotic variance, then the estimated generalized asymptotic variance at the reduced-bias estimates is always smaller than the corresponding estimated variance at the maximum likelihood estimates. Hence approximate confidence ellipsoids, based on asymptotic normality of the reduced-bias estimator, are reduced in volume.

4 Finiteness and shrinkage for non-logistic link functions

4.1 Finiteness

The results in Theorem 1 and Corollary 1 readily extend to more link functions than the logistic. Specifically, if \( G(\eta) = \frac{e^\eta}{1 + e^\eta} \) in model (1) is replaced by an at least twice differentiable and invertible function \( G: \mathbb{R} \to (0, 1) \), then the expected information matrix has again the form \( X^\top W(\beta) X \) but with working weights \( w_i(\beta) = m_i \omega(\eta_i(\beta)) \) (i = 1, ..., n) where \( \omega(\eta) = g(\eta)^2 / \{G(\eta)(1 - G(\eta))\} \) and \( g(\eta) = dG(\eta)/d\eta \). If the link function is such that \( \omega(\eta) \to 0 \) as \( \eta \) diverges to either \(-\infty\) or \( \infty \), then the proofs of Theorem 1 and Corollary 1 in the Appendix apply unaltered to show that when the penalty is Jeffreys’ invariant prior, \( \lim_{s \to \infty} |X^\top W(\beta(s)) X| = 0 \) and the penalized likelihood estimates have finite components. The logit, probit, complementary log-log, log-log and cauchit links are some commonly-used link functions for which \( \omega(\eta) \to 0 \). The functions \( G(\eta) \) and \( \omega(\eta) \) for each of the above link functions are shown in Table 1.

4.2 Shrinkage

The result that the determinant of the expected information matrix is maximized at zero in Theorem 2 holds also for more link functions than the logit. Let \( \bar{\omega}(z) = g(G^{-1}(z))^2 / \{z(1 - z)\} \). If the link function is such that \( \bar{\omega}(z) \) is maximized at some value \( z_0 \in (0, 1) \), then the same arguments as in the proof of result i) in Theorem 2 can be used to show that \( |X^\top \bar{W}(\pi) X| \) is globally maximized at \((z_0, \ldots, z_0)^\top \). Figure 2 illustrates that this condition is satisfied for the logit, probit, log-log, and complementary log-log link functions. In addition, directly from the proof of Theorem 2, a sufficient condition for the log-concavity of \( |X^\top \bar{W}(\pi) X| \) for non-logit link functions is that \( \bar{\omega}(z) \) is concave.

5 Maximum penalized likelihood as repeated maximum likelihood

The maximum penalized likelihood estimates, for full rank \( X \), can be computed by direct numerical optimization of the penalized log-likelihood \( l^\dag(\beta; a) \) in (4) or by using a quasi Newton-Raphson iteration as in Kosmidis and Firth (2010). Nevertheless, the particular form of the Jeffreys prior allows the convenient computation of penalized likelihood estimates by leveraging readily available maximum-likelihood implementations for binomial-response generalized linear models, such as the \texttt{glm} function in R (R Core Team, 2018) and the various implementations in the Python modules \texttt{statsmodels} (Seabold and Perktold, 2010) and \texttt{scikit-learn} (Pedregosa et al., 2011).

If \( G(\eta) = \frac{e^\eta}{1 + e^\eta} \) in model (1) is replaced by any invertible function \( G: \mathbb{R} \to (0, 1) \) that is at least twice differentiable, then differentiation of \( l^\dag(\beta; a) \) with respect to \( \beta_t \) (t = 1, ..., q)
gives that the penalized likelihood estimates are the roots of
\[ \sum_{i=1}^{n} \frac{w_i(\beta)}{d_i(\beta)} \left[ y_i + 2ah_i(\beta) \left( q_i(\beta) - \frac{1}{2} \right) - m_i\pi_i(\beta) \right] x_{it} = 0 \quad (t = 1, \ldots, p), \] (5)
where \( \pi_i(\beta) = G_i \circ \eta_i(\beta) \), \( d_i(\beta) = m_i g_i \circ \eta_i(\beta) \), \( q_i(\beta) = d'_i(\beta)/w_i(\beta) + \pi_i(\beta) \), and \( d'_i(\beta) = m_i g'_i \circ \eta_i(\beta) \) with \( g' (\eta) = d^2 G(\eta)/d\eta^2 \). The quantity \( h_i(\beta) \ (i = 1, \ldots, n) \) is the \( i \)th diagonal element of the ‘hat’ matrix \( H(\beta) = X (X^\top W(\beta) X)^{-1} X^\top W(\beta) \).

