Winkler:

Bootstrapping Goodness of Fit Statistics in Loglinear Poisson Models


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Bootstrapping Goodness of Fit Statistics in Loglinear Poisson Models

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Abstract

The possible discrepancy between a hypothesized model and the observed data is measured by so called Goodness of Fit Statistics. In order to decide whether the observed discrepancy is substantial, the distributions of these statistics under the hypothesized model are needed to perform a statistical test. Because of the difficulty to compute the exact distributions, just when the sample size is small, better approximations than provided by common asymptotic theory have to be found. In the case of a loglinear Poisson model we will do that by different bootstrap methods.

Keywords: Bootstrap, goodness of fit statistics, loglinear Poisson model, binary logit model, overdispersion.

1 Introduction

We consider cross-sectional regression data \((y_{ij}, x_j)\) for \(n_j = n\) individuals in each group \(j = 1, \ldots, g\). The responses \(y_{ij}\) are non-negative integer-valued, \(x_j\), the corresponding \(p\)-dimensional row vector of real-valued covariates common to the subjects of the \(j^{th}\) group and \(\beta\) is the \(p\)-dimensional column vector of unknown parameters. It is hypothesised that for given \(x_j\), the \(y_{ij}\)'s can be modelled as realisations of independent Poisson random variables \(Y_{ij}\), with parameter \(\mu_j = \exp(x_j \beta)\), respectively

\[
\text{IP}(Y_{ij} = y|x_j) = \frac{\exp(-\mu_j) \mu_j^y}{y!} = \exp(y \log(\mu_j) - \mu_j - \log(y!)) . \tag{1.1}
\]

This model is called a loglinear Poisson model, which belongs to the more general class of generalized linear models (GLMs).

The unknown parameter vector \(\beta\) can be estimated from the data by the maximum likelihood principle. Let \(\hat{\beta}\) denote the maximum likelihood estimator (MLE) of \(\beta\). For \(N = n \times g\) tending to infinity, a standardized respectively studentised version of the MLE has a standard normal distribution. For small \(n\) the distribution of the MLE might be poorly
approximated by the normal distribution. For various further details on GLMs see McCullagh & Nelder (1989) or Fahrmeir & Tutz (1994).

An interesting question is often whether the hypothesized model fits the data. To answer the question the expected response values, based on the hypothesized model, are compared with the observed response values. If there exists a substantial discrepancy the hypothesized model is rejected because of lack of fit. This discrepancy is measured by so called Goodness of Fit (GoF) statistics. We consider three such GoF statistics: the $\chi^2$-statistic, the deviance and the power divergence statistic. The definitions of these statistics are given in section 2. For an overview on GoF statistics for discrete data, in particular a discussion on power divergence statistics, see Read & Cressie (1988).

In order to decide whether the observed discrepancy is substantial, the distributions of these statistics under the hypothesized model are needed to perform a statistical test. The exact distributions are difficult to compute. Usually the asymptotic distributions of the GoF statistics for $n$, the number of subjects in each group, tending to infinity, are computed and used as approximations. Under certain regularity conditions it can be shown that their asymptotic distributions are $\chi^2$ distributed with $(g - p)$ degrees of freedom, i.e. they are asymptotically equal. However, when in fact $N$ is small, the approximation of the true distribution by the asymptotic distribution may be poor. Therefore better approximations than the asymptotic distributions have to be found. We will do that by bootstrap methods, described in the third section.

In the last section we describe the performed Monte Carlo simulations to assess the validity of the bootstrap for model (1.1) and compare it with the results, when there is overdispersion involved with the model. This could be of special interest because there exists no longer an asymptotic maximum likelihood theory but a quasi likelihood theory for GLMs.

For comparison we additionally test the bootstrap for small $N$ in the case of a binary logit model.
2 Goodness of Fit Statistics in GLMs

In this section we will introduce the three GoF statistics studied in this paper. First we consider the \( \chi^2 \) or Pearson GoF statistic.

