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# singleRcapture: An R Package for Single-Source Capture-Recapture Models

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#### Abstract

Population size estimation is a major challenge in official statistics, social sciences, and natural sciences. The problem can be tackled by applying capture-recapture methods, which vary depending on the number of sources used, particularly on whether a single or multiple sources are involved. This paper focuses on the first group of methods and introduces a novel R package: singleRcapture. The package implements state-ofthe-art single-source capture-recapture (SSCR) models (e.g. zero-truncated one-inflated regression) together with new developments proposed by the authors, and provides a user-friendly application programming interface (API). This self-contained package can be used to produce point estimates and their variance and implements several bootstrap variance estimators or diagnostics to assess quality and conduct sensitivity analysis. It is intended for users interested in estimating the size of populations, particularly those that are difficult to reach or measure, for which information is available only from one source and dual/multiple system estimation is not applicable. Our package serves to bridge a significant gap, as the SSCR methods are either not available at all or are only partially implemented in existing R packages and other open-source software. Furthermore, since many R users are familiar with countreg or VGAM packages, we have implemented a lightweight extension called singleRcaptureExtra which can be used to integrate singleRcapture with these packages.

*Keywords*: population size estimation, hidden populations, truncated distributuons, count regression models, R.

## 1. Introduction

Population size estimation is a methodological approach employed across multiple scientific disciplines, which serves as the basis for research, policy formulation, and decision-making

processes (cf. Böhning, Bunge, and Heijden 2018). In the field of statistics, particularly official statistics, precise population estimates are essential in order to develop robust economic models, optimize resource allocation, and inform evidence-based policy (cf. Baffour, King, and Valente 2013). Social scientists utilize advanced population estimation techniques to investigate hard-to-reach populations, such as homeless individuals or illicit drug users in an effort to overcome the inherent limitations of conventional census methodologies. These techniques are crucial for obtaining accurate data on populations that are typically under-represented or difficult to access using traditional sampling methods (cf. Vincent and Thompson 2022). In ecology and epidemiology, researchers focus on estimating the size of individual species or disease-affected populations within defined geographical regions as part of conservation efforts, ecosystem management, and public health interventions.

Population size estimation can be approached using various methodologies, each with distinct advantages and limitations. Traditional approaches include full enumeration (e.g. censuses) and comprehensive sample surveys, which, while providing detailed data, are often resource-intensive and may result in delayed estimates, particularly for human populations. Alternative methods leverage existing data sources, such as administrative registers or carefully designed small-scale studies in wildlife research, or census coverage surveys (cf. Wolter 1986; Zhang 2019). Information from these sources is often extracted by applying statistical methods, known as *capture-recapture* or *multiple system estimation*, which rely on data from multiple enumerations of the same population (cf. Dunne and Zhang 2024). This approach can be implemented using either a single source with repeated observations, two sources, or multiple sources.

In this paper we focus on methods that involve a single data source with multiple enumerations of the same units (cf. van der Heijden, Bustami, Cruyff, Engbersen, and van Houwelingen 2003). In human population studies, such data can be derived from police records, health system databases, or border control logs; in the case of non-human populations, data of this kind can come from veterinary records or specialized field data. These methods are often applied to estimate hard-to-reach or hidden populations, where standard sampling methods may be inappropriate because of prohibitive costs or problems with identifying population members.

While methods for two or more sources are implemented in various open-source software packages, for instance Rcapture (Baillargeon and Rivest 2007), marked (Laake, Johnson, Conn, and Isaac 2013) or VGAM (Yee, Stoklosa, and Huggins 2015), single-source capture-recapture (SSCR) methods are either not available at all or are only partially implemented in existing R packages. Therefore, the paper attempts to bridge this gap by introducing the singleRcapture and singleRcaptureExtra packages, which implement state-of-the-art SSCR methods and offer a user friendly API resembling existing R functions (e.g., glm). In the next subsection we describe existing R packages that could be used for estimating population size using SSCR methods.

#### 1.1. Software for capture-recapture with single and multiple sources

The majority of SSCR methods assume zero-truncated distributions or their extensions (e.g., inclusion of one-inflation). The **countreg** (Zeileis, Kleiber, and Jackman 2008), **VGAM** (Yee 2015) or **distributions3** (Hayes, Moller-Trane, Jordan, Northrop, Lang, and Zeileis 2024) implement some of those truncated distributions (e.g. **distributions3**::ZTPoisson

or countreg::zerotrunc) and the most general distributions, such as Generally Altered, Inflated, Truncated and Deflated, can be found in the VGAM package (e.g. VGAM::gaitdpoisson for the Poisson distribution, see Yee and Ma (2024) for a detailed description). However, the estimation of parameters of a given truncated (and possibly inflated) distribution is just the first step (as in the case of log-linear models in capture-recapture with two sources) and, to the best of our knowledge, there is no open-source software that can be used to estimate population size using on SSCR methods and includes variance estimators or diagnostics.

Therefore, the purpose of the **singleRcapture**, an R package, is to bridge this gap by providing scientists and other practitioners with a tool for estimating population size with SSCR methods. We have implemented state-of-the-art methods, as recently described by Böhning et al. (2018) or Böhning and Friedl (2024) and provided their extensions (e.g., inclusion of covariates, different treatment of one-inflation), which will be covered in detail in Section 2. The package implements variance estimation based on various methods, can be used to create custom models and diagnostic plots (e.g. rootograms) with parameters estimated using a modified iteratively reweighted least squares (IRLS) algorithm we have implemented for estimation stability. Furthermore, since many R users are familiar with **countreg** or **VGAM** packages, we have implemented a lightweight extension called **singleRcaptureExtra**, available through Github (https://github.com/ncn-foreigners/singleRcaptureExtra), which can be used to integrate **singleRcapture** with these packages. To the best of our knowledge, no existing open-source package allows the estimation of population size by selecting an appropriate SSCR model, conducting the estimation, and providing informative diagnostics of the results.

The remaining part of the paper is structured as follows. Section 2 contains a brief description of the theoretical background and information about fitting methods and available methods of variance estimation. Section 3 introduces the main functions of the package. Section 4 presents a case study and contains an assessment of its results, diagnostics and estimates of specific sub-populations. Section 5 describes classes and S3methods implemented in the package. Section 6 deals with how the package can be integrated with the countreg and VGAM packages using the singleRcaptureExtra package. The paper ends with conclusions and an appendix showing how to implement a custom model and how to use the estimatePopsizeFit function which is aimed to mimic the glm.fit or similar functions. This option could be of interest to users wishing to apply any new bootstrap methods not implemented in the package (see Appendix A.1).

# 2. Theoretical background

#### 2.1. How to estimate population size with a single register?

Let  $Y_k$  represent the number of times the k-th unit was observed in a register. Clearly, we only observe  $k: Y_k > 0$  and do not know how many units have been missed (i.e.  $Y_k = 0$ ), so the population size, denoted by N, needs to be estimated. In general, we assume that the conditional distribution of  $Y_k$  given a vector of covariates  $\boldsymbol{x}_k$  follows a version of the zero-truncated count data distribution (and its extensions). When we know the parameters of the distribution we can estimate the population size using a Horvitz-Thompson type estimator given by:

$$\hat{N} = \sum_{k=1}^{N} \frac{I_k}{\mathbb{P}[Y_k > 0 | \mathbf{X}_k]} = \sum_{k=1}^{N_{obs}} \frac{1}{\mathbb{P}[Y_k > 0 | \mathbf{X}_k]},$$
(1)

where  $I_k := \mathcal{I}_{\mathbb{N}}(Y_k)$ ,  $N_{obs}$  is the number of observed units and  $\mathcal{I}$  is the indicator function, while the maximum likelihood estimate of N is obtained after substituting regression parameters  $\boldsymbol{\beta}$  for  $\mathbb{P}[Y_k > 0 | \boldsymbol{x}_k]$  in (1).

The basic SSCR assumes independence between counts, which is a rather naive assumption, since the first capture may significantly influence the behavior of a given unit or limit the possibility of subsequent captures (e.g. due to incarceration).

To solve these issues, Godwin and Böhning (2017a) and Godwin and Böhning (2017b) introduced one-inflated distributions, which explicitly model the probability of singletons by giving additional mass  $\omega$  to singletons denoted as  $\mathcal{I}_{\{1\}}(y)$  (cf. Böhning and Friedl 2024). In other words they considered a new random variable  $Y^*$  that corresponds to the data collection process which exhibits one inflation:

$$\mathbb{P}[Y^* = y | Y^* > 0] = \omega \mathcal{I}_{\{1\}}(y) + (1 - \omega) \mathbb{P}[Y = y | Y > 0].$$

Analytic variance estimation is then performed by computing two parts of the decomposition according to the law of total variance given by:

$$\operatorname{var}[\hat{N}] = \mathbb{E}\left[\operatorname{var}\left[\hat{N}|I_1,\dots,I_n\right]\right] + \operatorname{var}\left[\mathbb{E}[\hat{N}|I_1,\dots,I_n]\right],\tag{2}$$

where the first part can be estimated using the multivariate  $\delta$  method given by:

$$\mathbb{E}\left[\operatorname{var}\left[\hat{N}|I_{1},\ldots,I_{n}\right]\right] = \left(\frac{\partial(N|I_{1},\ldots,I_{N})}{\partial\boldsymbol{\beta}}\right)^{\top}\operatorname{cov}\left[\hat{\boldsymbol{\beta}}\right]\left(\frac{\partial(N|I_{1},\ldots,I_{N})}{\partial\boldsymbol{\beta}}\right)\Big|_{\boldsymbol{\beta}=\hat{\boldsymbol{\beta}}},$$

while the second part of the decomposition in (2), assuming independence of  $I_k$ 's and after some omitted simplifications, is optimally estimated by:

$$\operatorname{var}\left[\mathbb{E}(\hat{N}|I_1,\ldots,I_n)\right] = \operatorname{var}\left[\sum_{k=1}^N \frac{I_k}{\mathbb{P}(Y_k > 0)}\right] \approx \sum_{k=1}^{N_{obs}} \frac{1 - \mathbb{P}(Y_k > 0)}{\mathbb{P}(Y_k > 0)^2},$$

which serves as the basis for interval estimation. Confidence intervals are usually constructed under the assumption of (asymptotic) normality of  $\hat{N}$  or asymptotic normality of  $\ln(\hat{N}-N)$  (or log normality of  $\hat{N}$ ). The latter is an attempt to address a common criticism of student type confidence intervals in SSCR, namely a possibly skewed distribution of  $\hat{N}$ , and results in the  $1-\alpha$  confidence interval given by:

$$\left(N_{obs} + \frac{\hat{N} - N_{obs}}{\xi}, N_{obs} + \left(\hat{N} - N_{obs}\right)\xi\right),\,$$

where:

$$\xi = \exp\left(z\left(1 - \frac{\alpha}{2}\right)\sqrt{\ln\left(1 + \frac{\widehat{\text{Var}}(\hat{N})}{\left(\hat{N} - N_{obs}\right)^2}\right)}\right),$$

and where z is the quantile function of the standard normal distribution. The estimator  $\hat{N}$  is best interpreted as being an estimator of the total number of <u>observable</u> units in the population, since we have no means of estimating the number of units in the population for which the probability of being included in the data is 0 (cf. van der Heijden *et al.* 2003).