If we temporarily omit the observation index and suppress the dependence of the various quantities on \( \beta \), the derivatives of \( l^1(\beta ; a) \) are the derivatives of the binomial log-likelihood \( l(\beta) \) with link function \( G(\eta) \), after adjusting the binomial response \( y \) to \( y + 2ah(q - 1/2) \). Hence, the penalized likelihood estimates can be conveniently computed through repeated maximum-likelihood fits where, at each repetition, i) the adjusted responses are computed at the current parameter values; and ii) the maximum likelihood estimates of \( \beta \) are computed at the current value of the adjusted responses.

However, depending on the sign and magnitude of \( 2ah(q - 1/2) \), the adjusted response can be either negative or greater than the binomial total \( m \). In such cases, standard implementations of maximum likelihood are either unstable or report an error. This is because the binomial log-likelihood is not necessarily concave when \( y < 0 \) or \( y > m \) for at least one observation, when a link function with concave \( \log (G(\eta)) \) and \( \log (1 - G(\eta)) \) is used (see, for example, Pratt, 1981, Section 5, for theorems on concavity of the log-likelihood in binomial-response models and discussion). Logit, probit, log-log and complementary log-log are link functions of this kind.

Such issues with the use of repeated maximum-likelihood fits can be avoided by noting that expression (5) results if, in the derivatives of the log-likelihood, \( y \) is replaced by an adjusted response
\[ \tilde{y} = y + 2ah(q - 1/2 + \pi b), \] (6)
and \( m \) is replaced by an adjusted total
\[ \tilde{m} = m + 2ahb. \] (7)
Here \( b \) is some arbitrarily chosen function of \( \beta \). The following theorem identifies one function \( b \) for which \( 0 \leq \tilde{y} \leq \tilde{m} \).

**Theorem 3:** Let \( I(A) \) be 1 if \( A \) holds and 0 otherwise. If
\[ b = 1 + \frac{q - 1/2}{\pi (1 - \pi)} \{ \pi - I(q \leq 1/2) \}, \]
then \( 0 \leq \tilde{y} \leq \tilde{m} \).

**Proof.** For \( b \) as in Theorem 3, the adjusted responses and totals (6, 7) have the form
\[ \tilde{y} = y + 2ah\pi \left\{ 1 + (q - 1/2) \frac{1 - I(q \leq 1/2)}{\pi (1 - \pi)} \right\}, \] (8)
\[ \tilde{m} = m + 2ah \left\{ 1 + (q - 1/2) \frac{\pi - I(q \leq 1/2)}{\pi (1 - \pi)} \right\}. \]
The result follows for any value of \( q \), because \( 0 \leq h \leq 1 \) and \( 0 \leq \pi \leq 1 \).

Algorithm 1 shows how repeated maximum-likelihood fits can be used to optimize the \( l^1(\beta ; a) \) for any supplied \( a \) and link function \( G(\eta) \). The variance-covariance matrix of the penalized likelihood estimator can be obtained as \( (R^\top R)^{-1} \), where \( R \) is the upper triangular matrix from the QR decomposition in step 17 of Algorithm 1 at the final iteration.
Algorithm 1 Repeated maximum-likelihood fits for the maximization of $l(\beta; a)$ in (4). The inputs $y, m, X, a, G, g_{\text{dash}}$ are $y = (y_1, \ldots, y_n)^T$, $m = (m_1, \ldots, m_n)^T$, $X$, $a$ in (4), $G(\eta)$, $g(\eta)$ and $g'(\eta)$, respectively, and $||| \|$ is the $L_2$ norm. The starting vector for $\beta$ is $b$ and $\epsilon$ is a small positive constant. ML is any maximum likelihood procedure.