\[
\chi^2(y, \hat{\beta}) = \sum_{j=1}^{g} \left( \sum_{i=1}^{n} (y_{ij} - n\hat{\mu}_{j})^T \Sigma_j^{-1}(\hat{\beta}) \sum_{i=1}^{n} (y_{ij} - n\hat{\mu}_{j}) \right) \tag{2.1}
\]

where \( \Sigma_j(\hat{\beta}) \) denotes the estimated covariance matrix of \( y_j \), the set of the original data of the \( j^{th} \) group and \( \hat{\mu}_{j} = \mu_j(\hat{\beta}) \) the estimated mean in the \( j^{th} \) group. In the case of the loglinear Poisson model the Pearson GoF statistic is given, with \( \hat{\mu}_j = exp(x_j^T\hat{\beta}) \), by

\[
\chi^2(y, \hat{\beta}) = \sum_{j=1}^{g} \frac{\left( \sum_{i=1}^{n} (y_{ij} - n\hat{\mu}_{j})^2 \right)^2}{n\hat{\mu}_{j}}. \tag{2.2}
\]

The second type of GoF statistic is the so called deviance

\[
D(y, \hat{\beta}) = 2 \sum_{j=1}^{g} \left( l_j \left( \sum_{i=1}^{n} y_{ij} \right) - l_j \left( n\hat{\mu}_{j} \right) \right) \tag{2.3}
\]

with \( l_j(\sum_{i=1}^{n} y_{ij}) \) the log-likelihood function of the GLM evaluated at the observed data and \( l_j(n\hat{\mu}_{j}) \) the log likelihood evaluated at the estimated value for the mean in the \( j^{th} \) group. In the case of the loglinear Poisson model the deviance is given by

\[
D(y, \hat{\beta}) = 2 \sum_{j=1}^{g} \sum_{i=1}^{n} y_{ij} \log \left( \frac{\sum_{i=1}^{n} y_{ij}}{n\hat{\mu}_{j}} \right) - \sum_{i=1}^{n} y_{ij} + n\hat{\mu}_{j}. \tag{2.4}
\]

The third type of GOF statistic is the power divergence statistic

\[
PD(y, \hat{\beta}; \kappa) = \frac{2}{\kappa(\kappa + 1)} \sum_{j=1}^{g} \sum_{i=1}^{n} y_{ij} \left[ \left( \frac{\sum_{i=1}^{n} y_{ij}}{n\hat{\mu}_{j}} \right)^\kappa - 1 \right]. \tag{2.5}
\]

The real-valued parameter \(-\infty < \kappa < \infty\) can be chosen by the user. The cases \( \kappa = 0 \) and \( \kappa = -1 \) are defined as the limits \( \kappa \to 0 \) and \( \kappa \to -1 \), respectively. When the observed and the expected data match exactly for each possible outcome, (2.5) is zero for any choice of \( \kappa \). In all other cases the statistic becomes larger as the observed and expected data "diverge". Two special cases of (2.5) are for \( \kappa = 1 \) the Pearson GoF statistic and as the limit of \( \kappa \to 0 \) the likelihood ratio statistic \( G^2 = D(y, \hat{\beta}) + \sum_{j=1}^{g} \left( \sum_{i=1}^{n} y_{ij} - n\hat{\mu}_{j} \right) \). Read & Cressie (1988) summarize the properties of the power divergence statistic.
3 Bootstrapping GLMs

There is a good basic account of literature on bootstrap in Moulton & Zeger (1991) regarding both theoretical and practical aspects in GLMs. Here we apply the bootstrap to obtain approximate distributions of the GoF statistics for finite $N$ via Monte Carlo simulation. The bootstrap itself is described by Efron & Tibshirani (1993) and Shao & Tu (1995).

3.1 A short review of the bootstrap idea

Suppose the data $y$ can be modelled as realisations of i.i.d random variables $\{Y_1, \ldots, Y_n\} = Y$, distributed according to $F(\beta)$, where $F$ is in our case the Poisson distribution and $\beta$ the unknown parameter vector. Furthermore, a GoF statistic $G(Y) = G(F)$ is given, whose distribution $\mathcal{L}(G(F))$ is of interest.

Now suppose some estimate $\hat{F}(\beta) = \hat{F}$ of $F(\beta)$ can be computed from the data. This could be the empirical distribution, or, when $F$ is known, $\hat{F}$ could be $F(\beta)$, which would then lead to the parametric bootstrap described in the next section. The bootstrap is then the idea of approximating $\mathcal{L}(G(F))$ by $\mathcal{L}(G(\hat{F}))$, shown in the following figure.

$$
\begin{array}{cccc}
F & \rightarrow & Y & \rightarrow \\
& & \downarrow & \\
G(Y) & \leftarrow & \mathcal{L}(G(F)) & \leftarrow \\
& & \downarrow & \\
\hat{F} & \rightarrow & Y^* & \\
\end{array}
$$

Figure 3.1: The bootstrap idea according to Efron & Tibshirani (1993)

Assume the model is correctly specified and $\hat{F}$ is given, $\mathcal{L}(G(\hat{F}))$ can usually be computed, at least approximately, via simulation given enough computer power. The simulation is based on some intelligent way of resampling from the original data.