#### 2.2. Available models

The full list of models implemented in **singleRcapture** along with corresponding expressions for probability density functions and point estimates can be found in the collective help file for all family functions:

#### R> ?ztpoisson

For the sake of simplicity, we only list the family functions together with brief descriptions. For more detailed information, please consult the relevant literature.

The current list of these family functions includes:

• Generalized Chao's (Chao 1987) and Zelterman's (Zelterman 1988) estimators via logistic regression on variable Z defined as Z = 1 if Y = 2 and Z = 0 if Y = 1 with  $Z \sim b(p)$  where  $b(\cdot)$  is the Bernoulli distribution and p can be modeled for each unit k by  $logit(p_k) = ln(\lambda_k/2)$  with Poisson parameter  $\lambda_k = x_k\beta$  (for a covariate extension see Böhning, Vidal-Diez, Lerdsuwansri, Viwatwongkasem, and Arnold (2013) and Böhning and van der Heijden (2009)):

$$\hat{N}_{\text{Chao}} = N_{obs} + \sum_{k=1}^{f_1 + f_2} \left( 2 \exp\left(\boldsymbol{x}_k \hat{\boldsymbol{\beta}}\right) + 2 \exp\left(2\boldsymbol{x}_k \hat{\boldsymbol{\beta}}\right) \right)^{-1}, \quad \text{(Chao's estimator)}$$

$$\hat{N}_{\text{Zelt}} = \sum_{k=1}^{N_{obs}} \left( 1 - \exp\left(-2 \exp\left(\boldsymbol{x}_k \hat{\boldsymbol{\beta}}\right)\right) \right)^{-1}. \quad \text{(Zelterman's estimator)}$$

where  $f_1$  and  $f_2$  denotes number of units observed once and twice.

• Zero-truncated (zt\*) and zero-one-truncated (zot\*) Poisson (cf. Böhning and van der Heijden 2019), geometric, NB type II (NB2) regression, where the non-truncated distribution is parameterized as:

$$\mathbb{P}[Y = y | \lambda, \alpha] = \frac{\Gamma(y + \alpha^{-1})}{\Gamma(\alpha^{-1}) y!} \left(\frac{\alpha^{-1}}{\alpha^{-1} + \lambda}\right)^{\alpha^{-1}} \left(\frac{\lambda}{\lambda + \alpha^{-1}}\right)^{y}.$$

• Zero-truncated one-inflated ( $ztoi^*$ ) modifications, where the count data variable  $Y^*$  is defined such that its distribution statisfies:

$$\mathbb{P}[Y^* = y] = \begin{cases} \mathbb{P}[Y = 0] & y = 0, \\ \omega (1 - \mathbb{P}[Y = 0]) + (1 - \omega) \mathbb{P}[Y = 1] & y = 1, \\ (1 - \omega) \mathbb{P}[Y = y] & y > 1, \end{cases}$$

$$\mathbb{P}[Y^* = y | Y^* > 0] = \omega \mathcal{I}_{\{1\}}(y) + (1 - \omega) \mathbb{P}[Y = y | Y > 0].$$

• One-inflated zero-truncated (oizt\*) modifications, where the count data variable  $Y^*$  is defined as:

$$\begin{split} \mathbb{P}\left[Y^* = y\right] &= \omega \mathcal{I}_{\{1\}}(y) + (1 - \omega) \mathbb{P}[Y = y], \\ \mathbb{P}\left[Y^* = y | Y^* > 0\right] &= \omega \frac{\mathcal{I}_{\{1\}}(y)}{1 - (1 - \omega) \mathbb{P}[Y = 0]} + (1 - \omega) \frac{\mathbb{P}[Y = y]}{1 - (1 - \omega) \mathbb{P}[Y = 0]}. \end{split}$$

Note that ztoi\* and oizt\* distributions are equivalent, in the sense that the maximum value of the likelihood function is equal for both of those distributions given any data, as shown by Böhning (2023) but population size estimators are different.

In addition, we propose two new approaches to model singletons in a similar way as in hurdle models. In particular, we have proposed the following:

 The zero-truncated hurdle model (ztHurdle\*) for Poisson, geometric and NB2 is defined as:

$$\mathbb{P}[Y^* = y] = \begin{cases} \frac{\mathbb{P}[Y=0]}{1 - \mathbb{P}[Y=1]} & y = 0, \\ \pi(1 - \mathbb{P}[Y=1]) & y = 1, \\ (1 - \pi)\frac{\mathbb{P}[Y=y]}{1 - \mathbb{P}[Y=1]} & y > 1, \end{cases}$$

$$\mathbb{P}\left[Y^* = y | Y^* > 0\right] = \pi \mathcal{I}_{\{1\}}(y) + (1 - \pi) \mathcal{I}_{\mathbb{N} \setminus \{1\}}(y) \frac{\mathbb{P}[Y = y]}{1 - \mathbb{P}[Y = 0] - \mathbb{P}[Y = 1]}.$$

where  $\pi$  denotes the conditional probability of observing singletons.

• The hurdle zero-truncated model (Hurdlezt\*) for Poisson, geometric and NB2 is defined as:

$$\begin{split} \mathbb{P}\left[Y^* = y\right] &= \begin{cases} \pi & y = 1, \\ (1 - \pi) \frac{\mathbb{P}[Y = y]}{1 - \mathbb{P}[Y = 1]} & y \neq 1, \end{cases} \\ \mathbb{P}\left[Y^* = y \middle| Y^* > 0\right] &= \begin{cases} \pi \frac{1 - \mathbb{P}[Y = 1]}{1 - \mathbb{P}[Y = 0] - \mathbb{P}[Y = 1]} & y = 1, \\ (1 - \pi) \frac{\mathbb{P}[Y = y]}{1 - \mathbb{P}[Y = 0] - \mathbb{P}[Y = 1]} & y > 1, \end{cases} \end{split}$$

where  $\pi$  denotes the unconditional probability of observing singletons.

The approaches presented above differ in their assumptions, computational complexity, or in the way they treat heterogeneity of captures and singletons. For instance, the dispersion parameter  $\alpha$  in the NB2 type models is often interpreted as measuring the *severity* of unobserved heterogeneity in the underlying Poisson process (cf. Cruyff and van der Heijden 2008). When using any truncated NB model, the hope is that given the class of models considered, the consistency is not lost despite the lack of information.

While not discussed in the literature, the interpretation of heterogeneous  $\alpha$  across the population (specified in controlModel) would be that the unobserved heterogeneity affects the accuracy of the prediction for the dependent variable Y more severely than others. The geometric model (NB with  $\alpha=1$ ) is singled out in the package and often considered in the literature because of inherent computational issues with NB models, which are exacerbated

by the fact that data used for SSCR are usually of rather low quality. Data sparsity is a particularly common problem in SSCR and a big challenge for all numerical methods for fitting the (zero-truncated) NB model.

The extra mass  $\omega$  in one-inflated models is an important extension to the researcher's toolbox for SSCR models, since the inflation at y=1 is likely to occur in many types of applications. For example, when estimating the number of active people who committed criminal acts in a given time period, the fact of being captured for the first time following an arrest is associated with the risk of no longer being able to be captured a second time. One constraint present in modelling via inflated models is that attempts to include both the possibility of one inflation and one deflation lead to both numerical and inferential problems since the parameter space (of  $(\omega, \lambda)$  or  $(\omega, \lambda, \alpha)$ ) is then given by  $\{(\omega, \lambda, \alpha) | \forall x \in \mathbb{N} : p(x|\omega, \lambda, \alpha) \geq 0\}$  for the probability mass function p. The boundary of this set is then a 1 or 2—dimentional manifold, transforming this parameter space into  $\mathbb{R}^3$  would require using "link" functions that depend on more than one parameter.

Hurdle models represent another approach to modelling one-inflation. They can also model deflation as well as inflation and deflation simultaneously, so they are more flexible and, in the case of hurdle zero-truncated models, appear to be more numerically stable.

Although the question of how to interpret regression parameters tends to be somewhat overlooked in SSCR studies, we should point out that the interpretation of the  $\omega$  inflation parameter (in ztoi\* or oizt\*) is more convenient than the interpretation of the  $\pi$  probability parameter (in hurdle models). Additionally, the interpretation of the  $\lambda$  parameter in (one) inflated models conforms to the following intuition: given that unit k comes from the noninflated part of the population, it follows a Poisson distribution (respectively geometric or negative binomial) with the  $\lambda$  parameter (or  $\lambda, \alpha$ ); no such interpretation exists for hurdle models. Interestingly, estimates from hurdle zero-truncated and one-inflated zero-truncated models tend to be quite close to one another, although more rigorous studies are required to confirm this observation.

#### 2.3. Fitting method

As previously noted, the **singleRcapture** package can be used to model the (linear) dependence of all parameters on covariates. A modified IRLS algorithm is employed for this purpose as presented in Algorithm 1; full details are available in Yee (2015). In order to apply the algorithm, a modified model matrix  $X_{\rm vlm}$  is created when the estimatePopsize function is called. In the context of the models implemented in **singleRcapture**, this matrix can be written as:

$$\boldsymbol{X}_{\text{vlm}} = \begin{pmatrix} \boldsymbol{X}_1 & \boldsymbol{0} & \dots & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{X}_2 & \dots & \boldsymbol{0} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{0} & \boldsymbol{0} & \dots & \boldsymbol{X}_p \end{pmatrix}$$
(3)

where each  $X_i$  corresponds to a model matrix associated with a user specified formula.

In the case of multi-parameter families, we get a matrix of linear predictors  $\eta$  instead of a vector, with the number of columns matching the number of parameters in the distribution.

## Algorithm 1: The modified IRLS algorithm used in the singleRcapture package

- 1 Initialize with iter $\leftarrow 1, \eta \leftarrow$ start,  $W \leftarrow I, \ell \leftarrow \ell(\beta)$ .
- 2 Store values from the previous step:  $\ell_- \leftarrow \ell, W_- \leftarrow W, \beta_- \leftarrow \beta$  (the last assignment is omitted during the first iteration), and assign values in the current iteration

$$oldsymbol{\eta} \leftarrow oldsymbol{X}_{ ext{vlm}}oldsymbol{eta} + oldsymbol{o}, oldsymbol{W}_{(k)} \leftarrow \mathbb{E}\left[ -rac{\partial^2 \ell}{\partial oldsymbol{\eta}_{(k)}^ op \partial oldsymbol{\eta}_{(k)}} 
ight], oldsymbol{Z}_{(k)} \leftarrow oldsymbol{\eta}_{(k)} + rac{\partial \ell}{\partial oldsymbol{\eta}_{(k)}} oldsymbol{W}_{(k)}^{-1} - oldsymbol{o}_{(k)},$$

where o denotes offset.

- 3 Assign the current coefficient value:  $\beta \leftarrow (X_{\text{vlm}}WX_{\text{vlm}})^{-1}X_{\text{vlm}}WZ$ .
- 4 If  $\ell(\beta) < \ell(\beta_-)$  try selecting the smallest value h such that for  $\beta_h \leftarrow 2^{-h} (\beta + \beta_-)$  the inequality  $\ell(\beta_h) > \ell(\beta_-)$  holds if this is successful  $\beta \leftarrow \beta_h$ , else stop the algorithm.
- 5 If convergence is achieved or iter is higher than maxiter, stop the algorithm, else iter ← 1+iter and return to step 2.