1: procedure JEFFREYSMPL$(y, m, X, a, G, g_{\text{dash}}, \text{ML}, b, \epsilon)$
2: k ← 0
3: n ← numberofrows$(X)$  \> Number of observations; must equal length$(y)$ and length$(m)$
4: p ← numberofcolumns$(X)$  \> Number of parameters; must equal length$(b)$
5: eta, pi, d, dd ← vector(n)
6: for i ∈ {1, 2, …, n} do
7: xi ← (X[i, 1], …, X[i, p])
8: eta[i] ← dotproduct(xi, b)  \> dot product of xi and b
9: pi[i] ← G(eta[i])
10: d[i] ← g(eta[i])
11: dd[i] ← g'(eta[i])
end for
13: w ← d * pi / ((1 − pi))  \> elementwise operations
14: q ← dd / w + pi  \> elementwise operations
15: j ← I(q ≤ 1/2)  \> elementwise inequality and indicator function
16: V ← diag([\sqrt{m}_1 * w[1], \ldots, \sqrt{m}_n * w[n]]) * X  \> · stands for matrix product
17: Q ← orthogonal matrix from the QR decomposition of V
18: h ← rowsums(Q * Q)  \> sum the elements in each row of the elementwise product Q * Q
19: y_adj ← y + 2 * a * h * pi * ((1 + (q − 1/2) / (1 − j) / pi / (1 − pi))  \> elementwise operations
20: m_adj ← m + 2 * a * h * ((1 + (q − 1/2) / (pi − j) / pi / (1 − pi))  \> elementwise operations
21: bp ← b
22: b ← ML(y_adj, m_adj, X, G)  \> Maximum likelihood fit on adjusted data with link G
23: if ||bp − b|| < \epsilon then
24: return b
25: else
26: k ← k + 1
27: Go to 6
28: end if
end procedure

If, in addition to full rank $X$, we require that $X$ has a column of ones and $g(\eta)$ is a unimodal density function, then it can be shown that if the starting value of the parameter vector $\beta$ in Algorithm 1 has finite components, then the values of $\beta$ computed at step 22 will also have finite components at all iterations. This is a consequence of the fact that, in that case, the adjusted responses and totals in (8) are such that $0 < \tilde{y} < \tilde{m}$ and, hence, solutions with infinite components are not possible. The strict inequalities $0 < \tilde{y} < \tilde{m}$ hold because, under the aforementioned conditions, $w_i(\beta) > 0$ and $X^TW(\beta)X$ is positive definite for $\beta$ with finite components. Then, Magnus and Neudecker (1999, Chapter 11, Theorem 4) on bounds for the Rayleigh quotient gives the inequality $h_i(\beta) \geq w_i(\beta)x_i^T x_i \lambda(\beta) > 0$ (1, …, n), where $\lambda(\beta) > 0$ is the minimum eigenvalue of $(X^TW(\beta)X)^{-1}$.

The iteration in Algorithm 1 has the correct fixed point even if, at its step 22, full maximum-likelihood estimation is replaced by a step that just increases the log-likelihood, such as a single step of iteratively reweighted least squares for the adjusted responses and totals (see, also, Firth, 1992, for a special case of such a scheme in logistic regressions with $a = 1/2$). There are currently no conclusive results on whether full maximum-likelihood iteration with reasonable
Table 2: The adjusted responses (top) and totals (bottom) for the first 6 games of Philadelphia 76ers (P76) at the first 6 iterations of Algorithm 1, when computing the reduced-bias fit in Figure 1. Figures are shown in 3 decimal digits. The home team is mentioned first in column names. The actual response is 1 if the home team wins and 0 otherwise. The acronyms for the opponents are IP (Indiana Pacers), MB (Milwaukee Bucks), MH (Miami Heat), HR (Houston Rockets), OR (Orlando Magic) and CB (Chicago Bulls). The starting values are the maximum likelihood estimates of the ability contrasts after adding 0.01 and 0.02 to the actual responses and totals (iteration 0).

| Iteration | P76 vs IP | P76 vs MB | MH vs P76 | HR vs P76 | OM vs P76 | CB vs P76 |
|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
|           | Adjusted responses |                   |           |           |           |           |
| 0         | 0.010     | 0.010     | 1.010     | 1.010     | 1.010     | 1.010     |
| 1         | 0.039     | 0.036     | 1.045     | 1.012     | 1.104     | 1.039     |
| 2         | 0.045     | 0.042     | 1.054     | 1.017     | 1.110     | 1.048     |
| 3         | 0.046     | 0.043     | 1.055     | 1.017     | 1.111     | 1.049     |
| 4         | 0.046     | 0.043     | 1.055     | 1.018     | 1.111     | 1.049     |
| 5         | 0.046     | 0.043     | 1.055     | 1.018     | 1.111     | 1.049     |
| 6         | 0.046     | 0.043     | 1.055     | 1.018     | 1.111     | 1.049     |