Using a random number generator, we can simulate pseudo data $\{y_1^*, \ldots, y_n^*\} = y^*$ which are supposed to be realisations of i.i.d. random variables $\{Y_1^*, \ldots, Y_n^*\} = Y^*$ with distribution $\hat{F}$. Using the pseudo data we can compute a realisation $G(y^*)$ of $G(Y^*) = G^*$. Repeating the whole procedure say $B$ times, we obtain realisations of random variables $G_1^*, \ldots, G_B^*$. The resulting empirical distribution of these random variables gives us an approximation of $\mathcal{L}(G(\hat{F}))$ via Monte Carlo simulation.
3.2 Methods for resampling in GLMs

According to Moulton & Zeger (1991) and Winkler (1991) we will introduce four different ways of resampling from the original data of a loglinear Poisson model to construct the bootstrap sample. The differences arise mainly in terms of different assumptions that are incorporated from the original model into the bootstrap.

The first method is the so called residual resampling method, which is based like in the classical linear model on resampling of some kind of modified Pearson residuals \( i = 1, 2, \ldots, n, \ j = 1, 2, \ldots, g \)

\[
r_{ij} = \frac{y_{ij} - \hat{\mu}_j}{\sqrt{\hat{\mu}_j(1 - \hat{\gamma}_j)}},
\]

where \( \hat{\gamma}_i = \hat{\gamma}_{i;j} \) denotes the \( i^{th} \) diagonal element of the estimated generalized hat matrix (Fahrmeir & Tutz (1994)). Then the components of the bootstrap sample \( \mathbf{y}^* \) are generated as

\[
y_{ij}^* = \hat{\mu}_j + \hat{\mu}_j r_{ij}^*,
\]

where \( \hat{F} \) would be the empirical distribution function of the \( r_{ij} \).

The second method is the so called vector resampling method, where we construct the bootstrap sample by drawing with replacement out of the original data \( \mathbf{y} \) and the corresponding covariate vectors \( \mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_g) \).

The last two methods are parametric bootstrap methods. It is also additionally assumed, that we know the kind of distribution \( F \) of the original data.

In the first case the pseudo data are generated as realisations of i.i.d. Poisson random variables

\[
Y_{ij}^* \overset{i.i.d.}{\sim} \text{Po}(\hat{\mu}_j \mid (\mathbf{Y}, \mathbf{X})).
\]

In the second case we additionally resample from the \( \mathbf{x}_j \)'s and generate the pseudo data, with \( \hat{\mu}_j^* = \exp(\hat{\beta} \mathbf{x}_j) \), as

\[
Y_{ij}^* \overset{i.i.d.}{\sim} \text{Po}(\hat{\mu}_j^* \mid (\mathbf{Y}, \mathbf{X}, \mathbf{x}_j^*)).
\]

The vector resampling method and (3.4) are recommended in the case of random covariates, because here additionally to the original data, resampling is done from the corresponding covariate values.
4 Monte Carlo Simulations

In our study, which is mainly empirical, we use Monte Carlo to simulate the truth, i.e. in our case the distributions of the GoF statistics and of the parameter estimators. Then we apply the bootstrap to obtain estimators for these distributions. For that we execute $MC = 500$ Monte Carlo runs to simulate the "true" distributions of the parameter estimator $\hat{\beta}$ of a loglinear Poisson model with given $\beta = (1.0, -0.5)^T$ and of the three GoF statistics (2.2), (2.4) and (2.5). Hereby the covariate values $x_j$ are generated once as $N(0, 1)$ pseudo random numbers and the response values $y_{ij}$ are generated as pseudo Poisson random numbers with parameter $\mu_j = \exp(x_j \beta)$ at each Monte Carlo step new. Then we apply 250 respectively 500 bootstrap simulations to obtain the bootstrap distributions of $\hat{\beta}$ and of the GoF statistics for each Monte Carlo step. The final bootstrap distribution is then computed as the average of the 500 single bootstrap distributions for $\hat{\beta}$ and for each GoF statistic. These simulations are performed with $g = 10$ and 20 and $n = 10, 20$ and 50. The parameter $\kappa$ of the power divergence statistic is chosen to be $2/3$ according to Read & Cressie (1988).