"Weights" (matrix  $\boldsymbol{W}$ ) are then modified to be information matrices  $\mathbb{E}\left[-\frac{\partial^2 \ell}{\partial \boldsymbol{\eta}_{(k)}^{\top} \partial \boldsymbol{\eta}_{(k)}}\right]$ , where  $\ell$  is the log-likelihood function and  $\boldsymbol{\eta}_{(k)}$  is the k-th row of  $\boldsymbol{\eta}$ , while in the typical IRLS they are scalars  $\mathbb{E}\left[-\frac{\partial^2 \ell}{\partial \eta_k^2}\right]$ , which is often just  $-\frac{\partial^2 \ell}{\partial \eta^2}$ .

## 2.4. Bootstrap variance estimators

We have implemented three types of bootstrap algorithms: parametric, semi-parametric and nonparametric. The nonparametric version is the usual bootstrap algorithm, as noted in Norris and Pollock (1996) and Zwane and Van der Heijden (2003). In this section, the focus is on the latter two approaches.

The idea of semi-parametric bootstrap is to modify the usual bootstrap to include the additional uncertainty resulting from the fact that the sample size is a random variable. This type of bootstrap is performed in steps listed in Algorithm 2.

#### Algorithm 2: Semi-parametric bootstrap

- 1 Draw a sample of size  $N'_{obs} \sim \text{Binomial}\left(N', \frac{N_{obs}}{N'}\right)$ , where  $N' = \lfloor \hat{N} \rfloor + \text{Bernoulli}\left(\lfloor \hat{N} \rfloor \hat{N}\right)$ .
- **2** Draw  $N'_{obs}$  units from the data uniformly without replacement.
- **3** Obtain a new population size estimate  $N_b$  using bootstrap data.
- 4 Repeat 1-3 steps B times.

In other words, we first draw a sample size and then a sample conditional on the sample size. Note that when using the semi-parametric bootstrap one implicitly assumes that the population size estimate  $\hat{N}$  is accurate. The last implemented bootstrap type is the parametric algorithm, which first draws a finite population of size  $\approx \hat{N}$  from the superpopulation model and then samples from this population according to the selected model, as described in Algorithm 3.

Note that in order for this type of algorithm to result in consistent standard error estimates, it is imperative that the estimated model for the entire superpopulation probability space is consistent, which may be much less realistic than in the case of the semi-parametric bootstrap. The parametric bootstrap algorithm is the default option in **singleRcapture**.

#### Algorithm 3: Parametric bootstrap

- 1 Draw the number of covariates equal to  $\lfloor \hat{N} \rfloor + \text{Bernoulli} \left( \lfloor \hat{N} \rfloor \hat{N} \right)$  proportional to the estimated contribution  $(\mathbb{P} [Y_k > 0 | \boldsymbol{x}_k])^{-1}$  with replacement.
- **2** Using the fitted model and regression coefficients  $\hat{\beta}$  draw for each covariate the Y value from the corresponding probability measure on  $\mathbb{N} \cup \{0\}$ .
- **3** Truncate units with the drawn Y value equal to 0.
- 4 Obtain a population size estimate  $N_b$  based on the truncated data.
- **5** Repeat 1-4 steps B times.

## 3. The main function

#### 3.1. The estimatePopsize function

The singleRcapture package is built around the estimatePopsize function. The main design objective was to make using estimatePopsize as similar as possible to the standard stats::glm function or packages for fitting zero-truncated regression models, such as countreg (e.g. countreg::zerotrunc function). The estimatePopsize function is used to first fit an appropriate (vector) generalized linear model and to estimate the population size along with its variance. It is assumed that the response vector (i.e. the dependent variable) corresponds to the number of times a given unit was observed in the source. The most important arguments are given in Table 1; the obligatory ones are formula, data, model.

An important step in using estimatePopsize is specifying the model parameter, which indicates the type of model that will be used for estimating the *unobserved* part of the population. For instance, to fit Chao's or Zelterman's model one should select chao or zelterman and, assuming that one-inflation is present, one can select one of the zero-truncated one-inflated (ztoi\*) or one-inflated zero-truncated (oizt\*) models, such as oiztpoisson for Poisson or ztoinegbin for NB2.

If it is assumed that heterogeneity is observed for NB2 models, one can specify the formula in the controlModel argument with the controlModel function and the alphaFormula argument. This enables the user to provide a formula for the dispersion parameter in the NB2 models. If heterogeneity is assumed for ztoi\* or oizt\*, one can specify the omegaFormula argument, which corresponds to the  $\omega$  parameter in these models. Finally, if covariates are assumed to be available for the hurdle models (ztHurdle\* or Hurdlezt\*), then piFormula can be specified, as it provides a formula for the probability parameter in these models.

#### 3.2. Controlling variance estimation with controlPopVar

The estimatePopsize function makes it possible to specify the variance estimation method via popVar (e.g. analytic or variance bootstrap) and control the estimation process by specifying controlPopVar. In the control function controlPopVar the user can specify the bootType argument, which has three possible values: "parametric", "semi-parametric" and "nonparametric". Additional arguments accepted by the contorlPopVar function, which are relevant to bootstrap, include:

alpha, B – the significance level and the number of bootstrap samples to be performed,

Argument	Description
formula	The main formula (i.e for the Poisson $\lambda$ parameter);
data	a data.frame (or data.frame coercible) object;
model	either a function a string or a family class object specifying which model should be used; possible values are listed in the documen-
	tation. The supplied argument should have the form model =
	"ztpoisson", model = ztpoisson, or if a link function should be
	specified, then model = ztpoisson(lambdaLink = "log") can
	be used;
method	a numerical method used to fit regression IRLS or optim;
popVar	a method for estimating variance of $\hat{N}$ and creating confidence in-
	tervals (either bootstrap, analytic or skipping the estimation en-
	tirely);
${\tt controlMethod},$	control parameters for numerical fitting, specifying additional for-
$\verb controlModel  or \\$	mulas (inflation, dispersion) and population size estimation, re-
${\tt controlPopVar}$	spectively;
offset	a matrix of offset values with the number of columns matching the
	number of distribution parameters providing offset values to each
	of linear predictors;
• • •	additional optional arguments passed to other methods eg.
	estimatePopsizeFit;

Table 1: A description of estimatePopsize function arguments

respectively, with 0.05 and 500 being the default options.

- cores the number of process cores to be used in bootstrap (1 by default); parallel computing is enabled by doParallel (Microsoft and Weston 2022a), foreach (Microsoft and Weston 2022b) and parallel packages (R Core Team 2023).
- keepbootStat a logical value indicating whether to keep a vector of statistics produced by the bootstrap.
- traceBootstrapSize, bootstrapVisualTrace logical values indicating whether sample and population size should be tracked (FALSE by default); these work only when cores = 1.
- fittingMethod, bootstrapFitcontrol the fitting method (by default the same as the one used in the original call) and control parameters (controlMethod) for model fitting in the bootstrap.

In addition, the user can specify the type of confidence interval by means of confType and the type of covariance matrix by using covType for the analytical variance estimator (observed or the Fisher information matrix).

In the next sections we present a case study involving the use of a simple zero-truncated Poisson regression and a more advanced model: one-inflated zero-truncated geometric regression with the cloglog link function. First, we present the example dataset, then we describe how

to estimate the population size and assess the quality and diagnostics measures. Finally, we show how to estimate the population size in user-specified sub-populations.

## 4. Data analysis example

The package can be installed in the standard manner using:

```
R> install.packages("singleRcapture")
```

Then, we need to load the package using the following code:

```
R> library(singleRcapture)
```

#### 4.1. Dataset

We use a dataset from van der Heijden *et al.* (2003), which contains information about immigrants in four Dutch cities (Amsterdam, Rotterdam, The Hague and Utrecht), who were staying in the country without a legal permit in 1995 and appeared in police records for that year. This dataset is included in the package called netherlandsimmigrant:

```
R> data(netherlandsimmigrant)
R> head(netherlandsimmigrant)
```

	capture	gender	age		reason		nation
1	1	male	<40yrs	Other	reason	${\tt North}$	${\tt Africa}$
2	1	male	<40yrs	Other	reason	${\tt North}$	${\tt Africa}$
3	1	male	<40yrs	Other	reason	${\tt North}$	${\tt Africa}$
4	1	male	<40yrs	Other	reason		Asia
5	1	${\tt male}$	<40yrs	Other	reason		Asia
6	2	${\tt male}$	<40yrs	Other	reason	North	Africa

The number of times each individual appeared in the records is included in the capture variable. The available covariates include gender, age, reason, nation; the last two represent the reason for being captured and the region of the world a given person comes from:

## R> summary(netherlandsimmigrant)

```
capture
                   gender
                                   age
                                                      reason
Min.
       :1.000
                female: 398
                               <40yrs:1769
                                             Illegal stay: 259
                male :1482
1st Qu.:1.000
                               >40yrs: 111
                                             Other reason:1621
Median :1.000
Mean
     :1.162
3rd Qu.:1.000
Max. :6.000
                   nation
```

American and Australia: 173
Asia : 284
North Africa :1023
Rest of Africa : 243
Surinam : 64
Turkey : 93

One notable characteristic of this dataset is that it contains a disproportionately large number of individuals who were observed only once (i.e. 1645).

## R> table(netherlandsimmigrant\$capture)

```
1 2 3 4 5 6
1645 183 37 13 1 1
```

The basic syntax of estimatePopsize is very similar to that of glm, the same can be said about the output of the summary method except for additional results of population size estimates (denoted as Population size estimation results).

```
R> basicModel <- estimatePopsize(
+ formula = capture ~ gender + age + nation,
+ model = ztpoisson(),
+ data = netherlandsimmigrant,
+ controlMethod = controlMethod(silent = TRUE)
+ )
R> summary(basicModel)
```

#### Call:

#### Pearson Residuals:

```
Min. 1st Qu. Median Mean 3rd Qu. Max. -0.486442 -0.486442 -0.298080 0.002093 -0.209444 13.910844
```

#### Coefficients:

-----

For linear predictors associated with: lambda

	Estimate	Std. Error	z value	P(> z )	
(Intercept)	-1.3411	0.2149	-6.241	4.35e-10	***
gendermale	0.3972	0.1630	2.436	0.014832	*
age>40yrs	-0.9746	0.4082	-2.387	0.016972	*
nationAsia	-1.0926	0.3016	-3.622	0.000292	***
nationNorth Africa	0.1900	0.1940	0.979	0.327398	

```
0.3008 -3.027 0.002468 **
nationRest of Africa -0.9106
nationSurinam
                     -2.3364
                                 1.0136
                                        -2.305 0.021159 *
                     -1.6754
nationTurkey
                                 0.6028 -2.779 0.005445 **
Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
AIC: 1712.901
BIC: 1757.213
Residual deviance: 1128.553
Log-likelihood: -848.4504 on 1872 Degrees of freedom
Number of iterations: 8
______
Population size estimation results:
Point estimate 12690.35
Observed proportion: 14.8% (N obs = 1880)
Std. Error 2808.165
95% CI for the population size:
         lowerBound upperBound
normal
           7186.449
                      18194.25
                      19718.31
logNormal
           8431.277
95% CI for the share of observed population:
          lowerBound upperBound
normal
           10.332933
                      26.16035
logNormal
           9.534288
                      22.29793
```

The output regarding the population size contains the point estimate, the observed proportion (based on the input dataset), the standard error and two confidence intervals: one relating to the point estimate, the second – to the observed proportion.