| Adjusted totals |                   |           |           |           |           |           |
|-----------------|--------------------|-----------|-----------|-----------|-----------|-----------|
| 0               | 1.020              | 1.020     | 1.020     | 1.020     | 1.020     | 1.020     |
| 1               | 1.114              | 1.105     | 1.067     | 1.018     | 1.158     | 1.059     |
| 2               | 1.128              | 1.120     | 1.081     | 1.025     | 1.170     | 1.073     |
| 3               | 1.130              | 1.122     | 1.083     | 1.026     | 1.171     | 1.075     |
| 4               | 1.131              | 1.122     | 1.084     | 1.026     | 1.172     | 1.075     |
| 5               | 1.131              | 1.122     | 1.084     | 1.026     | 1.172     | 1.075     |
| 6               | 1.131              | 1.122     | 1.084     | 1.026     | 1.172     | 1.075     |

Stopping criteria in step 22 is better or worse than, for example, a one-step iteration, in terms of the computational efficiency of Algorithm 1.

Our experience is that a satisfactory starting value $b$ for Algorithm 1 comes from the maximum likelihood estimates after adding a small positive constant to all binomial responses, and adding twice that constant to the totals.

Table 2 shows the values of the adjusted responses and totals for the first 6 games of Philadelphia 76ers at the first 6 iterations of Algorithm 1, when computing the reduced-bias fit shown in Figure 1. The starting values (iteration 0) are the maximum likelihood estimates of the ability contrasts after adding 0.01 and 0.02 to the actual responses and totals, respectively.

The R implementation of Algorithm 1 in the supplementary material has also been used to compute the reduced-bias estimates for a logistic regression model with $n = 1000$ binary responses and $p = 200$ covariates, as considered in Figure 2(b) of the supplementary information appendix of Sur and Candès (2019). That implementation is based on a full maximum-likelihood iteration using the R function glm.fit, and it takes approximately 2.73 seconds to converge to the reduced-bias estimates of the 200 parameters in 4 decimal places on a MacBook Pro laptop with 3.5GHz processor and 16GB of memory.

Finally, we note here that for $a = 1/2$, Algorithm 1 can be used to compute the posterior normalizing constant when implementing the importance sampling algorithm in Chen et al. (2008, Section 5) for posterior sampling of the parameters of Bayesian binomial-response generalized
Figure 2: Left: $\bar{\omega}(z)$ for various link functions. The dashed vertical line is at $z_0$. Right: Demonstration of how fitted probabilities from the penalized likelihood fit shrink relative to those of the maximum likelihood fit, from a complete enumeration of a saturated model where $\pi_i = G(\beta_1 + \beta_2 x_i)$ ($i = 1, 2$), $x_1 = -1$, $x_2 = 1$ and $m_1 = 9$ and $m_2 = 9$. The arrows point from the estimated probabilities based on the maximum likelihood estimates to those based on the penalized likelihood estimates. The grey curves are the contours of $\log |X^\top \bar{W}(\pi)X|$.

6 Illustrations

The left plot of Figure 2 shows $\bar{\omega}(z)$ and $z_0$ for the various links. The plot for the log-log link is the reflection of the one for the complementary log-log through $z = 0.5$. As is apparent, $\bar{\omega}(z)$ is concave for the logit, probit and complementary log-log links but not for the cauchit link. The right plot of Figure 2 visualizes the shrinkage induced by the penalization by Jeffreys’ invariant prior for the logit, probit, complementary log-log and cauchit links. For each link function, we obtain all possible fitted probabilities from a complete enumeration of a saturated model with $\pi_i = G(\beta_1 + \beta_2 x_i)$ ($i = 1, 2$), where $x_1 = -1$, $x_2 = 1$, $m_1 = 9$ and $m_2 = 9$. The grey curves are the contours of $\log |X^\top \bar{W}(\pi)X|$. An arrow is drawn from each pair of estimated probabilities based on the maximum likelihood estimates to the corresponding pair of estimated probabilities based on penalized likelihood estimates, to demonstrate the induced shrinkage towards $(z_0, z_0)^\top$.