The criteria we use to evaluate the quality of the Monte Carlo and the bootstrap approximations are bias with respect to the "true" value, i.e. $\hat{\beta} - \beta$ and $\hat{\beta}^* - \hat{\beta}$ for the parameter estimators and $G(Y^*) - G(Y)$ for the GoF statistics, standard deviation and 95%-quantile of the simulated distributions. Further we compute coverage and length of 95% bootstrap percentiles (Efron & Tibshirani (1993)) respectively asymptotic theory confidence intervals, if available, for the bootstrap respectively Monte Carlo estimators of the three GoF statistics and the parameter estimator $\hat{\beta}$.

To simulate a binary logit model, we use the same $\beta$ as for the loglinear Poisson model and simulate the data $y_{ij}$ as pseudo binomial random numbers with parameters $g$ and $\pi_j = \exp(x_j \beta)/(1 + \exp(x_j \beta))$.

For implementation of overdispersion we use a two-step procedure. With given $\phi = 2.0$ we assume for the loglinear Poisson model the parameter $\mu_j$ of the Poisson distribution to be $\Gamma(a_j, b)$ with $a_j = \exp(x_j \beta) \times \phi$, $b = 1/\phi$, which leads to a negative binomial distribution of the data with $E(y_{ij}) = \mu_j$ and $Var(y_{ij}) = \mu_j + \mu_j^2/b$. For the binary logit model we assume the parameter $\pi_j$ of the Binomial distribution to be $Beta(a_j, b)$ with $a_j = \pi_j \times (g - \phi)/(\phi - 1)$, $b = (1 - \phi) \times (g - \phi)/(\phi - 1)$, which leads to a beta-binomial distribution.
5 Results

In the following figures the step function always indicates the Monte Carlo distribution, which is estimated by the residual resampling bootstrap method (solid line, SR in the tables) and the parametric bootstrap method (3.3) (dashed line, P1 in the tables). If there exists an asymptotic theory, the corresponding asymptotic distribution always is a dotted line. In tables 5.1 to 5.4 the parameters of the Monte Carlo and the bootstrap distributions are displayed.

There are various ways of bootstrap resampling which compare rather different. Also there is a difference in robustness. For the loglinear Poisson model our favourite method is the parametric bootstrap (3.3) followed by the residual resampling (3.2). They perform equal or better than the other two methods. This result also holds in the case of a binary logit model and might be the same for other GLMs. For this reason we will concentrate on these two methods only.

Generally one can state, that method (3.3) in the case of a loglinear Poisson model always slightly overestimates the distribution of the GoF statistics, whereas for the binary logit model it’s vice versa. The simple bootstrap percentile confidence intervals are always smallest with method (3.2) and own the highest coverage.

For finite \( N \) the bootstrap yields approximations to the distributions of the parameter estimator and of the GoF statistics which are at least as good than the corresponding asymptotic theory shown in figures 5.1 to 5.4. The parameter estimators are displayed in table 5.1. This holds also for the binary logit model shown in figures 5.5 to 5.8 and in table 5.3.

For \( N \) large, the bootstrap yields approximations to the distributions of the parameter estimator and of the GoF statistics which are rather close to the results of the corresponding asymptotic theory. Acting for all large sample sizes table 5.2 and figures 5.9 to 5.12 show this fact.

In the case of overdispersion or random covariates, which is not explicitly treated here, the bootstrap yields acceptable approximations for the distribution of the parameter estimator and the distributions of the GoF statistics. Here method (3.2) beats (3.3), especially in estimating the
distributions of the GoF statistics. Acting for all overdispersed models, loglinear and binary, table 5.4 and figures 5.13 to 5.16 show, that method (3.2) estimates best the wide spread distributions of the GoF statistics. Whereas all two methods compete in the same way when estimating the parameter.

The power of the bootstrap estimates can be raised by enlarging the bootstrap replications $BC$ at the cost of computing time (tables 5.1 to 5.4). But for most of the estimates a number of $BC$ between 500 and 1000 will fullfill the needs.

There are no significant differences showing which GoF statistics are best in the case of a loglinear Poisson model. They all behave in the same way, also in the case of overdispersion. Figures 5.17 and 5.18 illustrate this fact for all sample sizes.

Figure 5.1: Bootstrap Distributions of the centered parameter estimators $\hat{\beta} - \beta$ for intercept and slope of a loglinear Poisson model with $g = n = 10$, $B = 500$. 
Figure 5.2: Bootstrap Distribution of the $\chi^2$ GoF statistic of a loglinear Poisson model with $g = n = 10$, $B = 500$.