According to this simple model, the population size is about 12,500, with about 15% of units observed in the register. The 95% CI under normality indicates that the true population size is likely to be between 7,000-18,000, with about 10-26% of the target population observed in the register.

Since there is a reasonable suspicion that the act of observing a unit in the dataset may lead to undesirable consequences for the person concerned (in this case, a possible deportation, detention or something similar). For these reasons, the user may consider one-inflated models, such as one-inflated zero-truncated geometric model (specified by oiztgeom family) and those presented below.

```
),
        popVar = "bootstrap",
        controlPopVar = controlPopVar(bootType = "semiparametric")
+ )
R> summary(modelInflated)
Call:
estimatePopsize.default(formula = capture ~ nation, data = netherlandsimmigrant,
     model = oiztgeom(omegaLink = "cloglog"), popVar = "bootstrap",
     controlModel = controlModel(omegaFormula = ~gender + age),
     controlPopVar = controlPopVar(bootType = "semiparametric"))
Pearson Residuals:
     Min. 1st Qu. Median Mean 3rd Qu.
-0.41643 -0.41643 -0.30127 0.00314 -0.18323 13.88376
Coefficients:
For linear predictors associated with: lambda
                          Estimate Std. Error z value P(>|z|)
(Intercept)
                         -1.2552 0.2149 -5.840 5.22e-09 ***

      nationAsia
      -0.8193
      0.2544
      -3.220
      0.00128
      **

      nationNorth Africa
      0.2057
      0.1838
      1.119
      0.26309

      nationRest of Africa
      -0.6692
      0.2548
      -2.627
      0.00862
      **

      nationSurinam
      -1.5205
      0.6271
      -2.425
      0.01532
      *

      nationTurkey
      -1.1888
      0.4343
      -2.737
      0.00619
      **

For linear predictors associated with: omega
              Estimate Std. Error z value P(>|z|)
(Intercept) -1.4577 0.3884 -3.753 0.000175 ***
gendermale -0.8738
                              0.3602 -2.426 0.015267 *
age>40yrs 1.1745 0.5423 2.166 0.030326 *
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
AIC: 1677.125
BIC: 1726.976
Residual deviance: 941.5416
Log-likelihood: -829.5625 on 3751 Degrees of freedom
Number of iterations: 10
 _____
Population size estimation results:
Point estimate 6699.953
Observed proportion: 28.1% (N obs = 1880)
Boostrap sample skewness: 1.621389
```

```
O skewness is expected for normally distributed variable
---
Bootstrap Std. Error 1719.353
95% CI for the population size:
lowerBound upperBound
5001.409 11415.969
95% CI for the share of observed population:
lowerBound upperBound
16.46816 37.58941
```

According to this approach, the population size is about 7000, which is about 5000 less than in the case of the naive Poisson approach. A comparison of AIC and BIC suggests that the one-inflation model fits the data better with BIC for oiztgeom 1727 and 1757 for ztpoisson. We can access population size estimates using the following code, which returns a list with numerical results.

```
R> popSizeEst(basicModel) #basicModel$populationSize
```

```
Point estimate: 12690.35 Variance: 7885790
```

95% confidence intervals:

lowerBound upperBound normal 7186.449 18194.25 logNormal 8431.277 19718.31

R> popSizeEst(modelInflated) #modelInflated\$populationSize

```
Point estimate: 6699.953
Variance: 2956175
95% confidence intervals:
lowerBound upperBound
5001.409 11415.969
```

The decision whether to use a zero-truncated Poisson or one-inflated zero-truncated geometric model should be based on the assessment of the model and the assumptions regarding the data generation process. One possible method of selection is based on the likelihood ratio test, which can be computed quickly and conveniently with the **lmtest** (Zeileis and Hothorn (2002)) interface:

```
R> library(lmtest)
```

Likelihood ratio test

```
Model 1: Basic model

Model 2: Inflated model

#Df LogLik Df Chisq Pr(>Chisq)

1 8 -848.45

2 9 -829.56 1 37.776 7.936e-10 ***
---

Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

However, the above is not a standard method of model selection in SSCR. The next sections are dedicated to a detailed description of how to assess the results using standard statistical tests and diagnostics.

#### 4.2. Testing marginal frequencies

A popular method of testing the model fit in single source capture-recapture studies consists in comparing the fitted marginal frequencies  $\sum_{j=1}^{N_{obs}} \hat{\mathbb{P}}[Y_j = k | \boldsymbol{x}_j, Y_j > 0]$  with the observed

marginal frequencies  $\sum_{j=1}^{N} \mathcal{I}_{\{k\}}(Y_j) = \sum_{j=1}^{N_{obs}} \mathcal{I}_{\{k\}}(Y_j)$  for  $k \geq 1$ . If the fitted model bears sufficient

resemblance to the real data collection process, these quantities should be quite close and both G and  $\chi^2$  tests can be used to test the statistical significance of the discrepancy with the following **singleRcapture** syntax for the Poisson model (rather poor fit):

```
R> margFreq <- marginalFreq(basicModel)
R> summary(margFreq, df = 1, drop15 = "group")
```

Test for Goodness of fit of a regression model:

```
Test statistics df P(>X^2)
Chi-squared test 50.06 1 1.5e-12
G-test 34.31 1 4.7e-09
```

-----

```
Cells with fitted frequencies of < 5 have been grouped Names of cells used in calculating test(s) statistic: 1 2 3
```

and for the one-inflated model (better fit):

```
R> margFreq_inf <- marginalFreq(modelInflated)
R> summary(margFreq_inf, df = 1, drop15 = "group")
```

Test for Goodness of fit of a regression model:

```
Test statistics df P(>X^2)
```

Chi-squared test	1.88	1	0.17
G-test	2.32	1	0.13

-----

```
Cells with fitted frequencies of < 5 have been grouped Names of cells used in calculating test(s) statistic: 1 2 3 4
```

where the drop15 argument is used to indicate how to handle cells with less than 5 fitted observations. Note, however, that currently there is no continuity correction.

## 4.3. Diagnostics

The singleRStaticCountData class has a plot method implementing several types of quick demonstrative plots, such as the rootogram (cf. Kleiber and Zeileis 2016), for comparing fitted and marginal frequencies, which can be generated with the following syntax:

```
R> plot( basicModel, plotType = "rootogram", main = "ZT Poisson model")
R> plot(modelInflated, plotType = "rootogram", main = "OI ZT Geometric model")
```

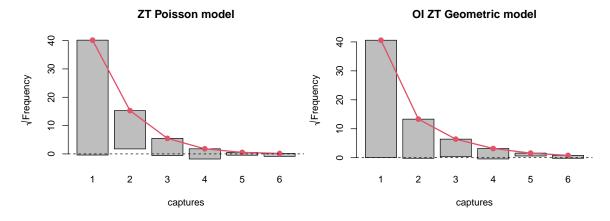


Figure 1: Rootograms for ztpoisson (left) and oiztgeom (right) models

The above plots suggest that the oiztgeom model fits the data better. Another important issue in population size estimation is to conduct model diagnostics in order to verify whether influential observations are present in the data. For this purpose the leave-one-out (LOO) diagnostic implemented in the dfbeta from the stats package has been adapted as shown below (multiplied by a factor of a hundred for better readability):

```
R> dfb <- dfbeta(basicModel)
R> round(t(apply(dfb, 2, quantile)*100), 4)
```

	0%	25%	50%	75%	100%
(Intercept)	-0.9909	-0.1533	0.0191	0.0521	8.6619
gendermale	-9.0535	-0.0777	-0.0283	0.1017	2.2135
age>40yrs	-2.0010	0.0179	0.0379	0.0691	16.0061

```
      nationAsia
      -9.5559
      -0.0529
      0.0066
      0.0120
      17.9914

      nationNorth Africa
      -9.6605
      -0.0842
      -0.0177
      0.0087
      3.1260

      nationRest of Africa
      -9.4497
      -0.0244
      0.0030
      0.0083
      10.9787

      nationSurinam
      -9.3138
      -0.0065
      0.0021
      0.0037
      99.3383

      nationTurkey
      -9.6198
      -0.0220
      0.0079
      0.0143
      32.0980
```

```
R> dfi <- dfbeta(modelInflated)
R> round(t(apply(dfi, 2, quantile)*100), 4)
```

```
0%
                                 25%
                                         50%
                                                 75%
                                                        100%
(Intercept)
                      -1.4640 0.0050
                                      0.0184
                                              0.0557
                                                      9.0600
nationAsia
                      -6.6331 -0.0346
                                              0.0347 12.2406
                                      0.0157
nationNorth Africa
                     -7.2770 -0.0768 -0.0170
                                              0.0085
                                                      1.9415
nationRest of Africa -6.6568 -0.0230 0.0081
                                              0.0262 7.1710
nationSurinam
                     -6.2308 -0.0124 0.0162
                                              0.0421 62.2045
nationTurkey
                     -6.4795 -0.0273 0.0204
                                              0.0462 21.1338
(Intercept):omega
                      -6.8668 -0.0193 0.0476
                                              0.0476 9.3389
gendermale:omega
                     -2.2733 -0.2227
                                      0.1313
                                              0.2482 11.1234
age>40yrs:omega
                    -30.2130 -0.2247 -0.1312 -0.0663
```

The result of the dfbeta can be further used in the dfpopsize function, which can be used to quantify LOO on the population size. Note the warning when the bootstap variance estimation is applied.

```
R> dfb_pop <- dfpopsize(basicModel, dfbeta = dfb)
R> dfi_pop <- dfpopsize(modelInflated, dfbeta = dfi)
R> summary(dfb_pop)
```

```
Min. 1st Qu. Median Mean 3rd Qu. Max. -4236.407 2.660 2.660 5.445 17.281 117.445
```

R> summary(dfi\_pop)

```
Min. 1st Qu. Median Mean 3rd Qu. Max. -456.6443 -3.1121 -0.7243 3.4333 5.1535 103.5949
```

Figure 2 shows a comparison of the effect of deleting an observation on the population size estimate and inverse probability weights, which refer to the contribution of a given observation to the population size estimate:

```
R> plot(basicModel, plotType = "dfpopContr",
+ dfpop = dfb_pop, xlim = c(-4500, 150))
R> plot(modelInflated, plotType = "dfpopContr",
+ dfpop = dfi_pop, xlim = c(-4500, 150))
```

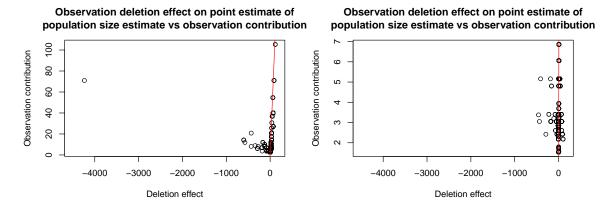


Figure 2: Results for ztpoisson (left) and oiztgeom (right) model

These plots show how the population size changes if a given observation is removed. For instance, if we remove observation 542, then the population size will increase by about 4236 for the ztpoisson model. In the case of oiztgeom, the largest change is equal to 457 for observation 900.

The full list of plot types along with the list of optional arguments that can be passed from the call to the plot method down to base R and **graphics** functions can be found in the help file of the plot method.

R> ?plot.singleRStaticCountData

## 4.4. The stratifyPopsize function

Researchers may be interested not only in the total population size but also in the size of specific sub-populations (e.g. males, females, particular age groups). For this reason we have created the stratifyPopsize function, which estimates the size by strata defined by the coefficients in the model (the default option). The following output presents results based on the ztpoisson and oiztgeom models.

