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

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Abstract

The estimation of population size represents a significant challenge within the domains of official statistics, social sciences, and natural sciences. In such situations capture-recapture methods can be applied, which can be classified according to the number of sources utilized, particularly whether a single or multiple sources are employed. This paper focuses on the first group of methods and introduces the package **singleRcapture**. The package implements state-of-the-art single-source capture-recapture models (e.g. zero-truncated one-inflated regression), new developments proposed by the authors, and provides a user-friendly application programming interface (API). The package is self-contained, providing point estimates and their variance, as well as implementing 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 from only one source and dual/multiple system estimation is not applicable.

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, serving as a basis for research, policy formulation, and decision-making processes (Böhning, Bunge, and Heijden 2018). In the field of statistics, particularly official statistics, precise population estimates are essential for developing robust economic models, optimizing resource allocation, and informing evidence-based policy formulation (cf. Baffour-Awuah 2009). Social scientists utilize advanced population estimation techniques to investigate hard-to-reach populations, such as homeless individuals or illicit drug users, thereby addressing 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 through traditional sampling methods (cf. Vincent and Thompson 2022). In ecology and epidemiology, researchers focus on estimating the size of specific species or disease-affected populations within defined geographical regions, which is vital for conservation efforts, ecosystem management, and public health interventions.

Population size estimation can be approached through various methodologies, each with distinct advantages and limitations. Traditional approaches include full enumeration (e.g. census operations) 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). Application of these sources often comes with statistical methods, known as capture-recapture or multiple system estimation, that utilizes data from multiple enumerations of the same population (cf. Dunne and Zhang 2024). This can be implemented using a single source with repeated observations, two, or multiple sources.

In this paper we focus methods that utilize 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 might be derived from police records, health system databases, or border control logs, while for non-human populations, veterinary records or specialized field data serve as analogous sources. These methods are often applied for hard-to-reach or hidden population where standard sampling methods may be inappropriate because of the costs or problems with identification of members of these populations.

While methods for two or more sources are implemented in various open-source software, for instance Rcapture (Baillargeon and Rivest 2007), marked (Laake, Johnson, Conn, and Isaac 2013) or VGAM (Yee, Stoklosa, and Huggins 2015) the single-source capture-recapture (SSCR) methods are not available at all or being only partially implemented in existing R packages. The goal of the paper is to introduce the singleRcapture and singleRcaptureExtra packages which by implementing state-of-the-art methods in SSCR and providing user friendly API which mimics existing R functions (e.g., glm) attempt to bridge this aforementioned gap. In the next subsection we describe the available R packages that could be used for estimating population size based on SSCR methods.

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

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::ztpoisson**) 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 poisson distribution), see Yee and Ma (2024) for recent description. However, estimation of parameters of a given truncated (and possibly inflated) distribution is just a first step (similarly as in log-linear models in capture-recapture with two sources) and to best of our knowledge there is no open-source software that allows to estimate population size based on SSCR method, including variance estimator or diagnostics.

Therefore, the goal of the **singleRcapture** is R language is to bridge this gap to provide scientists and other practitioners a tool for estimation of population size based on SSCR methods. The package implements state-of-the-art methods as recently described by Böhning *et al.* (2018) or Böhning and Friedl (2024) and its extensions (e.g., inclusion of covariates, different treatment of one-inflation) that we will cover in detail in Section 2. The package implements variance estimation based on various methods, allows for implementing custom models as well as diagnostics plots (e.g. rootograms) with parameters estimated using a modified IRLS algorithm implemented by us to for estimation stability. Furthermore, as many R users are familiar with **countreg** or **VGAM** we have implemented a lightweight extension **singleRcaptureExtra**, available through Github (https://github.com/ncn-foreigners/singleRcaptureExtra), that allows for integration of **singleRcapture** with those packages.

The remaining part of the paper is as follows. In Section 2 a brief description of the theoretical background is given and information on the fitting methods, the available methods and variance estimation is presented. In Section 3 the main functionalities of the package are introduced. Section 4 provides a case study along with assessment of results, diagnostics and estimation of specific sub-populations. Section 5 covers classes and S3methods implemented in the package. Section 6 covers integration with countreg and VGAM packages through singleRcaptureExtra package. The paper ends with conclusions and an appendix that shows how to a implement custom model and how one can use the estimatePopsizeFit which is faster than the main function but only estimates regression, which could be of interest to users interested in using any new bootstrap methods not programmed in the package (see Appendix A.1).