Despite the fact that $\bar{\omega}(z)$ is not concave for the cauchit link, the fitted probabilities still shrink towards $(z_0, z_0)^\top = (1/2, 1/2)^\top$. The plots in Figure 2 are invariant to the particular choice of $x_1$ and $x_2$, as long as $x_1 \neq x_2$. For either maximum likelihood or maximum penalized likelihood, if the estimates of $\beta_1$ and $\beta_2$ are $b_1$ and $b_2$ for $x_1 = -1$ and $x_2 = 1$, then the new estimates for any $x_1, x_2 \in \mathbb{R}$ with $x_1 \neq x_2$ are $b_1 - b_2 (x_1 + x_2)/(x_2 - x_1)$ and $2b_2/(x_2 - x_1)$, respectively. Hence, the fitted probabilities will be identical.

Another illustration of shrinkage follows from Example 1. Figure 3 shows the paths of the team ability contrasts as $a$ varies from 0 to 5. The estimates are obtained using Algorithm 1, starting at the maximum likelihood estimates of the ability contrasts after adding 0.01 and 0.02 to the actual responses and totals, respectively. In accord with the theoretical results in linear models with the Jeffreys prior.
Section 2 the estimated ability contrasts are finite for every $a > 0$; and, as expected from the results in Section 3, shrinkage towards equiprobability becomes stronger as $a$ increases.

7 Concluding remarks

This paper presents definitive results on the finiteness of the reduced-bias estimator of Firth (1993) in logistic regressions, and provides geometric insights on the shrinkage that penalization delivers. We have also discussed the direct implications that finiteness and shrinkage of the reduced-bias estimator have in inference, particularly when this is based on Wald-type procedures. As discussed in Section 4, the finiteness and shrinkage results extend directly to other link functions under general conditions on the limiting behaviour of the working weights and on their concavity when viewed as a function of the corresponding binomial probabilities.

A recent stream of literature investigates the use of the coefficient path defined by maximization of the penalized log-likelihood (4) for the prediction of rare events through logistic regression. Elgmati et al. (2015) study that path for $a \in (0, 1/2]$, and propose to take $a$ to be around 0.1, in order to handle issues related to infinite estimates, and they obtain predicted probabilities that are less biased than those based on the reduced-bias estimates ($a = 0.5$). More recently, Puhr et al. (2017) proposed two new methods for the prediction of rare events, and performed extensive simulation studies to compare performance with various methods, including maximum penalized likelihood with $a = 0.1$ and $a = 0.5$.

The coefficient path can be computed in an efficient manner by using Algorithm 1 with “warm” starts. For a grid of values $a_1 < \ldots < a_k$ with $a_j > 0$ ($j = 1, \ldots, k$), Algorithm 1 is first applied as described in Section 5 with $a = a_1$ to get the maximum penalized likelihood estimates $\beta(a_1)$; then, Algorithm 1 is applied again with $a = a_2$ but starting at $b = \beta(a_1)$, and so on, until $\beta(a_k)$ has been computed. This process supplies Algorithm 1 with the best available starting values, as it walks through the grid. The finiteness of the components of $\beta(a_1), \ldots, \beta(a_k)$ and the shrinkage properties described in Sections 3 and 4 contribute to the stability of the
overall process. The properties of the coefficient path for inference and prediction from binomial regression models, and the development of general procedures for selecting \( a \), are interesting, open research topics.

8 Acknowledgements

Ioannis Kosmidis and David Firth are supported by The Alan Turing Institute under the EPSRC grant EP/N510129/1. David Firth was partly supported also by EPSRC programme EP/K014463/1, Intractable Likelihood: New Challenges from Modern Applications.

9 Supplementary material

The supplementary material includes the R code and data to reproduce all numerical results and figures in the paper and is available for download at http://www.ikosmidis.com/files/finiteness-jeffreys-supplementary-v1.2.zip.

Appendix

Proof of Theorem 1

Since \( X \) has full rank, \( |X^\top W(\beta)X| \) is not trivially zero for all \( \beta \in \mathbb{R}^p \). Let \( R = \{1, \ldots, n\} \) and

\[
R_{(1)} = \{ i : \eta_i(\beta(s)) | \to \infty \text{ as } s \to \infty ; i \in R \}
\]

\[
R_{(2)} = \{ i : \eta_i(\beta(s)) \to c_i, |c_i| < \infty \text{ as } s \to \infty ; i \in R \} .
\]

Then \( R = R_{(1)} \cup R_{(2)} \) and \( R_{(1)} \cap R_{(2)} = \emptyset \), where \( \emptyset \) is the empty set.