```
R> popSizestrata <- stratifyPopsize(basicModel)</pre>
R> cols <- c("name", "Observed", "Estimated", "logNormalLowerBound",
+
             "logNormalUpperBound")
R> popSizestrata_report <- popSizestrata[, cols]</pre>
R> cols_custom <- c("Name", "Obs", "Estimated", "LowerBound", "UpperBound")
R> names(popSizestrata_report) <- cols_custom</pre>
R> popSizestrata_report
                              Name
                                     Obs
                                          Estimated LowerBound UpperBound
1
                    gender==female
                                    398
                                          3811.0911
                                                     2189.0443
                                                                   6902.133
2
                      gender==male 1482
                                          8879.2594
                                                     6090.7762
                                                                 13354.880
3
                       age==<40yrs 1769 10506.8971
                                                      7359.4155
                                                                  15426.455
                       age==>40yrs
4
                                     111
                                          2183.4535
                                                       872.0130
                                                                   5754.876
   nation==American and Australia
                                           708.3688
                                                       504.6086
                                                                   1037.331
                                     173
```

```
6
                     nation==Asia 284 2742.3147 1755.2548
                                                               4391.590
7
             nation==North Africa 1023 3055.2033 2697.4900
                                                               3489.333
           nation==Rest of Africa 243 2058.1533 1318.7466
                                                               3305.786
9
                  nation==Surinam
                                    64 2386.4513
                                                    505.2457
                                                              12287.983
                                    93 1739.8592
                                                               5068.959
10
                   nation==Turkey
                                                    638.0497
R> popSizestrata_inflated <- stratifyPopsize(modelInflated)</pre>
R> popSizestrata inflated report <- popSizestrata inflated[, cols]
R> names(popSizestrata_inflated_report) <- cols_custom</pre>
R> popSizestrata_inflated_report
```

```
Name Obs Estimated LowerBound UpperBound
1 nation==American and Australia 173 516.2432
                                                370.8463
                                                          768.4919
                    nation==Asia 284 1323.5377
                                                831.1601 2258.9954
3
            nation==North Africa 1023 2975.8801 2254.7071 4119.3050
          nation==Rest of Africa 243 1033.9753 667.6106 1716.4484
4
5
                 nation==Surinam
                                  64 354.2236 193.8891
                                                         712.4739
6
                                                283.1444 947.5309
                  nation==Turkey
                                  93 496.0934
7
                  gender==female 398 1109.7768
                                                778.7197 1728.7066
8
                    gender==male 1482 5590.1764 3838.4550 8644.0776
9
                     age==<40yrs 1769 6437.8154 4462.3472 9862.2147
                     age==>40yrs 111
10
                                     262.1379
                                                 170.9490
                                                           492.0347
```

The stratifyPopsize function prepared to handle objects of the singleRStaticCountData class, accepts three optional parameters strata, alpha, cov, which are used for specifying sub-populations, significance levels and the covariance matrix to be used for computing standard errors. An example of the full call is presented below.

```
R> library(sandwich)
R> popSizestrataCustom <- stratifyPopsize(</pre>
    object = basicModel,
    strata = ~ gender + age,
            = rep(c(0.1, 0.05), each=2),
    alpha
    cov
            = vcovHC(basicModel, type = "HC4")
+ )
R>
R> popSizestrataCustom_report <- popSizestrataCustom[, c(cols, "confLevel")]</pre>
R> names(popSizestrataCustom_report) <- c(cols_custom, "alpha")</pre>
R> popSizestrataCustom_report
            Name Obs Estimated LowerBound UpperBound alpha
1 gender==female 398
                       3811.091 2275.6416
                                            6602.161
                                                       0.10
    gender==male 1482 8879.259 6261.5125 12930.751
                                                       0.10
     age==<40yrs 1769 10506.897 7297.2081 15580.138 0.05
3
     age==>40yrs 111 2183.453
                                  787.0676
                                            6464.009 0.05
```

We have provided integration with the sandwich (Zeileis, Köll, and Graham 2020) package to correct the variance-covariance matrix in the  $\delta$  method. In the code we have used the vcovHC method for singleRStaticCountData class from the sandwich package, different significance levels for confidence intervals in each stratum and a formula to specify that we want estimates for both males and females to be grouped by nation and age. The strata parameter can be specified either as:

- a formula with the empty left hand side, as shown in the example above (e.g. ~ gender
   \* age),
- a logical vector with the number of entries equal to the number of rows in the dataset, in which case only one stratum will be created (e.g. netherlandsimmigrant\$gender == "male"),
- a vector of names of explanatory variables, which will result in every level of the explanatory variable having its own sub-population for each variable specified (e.g. c("gender", "age")),
- not supplied at all, in which case strata will correspond to levels of each factor in the data without any interactions (string vectors will be converted to factors for the convenience of the user),
- a (named) list where each element is a logical vector; names of the list will be used to specify variable names in the returned object, for example:

```
R> list(
+ "Stratum 1" = netherlandsimmigrant$gender == "male" &
+ netherlandsimmigrant$nation == "Suriname",
+ "Stratum 2" = netherlandsimmigrant$gender == "female" &
+ netherlandsimmigrant$nation == "North Africa"
+ )
```

One can also specify plotType = "strata" in the plot function, which results in a plot with point and CI estimates of the population size.

```
R> par(mar = c(2.5, 8.5, 4.1, 2.5), cex.main = .7, cex.lab = .6)
R> plot(basicModel, plotType = "strata")
R> plot(modelInflated, plotType = "strata")
```

Only the logNormal type of confidence interval is used for plotting since the studentized confidence intervals often result in negative lower bounds.

#### 5. Classes and S3Methods

We have created a number of classes: singleRStaticCountData, singleR in the package (for the time being the two classes are the same, the distinction is made for future development), singleRfamily, popSizeEstResults, summarysingleRStaticCountData and

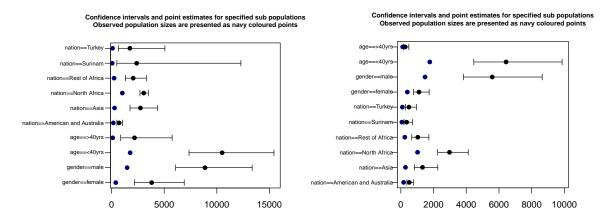


Figure 3: Population size by covariates for ztpoisson (left) and oiztgeom (right) model

summarysingleRmargin, which make it possible to extract relevant information regarding the population size.

For instance, the popSizeEst function can be used to extract information about the estimated size of the population as given below:

R> (popEst <- popSizeEst(basicModel))</pre>

Point estimate: 12690.35

Variance: 7885790

95% confidence intervals:

lowerBound upperBound normal 7186.449 18194.25 logNormal 8431.277 19718.31

and the resulting object popEst of the popSizeEstResults class contains the following fields:

- pointEstimate, variance numerics containing the point estimate and variance of this estimate.
- confidenceInterval a data.frame with confidence intervals.
- boot If the bootstrap was performed a numeric vector containing the  $\hat{N}$  values from the bootstrap, a character vector with value "No bootstrap performed" otherwise.
- control a controlPopVar object with controls used to obtain the object.

The only explicitly defined method for popSizeEstResults, summarysingleRmargin and summarysingleRStaticCountData classes is the print method, but the former one also accepts R primitives like coef:

R> coef(summary(basicModel))

```
Estimate Std. Error
                                          z value
                                                      P(>|z|)
(Intercept)
                   -1.3410661 0.2148870 -6.2407965 4.353484e-10
gendermale
                   age>40yrs
                   -0.9746058  0.4082420  -2.3873235  1.697155e-02
nationAsia
                   -1.0925990 0.3016259 -3.6223642 2.919228e-04
nationNorth Africa
                    0.1899980 0.1940007 0.9793677 3.273983e-01
nationRest of Africa -0.9106361 0.3008092 -3.0272880 2.467587e-03
nationSurinam
                   -2.3363949 1.0135639 -2.3051284 2.115938e-02
nationTurkey
                   -1.6753917 0.6027744 -2.7794674 5.444812e-03
```

analogously to glm from stats. The singleRfamily inherits the family class from stats and has explicitly defined print and simulate methods. Example usage is presented below

```
R> set.seed(1234567890)
R> N <- 10000
R> gender <- rbinom(N, 1, 0.2)
R> eta <- -1 + 0.5*gender
R> counts <- simulate(ztpoisson(), eta = cbind(eta), seed = 1)
R> summary(data.frame(gender, eta, counts))
     gender
                       eta
                                         counts
 Min.
        :0.0000
                  Min.
                          :-1.0000
                                     Min.
                                            :0.0000
 1st Qu.:0.0000
                  1st Qu.:-1.0000
                                     1st Qu.:0.0000
 Median :0.0000
                  Median :-1.0000
                                     Median :0.0000
 Mean
        :0.2036
                         :-0.8982
                                            :0.4196
                  Mean
                                     Mean
 3rd Qu.:0.0000
                  3rd Qu.:-1.0000
                                     3rd Qu.:1.0000
```

:-0.5000

The full list of explicitly defined methods for singleRStaticCountData methods is presented in Table 2.

Max.

:5.0000

# 6. Integration with the VGAM, countreg packages

As noted at the beginning, we provide an integration with the **VGAM** and **countreg** packages via the **singleRcaptureExtra** package available through Github at https://github.com/ncn-foreigners/singleRcaptureExtra.