2. Theoretical background

2.1. How do we estimate population size with a single register?

Let Y_k represent the number of times k-th unit was observed in a register. Clearly, we only observe $k: Y_k > 0$ and we do not know how many units are missed (i.e. $Y_k = 0$) and to find the population size denoted by N we need to estimate it. In general, we assume that conditional distribution of Y_k given a vector of covariates \boldsymbol{x}_k follows some version of zero-truncated count data distribution (and its extensions). Knowing the parameters of the distribution we may estimate the population size using Horowitz-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, and maximum likelihood estimate of N is obtained after substituting regression parameters $\boldsymbol{\beta}$ for $\mathbb{P}[Y_k > 0 | \boldsymbol{x}_k]$ into (1).

The basic SSCR assumes independence between counts which may be rather naive as the first capture may significantly influence the behaviour of a given unit or limit possibilities of further captures (e.g. due to incarceration).

To solve these issues, Godwin and Böhning (2017a) and Godwin and Böhning (2017b) introduced one-inflated distributions that explicitly model probability of the singletons by giving

additional mass ω for singletons denoted as $\mathcal{I}_{\{1\}}(y)$ (cf. Böhning and Friedl 2024)

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

The analytic variance estimation is then done by computing two parts of the decomposition due 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 δ method given by:

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

while the second part of the decomposition in (2) is under the assumption of 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 forms the basis for the 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 of which is an attempt to address a common criticism of student type confidence intervals in SSCR, that is a possibly skewed distribution of \hat{N} , and results in the $1-\alpha$ confidence interval given by:

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

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 quatile function of the standard normal distribution. The estimator \hat{N} is best interpreted as being an estimator for 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 implemented models in **singleRcapture** along with the 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 limit ourselves to just listing the family functions with the briefest descriptions and instead direct interested reader to the relevant literature for elaboration.

These family functions currently are:

• 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 covariate extension see Böhning, Vidal-Diez, Lerdsuwansri, Viwatwongkasem, and Arnold (2013) and Böhning and van der Heijden (2009)):

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

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

• 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 distributions where the new probability \mathbb{P}^* measure is defined in terms of count data measure \mathbb{P} with support on $\mathbb{N} \cup \{0\}$ as:

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

• One-inflated zero-truncated (oizt*) modifications distributions where the new probability \mathbb{P}^* measure is defined as:

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

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 have provided two new approaches that allow modelling singletons in a similar way as in Hurdle models. In particular we have proposed the following:

 Zero-truncated Hurdle model (ztHurdle*) for Poisson, geometric and NB2 is defined as:

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

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

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

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

The approaches presented above differ in terms of assumptions, computational complexity, or how they treat heterogeneity of captures and singletons. For instance, the dispersion parameter α in the NB2 type models is often interpreted as measuring the *severeness* 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 due to the class of models considered the consistency is not lost despite the lack of information.

While not discussed in the literature yet the interpretation of heterogeneous α 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 due to inherent computational issues with NB models which are exasperated by the fact that data in SSCR is usually of somewhat low quality. Sparseness of the data is in particular a common issue in SSCR and a big issue for all numerical methods for fitting the (zero-truncated) NB model.

The extra mass ω in the 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 in estimating the number active people who committed criminal acts in a given time period being observed naturally induces a risk of no longer being able to be observed for all units with possibility of arrest. One constraint present in modelling via inflated models is that trying to include both the possibility of one inflation and one deflation leads to both numerical and theoretical problems since the parameter space (of (ω, λ)) or $(\omega, \lambda, \alpha)$) is then a much more complicated set.

Hurdle models are another approach to modelling the one-inflation, they can also model deflation as well as both inflation and deflation simultaneously so they are more flexible and it seems that the Hurdle zero-truncated models are more numerically stable.