Figure 5.3: Bootstrap Distribution of the deviance GoF statistic of a loglinear Poisson model with $g = n = 10$, $B = 500$. 
Figure 5.4: Bootstrap Distribution of the power divergence GoF statistic of a loglinear Poisson model with $g = n = 10, B = 500$.

Figure 5.5: Bootstrap Distributions of the centered parameter estimators $\hat{\beta} - \beta$ for intercept and slope of a binary logit model with $g = n = 10, B = 500$. 
Figure 5.6: Bootstrap Distribution of the $\chi^2$ GoF statistic of a binary logit model with $g = n = 10, B = 500$.

Figure 5.7: Bootstrap Distribution of the deviance GoF statistic of a binary logit model with $g = n = 10, B = 500$. 
Figure 5.8: Bootstrap Distribution of the power divergence GoF statistic of a binary logit model with $g = n = 10$, $B = 500$.

Figure 5.9: Bootstrap Distributions of the centered parameter estimators $\hat{\beta} - \beta$ for intercept and slope of a loglinear Poisson model with $g = 20$, $n = 50$, $B = 500$. 
Figure 5.10: Bootstrap Distribution of the $\chi^2$ GoF statistic of a loglinear Poisson model with $g = 20$, $n = 50$, $B = 500$.

Figure 5.11: Bootstrap Distribution of the deviance GoF statistic of a loglinear Poisson model with $g = 20$, $n = 50$, $B = 500$. 
Figure 5.12: Bootstrap Distribution of the power divergence GoF statistic of a loglinear Poisson model with $g = 20$, $n = 50$, $B = 500$.

Figure 5.13: Bootstrap Distributions of the centered parameter estimators $\hat{\beta} - \beta$ for intercept and slope of an overdispersed loglinear Poisson model with $g = n = 10$, $B = 500$. 
Figure 5.14: Bootstrap Distribution of the $\chi^2$ GoF statistic of an overdispersed loglinear Poisson model with $g = n = 10$, $B = 500$.

Figure 5.15: Bootstrap Distribution of the deviance GoF statistic of an overdispersed loglinear Poisson model with $g = n = 10$, $B = 500$. 
Figure 5.16: Bootstrap Distribution of the power divergence GoF statistic of an overdispersed loglinear Poisson model with $g = n = 10$, $B = 500$.

Figure 5.17: Bootstrap Distributions of all three GoF statistic estimators of a loglinear Poisson model with $g = n = 10$, $B = 500$. 
Figure 5.18: Bootstrap Distributions of all three GoF statistic estimators of an overdispersed loglinear Poisson model with $g = n = 10$, $B = 500$. 
Table 5.1: Simulation results for a loglinear Poisson model with \( n = g = 10 \). The asymptotic theory distribution here is \( \chi^2(8) \) of which the 95\%-quantile is 15.5051.
Table 5.2: Simulation results for a loglinear Poisson model with \( n = 50, g = 20 \). The asymptotic theory distribution here is \( \chi^2(18) \) of which the 95%-quantile is 28.8693.
Table 5.3: Simulation results for a binary logit model with $n = g = 10$. The asymptotic theory distribution here is $\chi^2(8)$ of which the 95%-quantile is 15.5051.
<table>
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<th>n=g=10</th>
<th>B=250</th>
<th>B=500</th>
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<tbody>
<tr>
<td></td>
<td>MC=500</td>
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Mean of the Monte Carlo distribution:

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<tr>
<td>Mean</td>
<td>45.3331</td>
<td>45.5346</td>
<td>45.0142</td>
<td>48.3843</td>
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<td>-17.7600</td>
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Standard deviation:

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<tr>
<td>MC</td>
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<td>24.7806</td>
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95% quantile:

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Length of 95% confidence intervals:

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Coverage of 95% confidence intervals:

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Table 5.4: Simulation results for an overdispersed loglinear Poisson model with $n = g = 10$.  

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6 Conclusion

We showed how bootstrap methods can be successfully used in generalized linear models as a tool for estimating the "true" distribution of model diagnostic statistics in sparse data situations and in cases of overdispersion. The results can reliably be used in forthcoming model checking analyses. However these bootstrap methods are not implemented in standard software packages. In this paper we studied parametric models. Future work has to be done, to check the validity of the bootstrap in nonparametric regression.

References