```
R> install.packages("pak")
R> pak::pak("ncn-foreigners/singleRcaptureExtra")
```

The singleRcaptureExtra makes it possible to convert objects created by vglm, vgam, countreg functions from packages VGAM, countreg to a singleRStaticCountData via the respective estimatePopsize methods for their classes. The help files for all the methods and all the control functions can be accessed by

```
R> ?estimatePopsize.vgam
R> ?controlEstPopVgam
```

Max.

:1.0000

Max.

Function	Description		
fitted	it works almost exactly like glm counterparts but returns more infor-		
	mation, namely on fitted values for the truncated and non-truncated		
	probability distribution;		
logLik	compared to glm method, it has the possibility of returning not just the		
	value of the fitted log-likelihood but also the entire function (argument		
	type = "function") along with two first derivatives (argument deriv		
	= 0:2);		
model.matrix	it has the possibility of returning the $X_{\text{vlm}}$ matrix defined in 3;		
simulate	it calls the simulate method for the chosen model and fitted $\eta$ ;		
predict	it has the possibility of returning either fitted distribution parameters		
	for each unit (type = "response"), or just linear predictors (type =		
	"link"), or means of the fitted distributions of $Y$ and $Y Y>0$ (type		
	= "mean") or the inverse probability weights (type = "contr"). It is		
	possible to set the se.fit argument to TRUE in order to obtain standard		
	errors for each of those by using the $\delta$ method. Also, it is possible to use		
	a custom covariance matrix for standard error computation (argument		
	cov);		
${\tt redoPopEstimation}$	a function that applies all post-hoc procedures that were performed (such		
	as heteroscedastic consistent covariance matrix estimation via <b>countreg</b> )		
	to estimate the population size and standard errors;		
residuals	used for obtaining residuals of several types,		
	we refer interested readers to the manual		
	?singleRcapture:::residuals.singleRStaticCountData;		
stratifyPopsize,	compared to the glm class, summary has the possibility of adding con-		
summary	fidence intervals to the coefficient matrix (argument confint = TRUE)		
	and using a custom covariance matrix (argument cov = someMatrix);		
plot	it has been discussed above;		
popSizeEst	an extractor showcased above;		
cooks.distance	it works only for single predictor models		
dfbeta, dfpopsize	Multi-threading in dfbeta is available and dfpopsize calls dfbeta if no		
	dfbeta object was provided in the call;		
bread, estfun, vcovHC	for (almost) full <b>sandwich</b> compatibility;		
AIC, BIC, extractAIC,	it works exactly like glm counterparts.		
family, confint,			
df.residual,			
model.frame,			
hatvalues, nobs,			
print			

Table 2: S3Methods implemented in the singleRcapture

Below we present how to use the vglm, vgam class objects for population size estimation. The usage of zerotrunc class objects is almost exactly analogous. We use additive models with smooth terms for dataset from Böhning et al. (2013). Note that we use a different dataset than the one presented in the case study since our goal is to show the use of additive models and how it is handled in the singleRcapture package.

```
R> library(VGAM)
R> library(singleRcaptureExtra)
R> modelVgam <- vgam(</pre>
```

```
+ TOTAL_SUB ~ (s(log_size, df = 3) + s(log_distance, df = 2)) / C_TYPE,
+ data = farmsubmission,
+ # Using different link since
+ # VGAM uses parametrisation with 1/alpha
+ family = posnegbinomial(
+ lsize = negloglink
+ )
+ )
```

Estimation of the population size can be accomplished with the following simple syntax.

```
R> modelVgamPop <- estimatePopsize(modelVgam)</pre>
```

The resulting object is of class singleRforeign to indicate that the parameters were estimated outside the singleRcapture. The resulting object consists of the following elements:

```
R> str(modelVgamPop,1)
List of 5
 $ foreignObject :Formal class 'vgam' [package "VGAM"] with 43 slots
                : language estimatePopsize.vgam(formula = modelVgam)
 $ sizeObserved : int 12036
 $ populationSize:List of 5
  ..- attr(*, "class")= chr "popSizeEstResults"
                  :function (eta)
 $ derivFunc
 - attr(*, "class") = chr [1:4] "singleRadditive" "singleRforeign" "singleRStaticCountData"
Compare with a similar linear model from base singleRcapture:
R> modelBase <- estimatePopsize(</pre>
   TOTAL_SUB ~ (log_size + log_distance) * C_TYPE,
   data = farmsubmission,
  model = ztnegbin()
+ )
R> summary(modelBase)
Call:
estimatePopsize.default(formula = TOTAL_SUB ~ (log_size + log_distance) *
    C_TYPE, data = farmsubmission, model = ztnegbin())
Pearson Residuals:
     Min. 1st Qu.
                      Median
                                  Mean
                                         3rd Qu.
-0.729357 -0.317558 -0.152482 0.000609 0.148985 6.604269
Coefficients:
For linear predictors associated with: lambda
                        Estimate Std. Error z value P(>|z|)
```

```
0.45894 -3.870 0.000109 ***
(Intercept)
                      -1.77609
                                 0.02521 19.594 < 2e-16 ***
log size
                       0.49391
log_distance
                      C_TYPEDairy
                      -1.68591 0.55327 -3.047 0.002310 **
log_size:C_TYPEDairy
                     log_distance:C_TYPEDairy 0.08568
                                 0.04874 1.758 0.078762 .
For linear predictors associated with: alpha
          Estimate Std. Error z value P(>|z|)
(Intercept) 0.57673
                     0.07267 7.936 2.09e-15 ***
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
AIC: 34481.99
BIC: 34533.76
Residual deviance: 17611.16
Log-likelihood: -17233.99 on 24065 Degrees of freedom
Number of iterations: 9
_____
Population size estimation results:
Point estimate 38877
Observed proportion: 31% (N obs = 12036)
Std. Error 1749.448
95% CI for the population size:
        lowerBound upperBound
          35448.14 42305.85
normal
          35661.32 42530.37
logNormal
95% CI for the share of observed population:
         lowerBound upperBound
          28.44996 33.95382
normal
          28.29978 33.75085
logNormal
R> summary(modelVgamPop)
Call:
estimatePopsize.vgam(formula = modelVgam)
_____
Population size estimation results:
Point estimate 37760.01
Observed proportion: 31.9% (N obs = 12036)
Std. Error 1630.429
95\% CI for the population size:
         lowerBound upperBound
normal
          34564.42
                   40955.59
logNormal
          34757.77 41158.93
95% CI for the share of observed population:
         lowerBound upperBound
normal
          29.38793 34.82193
          29.24274 34.62823
logNormal
```

```
-- Summary of foreign object --
Call:
vgam(formula = TOTAL_SUB ~ (s(log_size, df = 3) + s(log_distance,
    df = 2))/C_TYPE, family = posnegbinomial(lsize = negloglink),
    data = farmsubmission)
Names of additive predictors: loglink(munb), negloglink(size)
Dispersion Parameter for posnegbinomial family:
Log-likelihood: -17214.62 on 24063.17 degrees of freedom
Number of Fisher scoring iterations: 11
DF for Terms and Approximate Chi-squares for Nonparametric Effects
                                                    Df Npar Df Npar Chisq
(Intercept):1
(Intercept):2
s(log_size, df = 3)
                                                     1
                                                                   51.949
                                                           1.8
s(\log_{distance}, df = 2)
                                                                    3.503
                                                     1
                                                           1.0
s(log_size, df = 3):s(log_distance, df = 2):C_TYPE
                                                      P(Chi)
(Intercept):1
(Intercept):2
```

The most important features of **singleRcapture** such as three types of bootstrap, **dfpopsize** and **stratifyPopsize** are extended for objects created by calling **estimatePopsize** on **vglm**, **vgam**, **zerotrunc** class object. We direct interested readers to the manual.

0.000000

0.063835

## 6.1. A note on implementation and differences

s(log\_size, df = 3):s(log\_distance, df = 2):C\_TYPE

 $s(log_size, df = 3)$ 

 $s(\log_{distance}, df = 2)$ 

One possible advantage of using vglm function from VGAM instead of estimatingPopsize is that in the latter one cannot fit models of the form analogous to:

$$\log(\lambda) = \beta_0 + \beta_1 X_1,$$
  
$$\operatorname{logit}(\omega) = (e^{-e})\beta_0 + \frac{1}{2}(\beta_0 + \beta_1)X_2,$$

for some explanatory variables  $X_1, X_2$ . It is possible to specify many quite "unusual" linear dependencies between elements of a coefficient matrix in the former function since implementation of **VGAM** allows the user to supply full constraint matrices (cf. Yee *et al.* (2015)) while **singleRcapture** "forces" the user to use formulas. We have decided to limit the number of possible models for the sake of simplicity since these more complicated dependencies seem not to be that frequently used in SSCR. Additionally it is worth remembering that much of the

implementation of the most computationally intensive code in VGAM is done in C making the implementation of vglm faster than that of estimatePopsize.

An advantage of using estimatingPopsize to fit the model as compared to calling it on vglm class object are that:

- The former is easier to use.
- Many SSCR specific diagnostics are not implemented as methods for vglm class (though the authors may consider implementing them if the demand is strong enough).
- Some important SSCR models such as oizt\* models are not implemented in VGAM.

Finally **singleRcapture** and **VGAM** implementation differ in how the expected information matrixes for negative binomial type distributions are calculated (the latter uses a randomized algorithm where as the former does not).

Comparison between singleRcapture and countreg is much simpler since as far as SSCR is concerned the latter offers just a small subset of what the former has to offer. In fact the implementation of bootstrap for zerotrunc uses estimatePopsizeFit function and not the original implementation which is not the case in vglm, vgam methods. So one would only use zerotrunc for fitting the model based on familiarity with the user interface.

# 7. Concluding remarks

In this paper we have introduced two packages for single source capture-recapture models, namely **singleRcapture** and **singleRcaptureExtra**. The packages implement state-of-the-art methods for estimating population size based on a single data set with multiple counts. The package implements different methods to account for heterogeneity in capture probabilities, modelled using covariates, as well as behavioral change, modelled using one-inflation. We have built the package to facilitate the implementation of new models using **family** objects; their application is exemplified in the Appendix A.2.

In future work we plan to implement Bayesian estimation using Stan (e.g. via the brms package; Carpenter, Gelman, Hoffman, Lee, Goodrich, Betancourt, Brubaker, Guo, Li, and Riddell (2017); Bürkner (2017)) and for one-inflation models we can use the recent approach proposed by Tuoto, Di Cecco, and Tancredi (2022) and implement our own families using the brms package.

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#### A. Detailed information

## A.1. The estimatePopsizeFit function

In this section we provide a step-by-step description of how to prepare data in order to use the estimatePopsizeFit function, which may be useful to some users, e.g. those wishing to make modifications to the  $\hat{N}$  estimate or to the bootstrap. In order to show how to apply the function we will fit a zero truncated geometric model on the data from Böhning et al. (2013) with covariate dependency:

```
\log(\lambda) = \beta_{1,1} + \beta_{1,2}\log_{\text{distance}} + \beta_{1,3}C_{\text{TYPE}} + \beta_{1,4}\log_{\text{size}},
\log_{\text{it}}(\omega) = \beta_{2,1} + \beta_{2,2}\log_{\text{distance}} + \beta_{2,3}C_{\text{TYPE}}.
```

This would be equivalent to the following esimatePopsize call:

```
R> estimatePopsize(
+ TOTAL_SUB ~ .,
+ data = farmsubmission,
+ model = ztoigeom(),
+ controlModel(
+ omegaFormula = ~ 1 + log_size + C_TYPE
+ )
+ )
```

1. Create a data matrix  $\boldsymbol{X}_{\text{vlm}}$ 

```
R> X <- matrix(data = 0, nrow = 2 * NROW(farmsubmission), ncol = 7)
```

2. Fill the first n rows with model.matrix according to the specified formula and specify the attribute attr(X, "hwm") that informs the function which elements of the design matrix correspond to which linear predictor (covariates for counts and covariates for one-inflation)

```
R> X[1:NROW(farmsubmission), 1:4] \leftarrow model.matrix( + ~ 1 + log_size + log_distance + C_TYPE, + farmsubmission + )
R> X[-(1:NROW(farmsubmission)), 5:7] \leftarrow model.matrix( + ~ 1 + log_distance + C_TYPE, + farmsubmission + )
R> attr(X, "hwm") <- c(4, 3)
```

3. Obtain starting  $\beta$  parameters using the glm.fit function.

1

2

-2.7845

0.6170

-2.5971

0.6163