Although interpretation of regression parameters tends to be somewhat overlooked in the SSCR studies we should point out that interpretation of the ω inflation parameter (in ztoi* or oizt*) is more convenient that the interpretation of the π probability parameter (in Hurdle models). Additionally the interpretation of the λ parameter in (one) inflated models conforms

to the intuition that given that unit k comes from the non-inflated part of the population then it follows a poisson distribution (respectively geometric or negative binomial) with the λ parameter (or λ, α), in hurdle models one loses that interpretation. It is somewhat interesting is that the estimates from Hurdle zero-truncated and one-inflated zero-truncated models are "usually" guite close to one another, this however require more studies.

2.3. Fitting method

As previously noted the **singleRcapture** package supports modelling (linear) dependence on covariates of all parameters. To that end a modified IRLS algorithm is employed, full details are available in Yee (2015). In order to employ the algorithm a modified model matrix is created X_{vlm} at call to estimatePopsize. 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 user specified formula.

In the context of multi-parameter families we have a matrix of linear predictors η instead of a vector, with the number of columns matching the number of parameters in the distribution.

"Weights" 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 ℓ is the log-likelihood function and $\boldsymbol{\eta}_{(k)}$ is the k 'th row of $\boldsymbol{\eta}$, while in the usual IRLS they are scalars

$$\mathbb{E}\left[-\frac{\partial^2 \ell}{\partial \eta_k^2}\right] \text{ which is often just } -\frac{\partial^2 \ell}{\partial \eta^2}.$$

Algorithm 1: A 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 current iteration
$$\boldsymbol{\eta} \leftarrow \boldsymbol{X}_{\text{vlm}} \boldsymbol{\beta} + \boldsymbol{o}, \boldsymbol{W}_{(k)} \leftarrow \mathbb{E} \left[-\frac{\partial^2 \ell}{\partial \boldsymbol{\eta}_{(k)}^\top \partial \boldsymbol{\eta}_{(k)}} \right], Z \leftarrow \boldsymbol{\eta}_{(k)} + \frac{\partial \ell}{\partial \boldsymbol{\eta}_{(k)}} \boldsymbol{W}_{(k)}^{-1} - \boldsymbol{o}_{(k)}.$$

- 3 Assign 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 end algorithm, else iter← 1+iter and return to step 2.

2.4. Bootstrap variance estimators

We have implemented three types of bootstrap algorithms: parametric, semi-parametric and nonparametric with the nonparametric being bootstrap being the usual bootstrap algorithm which as argued in Norris and Pollock (1996) and Zwane and Van der Heijden (2003).

The idea of semi-parametric bootstrap is to modify the usual bootstrap to include the additional uncertainty due to the sample size being a random variable. This type of bootstrap can be in short described as in the Algorithm 2.

Algorithm 2: Semi-parametric bootstrap

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

In other words, we first draw the sample size and then the sample conditional on the sample size. Note that in using 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 in short first draws the 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.

Algorithm 3: Parametric bootstrap

- 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 drawn Y value equal to 0.
- 4 Obtain population size estimate N_b based on the truncated data.
- **5** Repeat 1-4 steps B times.

Note that 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 semi-parametric bootstrap. The parametric bootstrap algorithm is the default in **singleRcapture**.

3. The main function

3.1. The estimatePopsize function

The main function that singleRcapture is built around is estimatePopsize. The leading design principle was to make using estimatePopsize as close to standard stats::glm as possible or packages for fitting zero-truncated regression models as countreg (e.g. countreg::zerotrunc function). This 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 with the formula, data, model being the three arguments which must be provided in the estimatePopsize syntax.

The most important part of the estimatePopsize is to specify the model parameter. This is a crucial part as it allows to select appropriate model to estimate the *unobserved* part of the population. For instance, to fit Chao's or Zelterman's model one should select chao or zelterman and if a researcher assumes that the one-inflation is present may select one of the zero-truncated one-inflated (ztoi*) or one-inflated zero-truncated (oizt*) such as oiztpoisson for Poisson or ztoinegbin for NB2.