We first consider the case where \( R_{(1)} \) and \( R_{(2)} \) are non-empty. Then, \( X \) and \( W(\beta) \) can be partitioned as

\[
X = \begin{bmatrix} X_{(1)} \\ X_{(2)} \end{bmatrix} \quad \text{and} \quad W(\beta) = \begin{bmatrix} W_{(1)}(\beta) & 0 \\ 0 & W_{(2)}(\beta) \end{bmatrix},
\]

where \( X_{(i)} \) has rows \( x_i \) with \( i \in R_{(i)} \) and \( W_{(i)}(\beta) = \text{diag} \{ m_i \omega(\eta_i(\beta)), i \in R_{(i)} \} \) (\( l = 1, 2 \)). We can then write

\[
X^\top W(\beta(s))X = X_{(1)}^\top W_{(1)}(\beta(s))X_{(1)} + X_{(2)}^\top W_{(2)}(\beta(s))X_{(2)}. \tag{9}
\]

The limit of the first term in the right hand side of (9), as \( s \to \infty \), is zero because the limit of \( \omega(\eta) = e^\eta/(1 + e^\eta)^2 \), as \( \eta \) grows to infinity in absolute value, is zero. For the second term, \( X_{(2)} \) is such that \( X_{(2)}(\beta(s)) \to c(s) \) as \( s \to \infty \) where \( c(s) \) has all of its components finite. There must exist vectors \( a \in \mathbb{R}^p \) and \( b \in \mathbb{R}^p \) with finite components such that \( a + bs \to \beta_0 \). So, \( X_{(2)}a + X_{(2)}bs \to c(s) \) as \( s \to \infty \) which is possible if and only if \( X_{(2)}b = 0 \). Hence \( X_{(2)} \) has rank smaller than \( p \) and \( |X_{(2)}^\top W_{(2)}(\beta(s))X_{(2)}| = 0 \) for all \( s \). The result follows because \( |X_{(2)}^\top W_{(2)}(\beta(s))X_{(2)}| = 0 \) for all \( s \) and \( |X_{(1)}^\top W_{(1)}(\beta(s))X_{(1)}| \to 0 \) as \( s \to \infty \).

Because \( X \) is of full rank and \( X_{(2)} \) has rank smaller than \( p \), \( R_{(1)} \) cannot be empty. Hence, we only need to also examine the case that \( R_{(2)} \) is empty and \( R_{(1)} \) is not. In this case the same arguments as above give \( |X^\top W(\beta(s))X| = |X_{(1)}^\top W_{(1)}(\beta(s))X_{(1)}| \to 0 \) as \( s \to \infty \).
Proof of Theorem 2

The sum of \( m \) independent Bernoulli distributions with probability \( \pi \) is binomial with index \( m \) and probability \( \pi \). For this reason and without any loss of generality, the proof proceeds with \( m_i = 1 \) so that \( w_i(\beta) = \omega(\eta_i(\beta)) \) \((i = 1, \ldots, n)\).

For proving \( i \) decompose \( X \) as \( X = QR \), where \( Q \) is a \( n \times p \) matrix with orthonormal columns \((Q^TQ = I_p \text{ where } I_p \text{ is the } p \times p \text{ identity matrix})\) and \( R \) is a \( p \times p \) non-singular matrix. This decomposition is always possible because \( X \) has full rank by assumption. Then \(|X^TW(\beta)X| = |Q^TW(\beta)Q|/|R|^2\). The functions \(|X^TW(\beta)X|\) and \(|Q^TW(\beta)Q|\) will have stationary points of the same kind and at the same values of \( \beta \), because \(|R|^2 > 0\) does not depend on \( \beta \).

Denote the ordered set of quadratic weights as \( w_{(1)}(\beta), \ldots, w_{(n)}(\beta) \) with \( w_{(1)}(\beta) \leq \ldots \leq w_{(n)}(\beta) \). The Poincaré separation theorem (see, for example Magnus and Neudecker, 1999, Chapter 11, Theorem 10 for statement) and the positive definiteness of \( W(\beta) \) for \( \beta \in \mathbb{R}^p \) imply that

\[
\prod_{t=1}^p w_{(t)}(\beta) \leq |Q^TW(\beta)Q| \leq \prod_{t=1}^p w_{(n-p+t)}(\beta).
\] (10)

Note that \( 0 \leq \omega(\eta) \leq 1/4 \), with the upper bound achieved when \( \eta = 0 \). It follows that \( \prod_{t=1}^p w_{(t)}(\beta) \leq 1/4^p \) and \( \prod_{t=1}^p w_{(n-p+t)}(\beta) \leq 1/4^p \) and that, at \( \beta = 0 \) inequalities (10) become \( 1/4^p \leq |Q^TW(0)Q| \leq 1/4^p \). The proof of \( i \) concludes by noting that \(|Q^TW(0)Q| = 1/4^p\) which is the maximum value that \(|Q^TW(\beta)Q|\) can take.