```
R> start <- glm.fit(# get starting points</pre>
   y = farmsubmission$TOTAL_SUB,
    x = X[1:NROW(farmsubmission), 1:4],
    family = poisson()
+ )$coefficients
R> start
4. Use the estimatePopsizeFit function to fit the model assuming a zero-truncated one-
    inflated geometric distribution as specified in the family argument.
R> res <- estimatePopsizeFit(</pre>
                 = farmsubmission$TOTAL_SUB,
+
    У
    Χ
                 = X,
                = "IRLS",
  method
  priorWeights = 1,
+ family
                = ztoigeom(),
  control
               = controlMethod(silent = TRUE),
  coefStart = c(start, 0, 0, 0),
   etaStart = matrix(X %*% c(start, 0, 0, 0), ncol = 2),
offset = cbind(rep(0, NROW(farmsubmission)).
                         rep(0, NROW(farmsubmission)))
+ )
  5. Compare our results with those obtained by applying the stats::optim function.
R> 11 <- ztoigeom() $makeMinusLogLike(y = farmsubmission $TOTAL_SUB, X = X)
R> res2 <- estimatePopsizeFit(</pre>
    y = farmsubmission$TOTAL_SUB,
   X = X
  method = "optim",
  priorWeights = 1,
+ family = ztoigeom(),
   coefStart = c(start, 0, 0, 0),
  control = controlMethod(silent = TRUE, maxiter = 10000),
    offset = cbind(rep(0, NROW(farmsubmission)), rep(0, NROW(farmsubmission)))
+ )
R> data.frame(IRLS = round(c(res$beta, -11(res$beta), res$iter), 4),
             optim = round(c(res2$beta, -11(res2$beta), res2$iter[1]), 4))
         IRLS
                    optim
```

3	-0.0646	-0.0825
4	0.5346	0.5431
5	-3.1745	-0.1504
6	0.1281	-0.1586
7	-1.0865	-1.0372
8	-17278.7613	-17280.1189
9	15.0000	1696.0000

The default maxiter parameter for "optim" fitting is 1000, but we needed to increase it since the optim does not converge in 1000 steps and "gets stuck" at a plateau, which results in a lower log-likelihood value compared to the standard "IRLS".

The above situation is rather typical. While we did not conduct any formal numerical analyses, it seems that when one attempts to model more than one parameter of the distribution as covariate dependent optim algorithms, both "Nelder-Mead" and "L-BFGS-B" seem to be ill-suited for the task despite being provided with the analytically computed gradient. This is one of the reasons why "IRLS" is the default fitting method.

# A.2. Structure of a family function

In this section we provide details regarding the family object for the singleRcapture package. This object contains additional parameters in comparison to the standard family object from the stats package.

Function	Description
makeMinusLogLike	A factory function for creating the following functions:
	$\ell(\boldsymbol{\beta}), \frac{\partial \ell}{\partial \boldsymbol{\beta}}, \frac{\partial^2 \ell}{\partial \boldsymbol{\beta}^\top \partial \boldsymbol{\beta}}$
	from the $y$ vector and the $X_{vlm}$ matrix, which has the deriv argument with possible values in $c(0, 1, 2)$ that determine which derivative to return; the default value is 0, which represents the minus log-likelihood;
links	A list with link functions;
mu.eta, variance	Functions of linear predictors that return the expected value and variance. The type argument with 2 possible values ("trunc" and "nontrunc") specifies whether to return $\mathbb{E}[Y Y>0]$ , var $[Y Y>0]$ or $\mathbb{E}[Y]$ , var $[Y]$ respectively; the deriv argument with values in c(0, 1, 2) is used for indicating the derivative with respect to the linear predictors, which is used for providing standard errors in the predict method;
family	A string that specifies the model name;
valideta, validmu	For now it only returns TRUE. In the near future, it will be used to check whether applied linear predictors are valid (i.e. are transformed into some elements of the parameter space subjected to the inverse link function);
funcZ, Wfun	Functions that create pseudo residuals and working weights used in the IRLS algorithm;
devResids	A function that returns deviance residuals given a vector of prior weights of linear predictors and the response vector;
pointEst, popVar	Functions that return the point estimate for the population size and analytic estimation of its variance given prior weights of linear predictors and, in the later case, also estimates of $cov(\hat{\beta})$ and $X_{vlm}$ matrix. There is an additional boolean parameter $contr$ in the former function, which, if set to TRUE, returns the contribution of each unit;
etaNames	Names of linear predictors;
densityFunction	A function that returns the value of PMF at values of x given linear predictors. The type argument specifies whether to return $\mathbb{P}[Y Y>0]$ or $\mathbb{P}[Y]$ ;
simulate	A function that generates values of a dependent vector given linear predictors;
getStart	An expression for generating starting points;

## B. Implementing a custom singleRcapture family function

Suppose we want to implement a very specific zero truncated family function in the **singleR-capture**, which corresponds to the following "untruncated" distribution:

$$\mathbb{P}[Y=y|\lambda,\pi] = \begin{cases} 1 - \frac{1}{2}\lambda - \frac{1}{2}\pi & \text{when: } y=0\\ \frac{1}{2}\pi & \text{when: } y=1\\ \frac{1}{2}\lambda & \text{when: } y=2, \end{cases}$$
(4)

with  $\lambda, \pi \in (0,1)$  being dependent on covariates.

The following would be one way of implementing it, with lambda, pi in the code meaning  $\frac{1}{2}\lambda, \frac{1}{2}\pi$  in the equation above.

```
R> myFamilyFunction <- function(lambdaLink = c("logit", "cloglog", "probit"),
                                         = c("logit", "cloglog", "probit"),
                                piLink
                                ...) {
    if (missing(lambdaLink)) lambdaLink <- "logit"</pre>
   if (missing(piLink)) piLink <- "logit"</pre>
   links <- list()
   attr(links, "linkNames") <- c(lambdaLink, piLink)</pre>
    lambdaLink <- switch(lambdaLink,</pre>
      "logit" = singleRcapture:::singleRinternallogitLink,
      "cloglog" = singleRcapture:::singleRinternalcloglogLink,
      "probit" = singleRcapture:::singleRinternalprobitLink
    piLink <- switch(piLink,</pre>
      "logit" = singleRcapture:::singleRinternallogitLink,
      "cloglog" = singleRcapture:::singleRinternalcloglogLink,
      "probit" = singleRcapture:::singleRinternalprobitLink
   links[1:2] <- c(lambdaLink, piLink)</pre>
   mu.eta <- function(eta, type = "trunc", deriv = FALSE, ...) {</pre>
                    piLink(eta[, 2], inverse = TRUE) / 2
      lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2</pre>
     if (!deriv) {
        switch (type,
          "nontrunc" = pi + 2 * lambda,
          "trunc" = 1 + lambda / (pi + lambda)
        )
     } else {
        # Only necessary if one wishes to use standard errors in predict method
        switch (type,
          "nontrunc" = {
            matrix(c(2, 1) * c(
              lambdaLink(eta[, 1], inverse = TRUE, deriv = 1) / 2,
                  piLink(eta[, 2], inverse = TRUE, deriv = 1) / 2
```

```
), ncol = 2)
          },
          "trunc" = {
            matrix(c(
              pi / (pi + lambda) ^ 2,
              -lambda / (pi + lambda) ^ 2
            ) * c(
              lambdaLink(eta[, 1], inverse = TRUE, deriv = 1) / 2,
                  piLink(eta[, 2], inverse = TRUE, deriv = 1) / 2
            ), ncol = 2)
          }
+
        )
+
     }
    }
    variance <- function(eta, type = "nontrunc", ...) {</pre>
                   piLink(eta[, 2], inverse = TRUE) / 2
      lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2</pre>
     switch (type,
      "nontrunc" = pi * (1 - pi) + 4 * lambda * (1 - lambda - pi),
      "trunc" = lambda * (1 - lambda) / (pi + lambda)
    }
    Wfun <- function(prior, y, eta, ...) {
                    piLink(eta[, 2], inverse = TRUE) / 2
             <-
      lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2</pre>
      G01 \leftarrow ((lambda + pi) ^ (-2)) * piLink(eta[, 2], inverse = TRUE, deriv = 1) *
       lambdaLink(eta[, 1], inverse = TRUE, deriv = 1) * prior / 4
      G00 <- ((lambda + pi) ^ (-2)) - (pi ^ (-2)) - lambda / ((lambda + pi) * (pi ^ 2))
      G00 \leftarrow G00 * prior * (piLink(eta[, 2], inverse = TRUE, deriv = 1) ^ 2) / 4
      G11 <- ((lambda + pi) ^ (-2)) - (((lambda + pi) * lambda) ^ -1)
      G11 \leftarrow G11 * prior * (lambdaLink(eta[, 1], inverse = TRUE, deriv = 1) ^ 2) / 4
      matrix(
       -c(G11, # lambda)
           G01, # mixed
           GO1, # mixed
           G00 # pi
        dimnames = list(rownames(eta), c("lambda", "mixed", "mixed", "pi")),
        ncol = 4
   }
   funcZ <- function(eta, weight, y, prior, ...) {</pre>
                    piLink(eta[, 2], inverse = TRUE) / 2
            <-
      lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2</pre>
```

```
+
      weight <- weight / prior
      GO \leftarrow (2 - y) / pi - ((lambda + pi) ^ -1)
      G1 \leftarrow (y - 1) / lambda - ((lambda + pi) ^ -1)
      G1 <- G1 * lambdaLink(eta[, 1], inverse = TRUE, deriv = 1) / 2
                     piLink(eta[, 2], inverse = TRUE, deriv = 1) / 2
      GO <- GO *
      uMatrix \leftarrow matrix(c(G1, G0), ncol = 2)
      weight <- lapply(X = 1:nrow(weight), FUN = function (x) {</pre>
       matrix(as.numeric(weight[x, ]), ncol = 2)
      })
      pseudoResid <- sapply(X = 1:length(weight), FUN = function (x) {</pre>
       #xx <- chol2inv(chol(weight[[x]])) # less computationally demanding</pre>
        xx <- solve(weight[[x]]) # more stable</pre>
       xx %*% uMatrix[x, ]
      pseudoResid <- t(pseudoResid)</pre>
      dimnames(pseudoResid) <- dimnames(eta)</pre>
     pseudoResid
   minusLogLike <- function(y, X, offset,</pre>
                              weight
                                         = 1,
                                         = FALSE,
                              NbyK
                              vectorDer = FALSE,
                              deriv
                                         = 0,
                               ...) {
      y <- as.numeric(y)</pre>
      if (is.null(weight)) {
       weight <- 1
      if (missing(offset)) {
        offset \leftarrow cbind(rep(0, NROW(X) / 2), rep(0, NROW(X) / 2))
      if (!(deriv %in% c(0, 1, 2)))
        stop("Only score function and derivatives up to 2 are supported.")
      deriv <- deriv + 1
      switch (deriv,
        function(beta) {
          eta <- matrix(as.matrix(X) %*% beta, ncol = 2) + offset
          pi <- piLink(eta[, 2], inverse = TRUE) / 2</pre>
          lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2</pre>
          -sum(weight * ((2 - y) * log(pi) + (y - 1) * log(lambda) - log(pi + lambda)))
        },
        function(beta) {
          eta <- matrix(as.matrix(X) %*% beta, ncol = 2) + offset
                <- piLink(eta[, 2], inverse = TRUE) / 2</pre>
         lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2</pre>
```