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

Argument	Description
formula	The main formula (i.e for the Poisson λ parameter)
data	the 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 documentation. The supplied argument should have the form model = "ztpoisson", model = ztpoisson or if link function should be specified then model = ztpoisson(lambdaLink = "log") can be used
method	numerical method used to fit regression IRLS or optim
popVar	a method for estimating variance of \hat{N} and confidence interval creation (either bootstrap, analytic or skipping the estimation entirely)
controlMethod, controlModel or controlPopVar	control parameters for numerical fitting, specifying additional formulas (inflation, dispersion) and population size estimation respectively
offset	a matrix of offset values with 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: estimatePopsize function arguments description

3.2. Controlling the variance estimation with the controlPopVar

The estimatePopsize function allows to specify the variance estimation method via the popVar (e.g. analytic or variance bootstrap) as well as controlling the estimation process by specifying controlPopVar. In the control function controlPopVar user may 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 are:

- alpha, B significance level and number of bootstrap samples to be performed respectively with 0.05 and 500 being the default options.
- cores number of process cores to use in bootstrap (1 by default) parallel computing is done via doParallel (Microsoft and Weston 2022a), foreach (Microsoft and Weston 2022b) or parallel packages (R Core Team 2023).
- keepbootStat logical value indicating whether to keep a vector of statistics produced by 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 fitting method (by default the same as used in the original call) and control parameters (controlMethod) for model fitting in bootstrap.

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

In the next sections we provide a case study on the usage of a simple zero-truncated Poisson regression and a more advanced model: one-inflated zero-truncated geometric regression with cloglog link function. First, we describe example dataset, then we present how to estimate the population size and assess the quality and diagnostics measures. Finally, we show how to estimate population size in a user-specified sub-populations.

4. Data analysis example

The package can be installed in a standard way using:

R> install.packages("singleRcapture")

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

R> library(singleRcapture)

4.1. Dataset

We will use dataset from van der Heijden et al. (2003) that contains information about immigrants in four cities (Amsterdam, Rotterdam, The Hague and Utrecht) in Netherlands that have been staying in the country without a legal permit in 1995 and have appeared in police records that year. This dataset is included in the package under the name netherlandsimmigrant:

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

```
capture gender
                                            nation
                    age
                               reason
1
        1
            male <40yrs Other reason North Africa
2
            male <40yrs Other reason North Africa
3
            male <40yrs Other reason North Africa
            male <40yrs Other reason
4
5
            male <40yrs Other reason
        1
                                              Asia
            male <40yrs Other reason North Africa
```

The number of times each individual appeared in the records is included in the capture variable with the available covariates being gender, age, reason, nation being respectively the persons gender and age, reason for being captured and region of the world from which each person comes:

R> summary(netherlandsimmigrant)

```
capture
                    gender
                                    age
                                                        reason
Min.
       :1.000
                 female: 398
                                <40yrs:1769
                                              Illegal stay: 259
1st Qu.:1.000
                 male :1482
                                >40yrs: 111
                                              Other reason:1621
Median :1.000
       :1.162
Mean
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 point which we should make while analysing this data set is that there is a disproportionate 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 is vary similar to that of glm with the output of the summary method being also quite similar except for the additional results of the population size estimates (denoted as Population size estimation results).

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

```
Call:
```

```
estimatePopsize.default(formula = capture ~ gender + age + nation,
    data = netherlandsimmigrant, model = ztpoisson())
```

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	
nationRest of Africa	-0.9106	0.3008	-3.027	0.002468	**
nationSurinam	-2.3364	1.0136	-2.305	0.021159	*
nationTurkey	-1.6754	0.6028	-2.779	0.005445	**
Signif. codes: 0 '**	**' 0.001	'**' 0.01	·*' 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 2808.169

95% CI for the population size:

lowerBound upperBound

normal 7186.444 18194.26 logNormal 8431.275 19718.32

95% CI for the share of observed population:

lowerBound upperBound

normal 10.332927 26.16037 logNormal 9.534281 22.29793

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

According to this simple model the population size is about 12.5k with about 15% of units observed in the register. The 95% CI under normality indicate that the true population size may be between 7k-18k with about 10% to 26% observed in the register.

Since there is a reasonable suspicion that the act of observing a unit in the dataset may led to undesirable consequences from the point of view of the subject of the observation (here possible deportation, detainment or similar). For those reason researcher may consider one-inflated models such as oiztgeom and presented below.