For proving \( ii \), note that \( \bar{\omega}(z) = z(1-z) \) is concave. Hence, for \( \theta \in (0,1), \theta^* = 1 - \theta \) and any pair of \( n \)-vectors of probabilities \( \pi \) and \( \rho \) \( \bar{\omega}(\theta\pi_i + \theta^*\rho_i) \geq \bar{\omega}(\theta\pi_i) + \bar{\omega}(\theta^*\rho_i) \) \((i = 1, \ldots, n)\).

Lemma 1 can then be used to show that

\[
|X^TW(\theta\pi + \theta^*\rho)X| \geq |\theta X^TW(\pi)X + \theta^* X^TW(\rho)X|.
\]

The result in \( ii \) follows from Magnus and Neudecker (1999, Chapter 11, Theorem 25) which can be used to show that

\[
|\theta X^TW(\pi)X + \theta^* X^TW(\rho)X| \geq |X^TW(\pi)X|^{\theta} |X^TW(\rho)X|^{\theta^*}.
\]

Lemma 1. If \( A \) and \( B \) are both diagonal \( n \times n \) matrices with non-negative diagonal elements \( \{a_r\} \) and \( \{b_r\} \), respectively, and \( a_r \geq b_r \), for every \( r \in \{1, \ldots, n\} \), then, if \( X \) is a \( n \times p \) matrix, \(|X^TAX| > |X^TAX|\).

Proof. Since \( A \geq B \), elementwise, \( A = B + C \), where \( C \) is a diagonal matrix with non-negative entries. Furthermore, \( X^TAX \), \( X^TAX \) and \( X^TAX \) are positive semidefinite, by the non-negativity of the diagonal elements of \( A \), \( B \) and \( C \), respectively. Hence, by Magnus and Neudecker (1999, Chapter 11, Theorem 9), \( \lambda_t(X^TAX) \geq \lambda_t(X^TAX) \) \((t = 1, \ldots, p)\), where \( \lambda_t(D) \) denotes the \( t \)th eigenvalue of the matrix \( D \). Since the determinant of a matrix is the product of its eigenvalues the result follows.

References

Agresti, A. (2012). *Categorical Data Analysis* (3rd ed.). Hoboken, NJ: John Wiley & Sons.

Albert, A. and J. Anderson (1984). On the existence of maximum likelihood estimates in logistic regression models. *Biometrika* 71(1), 1–10.

Bradley, R. A. and M. E. Terry (1952). Rank analysis of incomplete block designs: I. The method of paired comparisons. *Biometrika* 39(3/4), 324–345.
Bull, S. B., J. B. Lewinger, and S. S. F. Lee (2007). Confidence intervals for multinomial logistic regression in sparse data. *Statistics in Medicine* 26, 903–918.

Bull, S. B., C. Mak, and C. M. Greenwood (2002). A modified score function estimator for multinomial logistic regression in small samples. *Computational Statistics & Data Analysis* 39(1), 57–74.

Chen, M.-H., J. G. Ibrahim, and S. Kim (2008). Properties and implementation of Jeffreys’s prior in binomial regression models. *Journal of the American Statistical Association* 103(484), 1659–1664.

Copas, J. B. (1988). Binary regression models for contaminated data (with discussion). *Journal of the Royal Statistical Society, Series B: Methodological* 50(2), 225–265.

Cordeiro, G. M. and P. McCullagh (1991). Bias correction in generalized linear models. *Journal of the Royal Statistical Society, Series B: Methodological* 53(3), 629–643.

Cox, D. R. (1972). Regression models and life-tables. *Journal of the Royal Statistical Society: Series B (Methodological)* 34(2), 187–202.

Elgmati, E., R. L. Fiaccone, R. Henderson, and J. N. S. Matthews (2015). Penalised logistic regression and dynamic prediction for discrete-time recurrent event data. *Lifetime Data Analysis* 21(4), 542–560.