```
GO \leftarrow (2 - y) / pi - ((lambda + pi) ^ -1)
  G1 \leftarrow (y - 1) / lambda - ((lambda + pi) ^ -1)
  G1 <- G1 * weight * lambdaLink(eta[, 1], inverse = TRUE, deriv = 1) / 2
                         piLink(eta[, 2], inverse = TRUE, deriv = 1) / 2
  GO <- GO * weight *
  if (NbyK) {
    XX <- 1:(attr(X, "hwm")[1])</pre>
    return(cbind(as.data.frame(X[1:nrow(eta), XX]) * G1,
                 as.data.frame(X[-(1:nrow(eta)), -XX]) * GO))
  }
  if (vectorDer) {
    return(cbind(G1, G0))
  as.numeric(c(G1, G0) \%*\% X)
},
function (beta) {
  lambdaPredNumber <- attr(X, "hwm")[1]</pre>
  eta <- matrix(as.matrix(X) %*% beta, ncol = 2) + offset
                piLink(eta[, 2], inverse = TRUE) / 2
  lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2</pre>
  res <- matrix(nrow = length(beta), ncol = length(beta),
                 dimnames = list(names(beta), names(beta)))
  # pi^2 derivative
  dpi <- (2 - y) / pi - (lambda + pi) ^ -1
  G00 \leftarrow ((lambda + pi) ^ (-2)) - (2 - y) / (pi ^ 2)
  G00 \leftarrow t(as.data.frame(X[-(1:(nrow(X) / 2)), -(1:lambdaPredNumber)] *
  (G00 * ((piLink(eta[, 2], inverse = TRUE, deriv = 1) / 2) ^ 2) +
  dpi * piLink(eta[, 2], inverse = TRUE, deriv = 2) / 2) * weight)) %*%
  as.matrix(X[-(1:(nrow(X) / 2)), -(1:lambdaPredNumber)])
  # mixed derivative
  G01 < - (lambda + pi) ^ (-2)
  G01 \leftarrow t(as.data.frame(X[1:(nrow(X) / 2), 1:lambdaPredNumber]) *
  GO1 * (lambdaLink(eta[, 1], inverse = TRUE, deriv = 1) / 2) *
  (piLink(eta[, 2], inverse = TRUE, deriv = 1) / 2) * weight) %*%
  as.matrix(X[-(1:(nrow(X) / 2)), -(1:lambdaPredNumber)])
  # lambda^2 derivative
  G11 \leftarrow ((lambda + pi) ^ (-2)) - (y - 1) / (lambda ^ 2)
  dlambda <- (y - 1) / lambda - ((lambda + pi) ^ -1)
  G11 <- t(as.data.frame(X[1:(nrow(X) / 2), 1:lambdaPredNumber] *</pre>
  (G11 * ((lambdaLink(eta[, 1], inverse = TRUE, deriv = 1) / 2) ^ 2) +
  dlambda * lambdaLink(eta[, 1], inverse = TRUE, deriv = 2) / 2) * weight)) %*%
  X[1:(nrow(X) / 2), 1:lambdaPredNumber]
  res[-(1:lambdaPredNumber), -(1:lambdaPredNumber)] <- G00</pre>
  res[1:lambdaPredNumber, 1:lambdaPredNumber] <- G11</pre>
```

```
res[1:lambdaPredNumber, -(1:lambdaPredNumber)] <- t(G01)</pre>
      res[-(1:lambdaPredNumber), 1:lambdaPredNumber] <- G01</pre>
      res
    }
  )
}
validmu <- function(mu) {</pre>
  (sum(!is.finite(mu)) == 0) \&\& all(0 < mu) \&\& all(2 > mu)
# this is optional
devResids <- function(y, eta, wt, ...) {</pre>
}
pointEst <- function (pw, eta, contr = FALSE, ...) {</pre>
        <-
                piLink(eta[, 2], inverse = TRUE) / 2
  lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2</pre>
  N \leftarrow pw / (lambda + pi)
  if(!contr) {
    N \leftarrow sum(N)
  }
  Ν
}
popVar <- function (pw, eta, cov, Xvlm, ...) {</pre>
  pi <-
               piLink(eta[, 2], inverse = TRUE) / 2
  lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2</pre>
  bigTheta1 <- -pw / (pi + lambda) ^ 2 # w.r to pi
  bigTheta1 <- bigTheta1 * piLink(eta[, 2], inverse = TRUE, deriv = 1) / 2</pre>
  bigTheta2 \leftarrow -pw / (pi + lambda) ^ 2 # w.r to lambda
  bigTheta2 <- bigTheta2 * lambdaLink(eta[, 1], inverse = TRUE, deriv = 1) / 2 # w.r to lambda
  bigTheta <- t(c(bigTheta2, bigTheta1) %*% Xvlm)</pre>
  f1 <- t(bigTheta) %*% as.matrix(cov) %*% bigTheta
  f2 <- sum(pw * (1 - pi - lambda) / ((pi + lambda) ^ 2))
  f1 + f2
}
dFun <- function (x, eta, type = c("trunc", "nontrunc")) {
  if (missing(type)) type <- "trunc"</pre>
                 piLink(eta[, 2], inverse = TRUE) / 2
  lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2</pre>
  switch (type,
    "trunc" = {
      (pi * as.numeric(x == 1) + lambda * as.numeric(x == 2)) / (pi + lambda)
```

```
},
    "nontrunc" = {
      (1 - pi - lambda) * as.numeric(x == 0) +
      pi * as.numeric(x == 1) + lambda * as.numeric(x == 2)
  )
}
simulate <- function(n, eta, lower = 0, upper = Inf) {</pre>
         <-
                 piLink(eta[, 2], inverse = TRUE) / 2
  lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2</pre>
  CDF <- function(x) {
    ifelse(x == Inf, 1,
    ifelse(x < 0, 0,
    ifelse(x < 1, 1 - pi - lambda,
    ifelse(x < 2, 1 - lambda, 1))))
  }
  1b <- CDF(lower)</pre>
  ub <- CDF(upper)</pre>
  p_u <- stats::runif(n, lb, ub)</pre>
  sims \leftarrow rep(0, n)
  cond <- CDF(sims) <= p_u</pre>
  while (any(cond)) {
    sims[cond] <- sims[cond] + 1</pre>
    cond <- CDF(sims) <= p_u</pre>
  }
  sims
}
getStart <- expression(</pre>
  if (method == "IRLS") {
    etaStart <- cbind(</pre>
      family links[[1]] (mean(observed == 2) * (1 + 0 * (observed == 2))), # lambda
      family$links[[2]](mean(observed == 1) * (1 + 0 * (observed == 1))) # pi
    ) + offset
  } else if (method == "optim") {
    init <- c(
      family$links[[1]](weighted.mean(observed == 2, priorWeights) * 1 + .0001),
      family$links[[2]](weighted.mean(observed == 1, priorWeights) * 1 + .0001)
    if (attr(terms, "intercept")) {
      coefStart <- c(init[1], rep(0, attr(Xvlm, "hwm")[1] - 1))</pre>
    } else {
      coefStart <- rep(init[1] / attr(Xvlm, "hwm")[1], attr(Xvlm, "hwm")[1])</pre>
    if ("(Intercept):pi" %in% colnames(Xvlm)) {
      coefStart <- c(coefStart, init[2], rep(0, attr(Xvlm, "hwm")[2] - 1))</pre>
      coefStart <- c(coefStart, \ rep(init[2] \ / \ attr(Xvlm, \ "hwm")[2], \ attr(Xvlm, \ "hwm")[2]))
  }
)
```

```
structure(
     list(
       makeMinusLogLike = minusLogLike,
       densityFunction = dFun,
       links
                = links,
                = mu.eta,
       mu.eta
       valideta = function (eta) {TRUE},
       variance = variance,
       Wfun
               = Wfun,
      funcZ = funcZ,
      devResids = devResids,
      validmu = validmu,
      pointEst = pointEst,
      popVar = popVar,
      family = "myFamilyFunction",
      etaNames = c("lambda", "pi"),
       simulate = simulate,
      getStart = getStart,
      extraInfo = c(
                   = "pi / 2 + lambda",
        variance = paste0("(pi / 2) * (1 - pi / 2) + 2 * lambda * (1 - lambda / 2 - pi / 2)"),
        popSizeEst = "(1 - (pi + lambda) / 2) ^ -1",
                 = "1 + lambda / (pi + lambda)",
         varianceTr = pasteO("lambda * (1 - lambda / 2) / (pi + lambda)")
       )
     class = c("singleRfamily", "family")
+ }
A quick tests shows us that this implementation in fact works:
R> set.seed(123)
R> Y <- simulate(</pre>
      myFamilyFunction(lambdaLink = "logit", piLink = "logit"),
      nsim = 1000, eta = matrix(0, nrow = 1000, ncol = 2),
      truncated = FALSE
+ )
R> mm <- estimatePopsize(</pre>
      formula = Y \sim 1,
      data = data.frame(Y = Y[Y > 0]),
      model = myFamilyFunction(lambdaLink = "logit",
                                piLink = "logit"),
      # the usual observed information matrix
      # is ill-suited for this distribution
      controlPopVar = controlPopVar(covType = "Fisher")
+ )
R> summary(mm)
```

Call:

```
estimatePopsize.default(formula = Y ~ 1, data = data.frame(Y = Y[Y >
    0]), model = myFamilyFunction(lambdaLink = "logit", piLink = "logit"),
    controlPopVar = controlPopVar(covType = "Fisher"))
Pearson Residuals:
   Min. 1st Qu. Median Mean 3rd Qu.
                                            Max.
-0.8198 -0.8198 0.8099 0.0000 0.8099 0.8099
Coefficients:
For linear predictors associated with: lambda
            Estimate Std. Error z value P(>|z|)
(Intercept) 0.01217 0.20253 0.06 0.952
For linear predictors associated with: pi
            Estimate Std. Error z value P(>|z|)
(Intercept) -0.01217 0.08926 -0.136 0.892
AIC: 687.4249
BIC: 695.8259
Residual deviance: 0
Log-likelihood: -341.7124 on 984 Degrees of freedom
Number of iterations: 2
Population size estimation results:
Point estimate 986
Observed proportion: 50% (N obs = 493)
Std. Error 70.30092
95% CI for the population size:
          lowerBound upperBound
            848.2127 1123.787
normal
logNormal
            866.3167
                       1144.053
95% CI for the share of observed population:
          lowerBound upperBound
            43.86951
                       58.12221
normal
logNormal
            43.09241
                       56.90759
where the link functions, such as singleRcapture:::singleRinternalcloglogLink, are just
internal functions in singleRcapture that compute link functions, their inverses and derivatives
of both links and inverse links up to the third order:
R> singleRcapture:::singleRinternalcloglogLink
function (x, inverse = FALSE, deriv = 0)
{
   deriv <- deriv + 1
   if (isFALSE(inverse)) {
```

One could, of course, include the code for computing them manually.

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