```
R> set.seed(123456)
R> modelInflated <- estimatePopsize(</pre>
     formula = capture ~ nation,
     model
            = oiztgeom(omegaLink = "cloglog"),
             = netherlandsimmigrant,
     data
     controlModel = controlModel(
         omegaFormula = ~ gender + age
     ),
     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
                               0.4343 -2.737 0.00619 **
                    -1.1888
nationTurkey
For linear predictors associated with: omega
           Estimate Std. Error z value P(>|z|)
(Intercept) -1.4577 0.3884 -3.753 0.000175 ***
                     0.3602 -2.426 0.015267 *
gendermale
           -0.8738
```

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

This approach suggest that the population size is about 7k which is about 5k less than the naive Poisson approach. Comparison of AIC and BIC suggest that the one-inflation model fits the data better with BIC for oiztgeom 1727 and 1757 for ztpoisson.

We can access the results of population size estimation using the following code which returns list with numerical results.

R> popSizeEst(basicModel) #basicModel\$populationSize

95% CI for the share of observed population:

37.58941

Point estimate: 12690.35

lowerBound upperBound

16.46816

Variance: 7885812

95% confidence intervals:

lowerBound upperBound normal 7186.444 18194.26 logNormal 8431.275 19718.32

R> popSizeEst(modelInflated) #modelInflated\$populationSize

Point estimate: 6699.953

Variance: 2956175

95% confidence intervals: lowerBound upperBound 5001.409 11415.969 Decision whether to use zero-truncated Poisson or one-inflated zero-truncated geometric should be on the assessment of the model and the assumptions on the data generation process. One possible method of method selection is based on likelihood ratio test which can be computed quickly and conveniently with the **lmtest** (Zeileis and Hothorn (2002)) interface:

this is however not a standard method of model selection in SSCR. The next sections are dedicated to providing details how to assess the results using more standard statistical tests and diagnostics.

4.2. Testing marginal frequencies

A popular method of testing the model fit in single source capture-recapture studies is 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 $\sum_{j=1}^{N} \mathcal{I}_{\{k\}}(Y_k) = \sum_{j=1}^{N_{obs}} \mathcal{I}_{\{k\}}(Y_k)$ for $k \geq 1$. If a fitted model bears sufficient resembles of the following sufficient resembles on the following sufficient resembles of the fo

blance to the real data collection process these quantities should be quite close and both G and χ^2 tests may be employed in order to test the statistical significance of the discrepancy with the following **singleRcapture** syntax for the Poisson model (rather poor fit):

```
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 the 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 the fitted and marginal frequencies which we can get with the syntax:

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

Plots suggest that the oiztgeom model fits the data better. Furthermore, important issue in population size estimation is the diagnostics of the models in order to verify whether influential observations are present in the data. For this purpose leave-one-out (LOO) diagnostic implemented in the dfbeta from the stats package was adapted and demonstrated below:

```
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

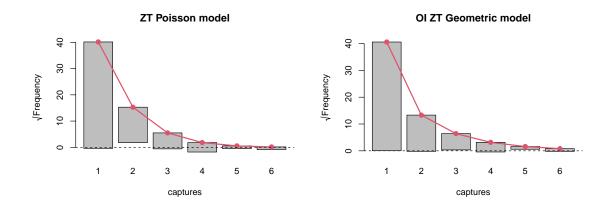


Figure 1: Rootograms for ztpoisson (left) and oiztgeom (right) models

```
      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
      -9.3140
      -0.0066
      0.0020
      0.0035
      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	0.0157	0.0347	12.2406
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	2.0393

Furthermore, result of the dfbeta can be further used in the function dfpopsize which allows for quantification of 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)</pre>
```

Warning in dfpopsize.singleRStaticCountData(modelInflated, dfbeta = dfi): dfpopsize may (in some cases) not work correctly when bootstrap was chosen as population variance estimate.