Firth, D. (1992). Bias reduction, the Jeffreys prior and GLIM. In L. Fahrmeir, B. Francis, R. Gilchrist, and G. Tutz (Eds.), *Advances in GLIM and Statistical Modelling: Proceedings of the GLIM 92 Conference, Munich*, New York, pp. 91–100. Springer.

Firth, D. (1993). Bias reduction of maximum likelihood estimates. *Biometrika* 80(1), 27–38.

Green, P. J. (1984). Iteratively reweighted least squares for maximum likelihood estimation, and some robust and resistant alternatives. *Journal of the Royal Statistical Society, Series B: Methodological* 46(2), 149–192.

Heinze, G. and M. Ploner (2003). Fixing the nonconvergence bug in logistic regression with SPLUS and SAS. *Computer Methods and Programs in Biomedicine* 71(2), 181–187.

Heinze, G. and M. Ploner (2018). *logistf: Firth’s Bias-Reduced Logistic Regression*. R package version 1.23, https://CRAN.R-project.org/package=logistf.

Heinze, G. and M. Schemper (2001). A solution to the problem of monotone likelihood in Cox regression. *Biometrics* 57(1), 114–119.

Heinze, G. and M. Schemper (2002). A solution to the problem of separation in logistic regression. *Statistics in Medicine* 21, 2409–2419.

Hosmer, D. W., S. Lemeshow, and R. X. Sturdivant (2013). *Applied Logistic Regression* (3rd ed.). Hoboken, NJ: John Wiley & Sons.

Ibrahim, J. G. and P. W. Laud (1991). On Bayesian analysis of generalized linear models using Jeffreys’s prior. *Journal of the American Statistical Association* 86(416), 981–986.

Konis, K. (2007). *Linear programming algorithms for detecting separated data in binary logistic regression models*. Ph. D. thesis, University of Oxford.

Kosmidis, I. (2014). Improved estimation in cumulative link models. *Journal of the Royal Statistical Society, Series B: Methodological* 76(1), 169–196.
Kosmidis, I. (2018). *brglm2: Bias Reduction in Generalized Linear Models*. R package version 0.1.8, https://CRAN.R-project.org/package=brglm2.

Kosmidis, I. and D. Firth (2010). A generic algorithm for reducing bias in parametric estimation. *Electronic Journal of Statistics* 4(0), 1097–1112.

Lunardon, N. (2018). On bias reduction and incidental parameters. *Biometrika* 105(1), 233–238.

Magnus, J. R. and H. Neudecker (1999). *Matrix Differential Calculus with Applications in Statistics and Econometrics*. Chichester: Wiley.

Mansournia, M. A., A. Geroldinger, S. Greenland, and G. Heinze (2018). Separation in logistic regression: Causes, consequences, and control. *American Journal of Epidemiology* 187(4), 864–870.

McCullagh, P. and J. A. Nelder (1989). *Generalized Linear Models* (2nd ed.). London: Chapman and Hall.

Pedregosa, F., G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, and E. Duchesnay (2011). Scikit-learn: Machine learning in Python. *Journal of Machine Learning Research* 12, 2825–2830.

Pratt, J. W. (1981). Concavity of the log likelihood. *Journal of the American Statistical Association* 76(373), 103–106.

Puhr, R., G. Heinze, M. Nold, L. Lusa, and A. Geroldinger (2017). Firth’s logistic regression with rare events: accurate effect estimates and predictions? *Statistics in Medicine* 36(14), 2302–2317.

R Core Team (2018). *R: A Language and Environment for Statistical Computing*. Vienna, Austria: R Foundation for Statistical Computing.

Sartori, N. (2003). Modified profile likelihoods in models with stratum nuisance parameters. *Biometrika* 90(3), 533–549.

Seabold, S. and J. Perktold (2010). Statsmodels: Econometric and statistical modeling with Python. In S. van der Walt and J. Millman (Eds.), *Proceedings of the 9th Python in Science Conference*, pp. 57–61.

Silvapulle, M. J. (1981). On the existence of maximum likelihood estimators for the binomial response models. *Journal of the Royal Statistical Society, Series B: Methodological* 43(3), 310–313.

Sur, P. and E. J. Candès (2019). A modern maximum-likelihood theory for high-dimensional logistic regression. *Proceedings of the National Academy of Sciences* 116(29), 14516–14525.

Zorn, C. (2005). A solution to separation in binary response models. *Political Analysis* 13(2), 157–170.