```
R> summary(dfb_pop)
```

```
Min.
             1st Qu.
                          Median
                                       Mean
                                               3rd Qu.
                                                             Max.
-4236.412
               2.664
                           2.664
                                      5.448
                                                17.284
                                                          117.448
R> summary(dfi_pop)
     Min.
             1st Qu.
                          Median
                                       Mean
                                               3rd Qu.
                                                             Max.
-456.6443
             -3.1121
                         -0.7243
                                     3.4333
                                                5.1535
                                                         103.5949
```

The comparison of deletion effect on population size estimate and inverse probability weights, which refer to the contribution of a given observation to the population size estimation, is presented in the Figure bellow:

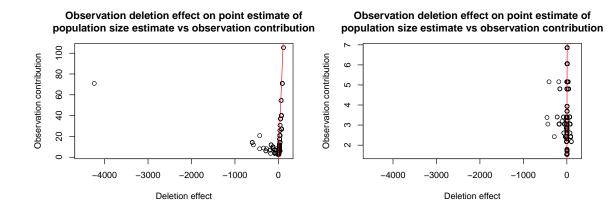


Figure 2: Results for ztpoisson (left) and oiztgeom (right) model

These plot informs on the change of the population size if a given observation will be removed. For instance if we remove observation 542 from the data then population size will rise by about 4236 for the ztpoisson model. While for the oiztgeom the largest change is 457 for the 900 observation.

The full list of plot types along with the list of optional arguments which may be passed from the call to the plot method down to base R and graphics functions is listed in the help file of the plot method.

R> ?plot.singleRStaticCountData

4.4. The stratifyPopsize function

Researchers may be interested on only in the total population size but also in specific sub-populations (e.g. males, females, group pages). For that reason we have created the

stratifyPopsize function which allows to estimate the size by stratas defined by the coefficients in the model (the default option). In the output below we present results based on the ztpoisson and oiztgeom models.

R> popSizeStratas <- stratifyPopsize(basicModel)</pre>

10

```
R> cols <- c("name", "Observed", "Estimated", "logNormalLowerBound",
            "logNormalUpperBound")
R> popSizeStratas_report <- popSizeStratas[, cols]</pre>
R> cols_custom <- c("Name", "Obs", "Estimated", "LowerBound", "UpperBound")
R> names(popSizeStratas_report) <- cols_custom</pre>
R> popSizeStratas_report
                                    Obs Estimated LowerBound UpperBound
                              Name
1
                   gender==female
                                    398
                                         3811.0924
                                                     2189.0439
                                                                  6902.140
2
                      gender==male 1482
                                         8879.2613
                                                     6090.7752
                                                                 13354.889
3
                       age==<40yrs 1769 10506.8994
                                                     7359.4140
                                                                 15426.465
4
                       age==>40yrs
                                    111
                                          2183.4543
                                                      872.0130
                                                                  5754.881
5
  nation == American and Australia
                                    173
                                           708.3688
                                                      504.6086
                                                                  1037.331
6
                      nation==Asia
                                    284
                                         2742.3147
                                                     1755.2548
                                                                  4391.590
                                         3055.2033
7
             nation==North Africa 1023
                                                     2697.4900
                                                                  3489.333
8
           nation==Rest of Africa 243
                                         2058.1533
                                                     1318.7466
                                                                  3305.786
9
                  nation==Surinam
                                     64
                                         2386.4544
                                                      505.2460
                                                                 12288.008
10
                   nation==Turkey
                                     93
                                         1739.8592
                                                      638.0497
                                                                  5068.959
R> popSizeStratas_inflated <- stratifyPopsize(modelInflated)</pre>
R> popSizeStratas_inflated_report <- popSizeStratas_inflated[, cols]</pre>
R> names(popSizeStratas_inflated_report) <- cols_custom</pre>
R> popSizeStratas_inflated_report
                              Name
                                    Obs Estimated LowerBound UpperBound
   nation == American and Australia
                                    173 516.2432
                                                     370.8463
                                                                 768.4919
1
2
                     nation==Asia 284 1323.5377
                                                     831.1601
                                                                2258.9954
3
             nation==North Africa 1023 2975.8801
                                                    2254.7071
                                                               4119.3050
4
           nation==Rest of Africa 243 1033.9753
                                                               1716.4484
                                                     667.6106
5
                  nation==Surinam
                                                     193.8891
                                                                712.4739
                                     64
                                         354.2236
6
                   nation==Turkey
                                     93 496.0934
                                                     283.1444
                                                                947.5309
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
```

The function stratifyPopsize, that is prepared for the objects of the singleRStaticCountData class, accepts three optional parameters stratas, alpha, cov which correspond to specification of sub-populations, the significance levels and the covariance matrix that will be used to compute standard errors. An example of the full call is presented below.

262.1379

170.9490

492.0347

```
R> library(sandwich)
R> popSizeStratasCustom <- stratifyPopsize(</pre>
    object = basicModel,
    stratas = ~ gender + age,
           = rep(c(0.1, 0.05), each=2),
            = vcovHC(basicModel, type = "HC4")
+ )
R>
R> popSizeStratasCustom report <- popSizeStratasCustom[, c(cols, "confLevel")]
R> names(popSizeStratasCustom_report) <- c(cols_custom, "alpha")
R> popSizeStratasCustom_report
                 Obs Estimated LowerBound UpperBound alpha
                       3811.092 2275.6410
1 gender==female 398
                                             6602.168
                                                       0.10
   gender==male 1482 8879.261
                                 6261.5109
                                            12930.760
                                                       0.10
3
     age==<40yrs 1769 10506.899
                                7297.2057
                                            15580.151
                                                       0.05
     age==>40yrs 111
                       2183.454
                                  787.0673
                                             6464.016
                                                       0.05
```

We provide integration with the sandwich (Zeileis, Köll, and Graham 2020) package to correct variance-covariance matrix in the δ 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 strata and a formula to specify that we wanted estimates for both males and females subdivided by nation and age. The stratas parameter may be specified either as:

- a formula with empty left hand side which we have seen here (e.g. ~ gender * age),
- a logical vector with number of entries equal to number of rows in the dataset in which case only one strata will be created (e.g. netherlandsimmigrant\$gender == "male"),
- a (named) list where each element is a logical vector, names of the list will be used to specify names variable in returned object, for example: "'=latex

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

- a vector of names of explanatory variables which will result in every level of explanatory variable having its own sub population for each variable specified (e.g. c("gender", "age")),
- or not supplied at all in which case stratas 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).

One may 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")
```

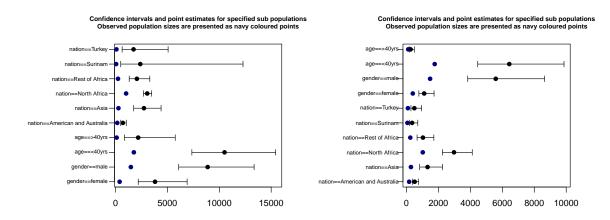


Figure 3: Population size by covariates for ztpoisson (left) and oiztgeom (right) model

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

5. Classes and S3methods

For the purpose of the package we have created classes singleRStaticCountData, singleR (for now the two former classes are the same, the distinction is made for future development), singleRfamily, popSizeEstResults, summarysingleRStaticCountData and summarysingleRmargin which allows for extracting relevant information regarding the population size.

For instance, function popSizeEst allows to extract information on the estimated size of the population as given below:

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

Point estimate: 12690.35

Variance: 7885812

95% confidence intervals:

lowerBound upperBound 7186.444 18194.26

normal 7186.444 18194.26 logNormal 8431.275 19718.32

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

- pointEstimate, variance numerics containing point estimate and variance of this estimate.
- confidenceInterval a data.frame with confidence intervals.
- boot If 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 obtained 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
                  -2.3363962 1.0135645 -2.3051282 2.115939e-02
nationSurinam
                  -1.6753917 0.6027744 -2.7794674 5.444812e-03
nationTurkey
```

analogously to glm from stats. The singleRfamily inherits the family class from stats and has explicitly defined print and simulate methods defined. 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		et	ta	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	Mean	:-0.8982	Mean	:0.4196
3rd Qu	.:0.0000	3rd Qu	.:-1.0000	3rd Qu	.:1.0000
Max.	:1.0000	Max.	:-0.5000	Max.	:5.0000

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

Function	Description
fitted	Which work almost exactly like glm counterparts but return more information, namely on fitted values for the truncated and non-truncated probability distribution.
logLik	which compared to glm method 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	which has the possibility of returning the $X_{\rm vlm}$ matrix defined in 3
simulate	which calls simulate method for the chosen model and fitted η
predict	which has the possibility of returning either of fitted ditribution parameters for each unit (type = "response"), just linear predictors (type = "link"), means of the fitted distributnios of Y and $Y Y>0$ (type = "mean") and the inverse probability weights (type = "contr"). There us also the se.fit argument which can be set to TRUE to obtain standard errors for each of those by using the δ method. Also it is possible to use a custom covariance matrix for standard error computation (argument cov).
redoPopEstimation	A function that applies all post-hoc procedures that were taken (such as heteroscedastic consistent covariance matrix estimation via countreg) to population size estimation and standard error estimation.
residuals	for obtaining residuals of several types, we refer interested readers to the manual ?singleRcapture:::residuals.singleRStaticCountData.
stratifyPopsize,	which were already discussed. Compared to glm class summary has the
summary	possibility of adding confidence interval to the coefficient matrix (argument confint = TRUE) and using custom covariance matrix (argument cov = someMatrix)
plot	which was already discussed
popSizeEst	an extractor showcased above.
cooks.distance	which works only for single predictor models
dfbeta, dfpopsize	Multithreading in dfbeta is available and dfpopsize calls dfbeta if no dfbeta object was provided at call.
bread, estfun, vcovHC	for (almost) full sandwich compatibility.
AIC, BIC, extractAIC, family, confint,	Which work exactly like glm counterparts.
df.residual,	
model.frame,	
hatvalues, nobs, print	

Table 2: S3Methods implemented in the singleRcapture

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 allows for converting 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 are accessed by

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

Using the fitted zerotrunc, vglm, vgam class objects in population size estimation such as the one 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 as our goal is to show usage of additive models and how it handled in the singleRcapture package.

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

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

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

The resulting object is of class singleRforeign to underline that the parameters were estimated outside the singleRcapture. Resulting object consist of the following elements

```
R> str(modelVgamPop,1)

List of 5
$ foreignObject :Formal class 'vgam' [package "VGAM"] with 43 slots
$ call : language estimatePopsize.vgam(formula = modelVgam)
$ sizeObserved : int 12036
$ populationSize:List of 5
..- attr(*, "class")= chr "popSizeEstResults"
$ derivFunc : function (eta)
- 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|)
                      (Intercept)
                      0.49391 0.02521 19.594 < 2e-16 ***
-0.14106 0.04098 -3.442 0.000578 ***
log size
log_distance
C_TYPEDairy
                      -1.68591 0.55327 -3.047 0.002310 **
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
logNormal
           35661.32 42530.37
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
           29.38793 34.82193
normal
logNormal 29.24274 34.62823
-- Summary of foreign object --
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
                                                     1
s(log_size, df = 3)
                                                     1
                                                           1.8
                                                                   51.949
s(\log_{distance}, df = 2)
                                                           1.0
                                                                    3.503
s(log_size, df = 3):s(log_distance, df = 2):C_TYPE 2
                                                      P(Chi)
(Intercept):1
(Intercept):2
s(log_size, df = 3)
                                                    0.000000
s(log_distance, df = 2)
                                                    0.063835
s(log_size, df = 3):s(log_distance, df = 2):C_TYPE
```

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 allows for different methods to account for heterogeneity in capture probabilities, modelled using covariates, as well as behavioural change, modelled using one-inflation. We have build the package in a such way that it is easy to implement new models using **family** objects which is demonstrated in the Appendix A.2.

In future work we plan on implementing 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 may use the recent approach proposed by Tuoto, Di Cecco, and Tancredi (2022) and implement our own families using the brms package.

8. Acknowledgements

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A. Detailed information

A.1. The estimatePopsizeFit function

In this section we provide step-by-step description how to prepare data to use the estimatePopsizeFit function that may be useful to some user e.g. those wishing to make modifications to \hat{N} estimate or to the bootstrap. In order to demonstrate the usage 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{t}}(\omega) = \beta_{2,1} + \beta_{2,2}\log_{\text{distance}} + \beta_{2,3}C_{\text{TYPE}}.
```

This would be equivalent to esimatePopsize call:

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

1. Create data matrix $X_{\rm vlm}$

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

3. Obtain starting β parameters using glm.fit function.

```
R> start <- glm.fit(# get starting points
+ y = farmsubmission$TOTAL_SUB,
+ x = X[1:NROW(farmsubmission), 1:4],
+ family = poisson()
+ )$coefficients
R> start
```

[1] -0.82583943 0.33254499 -0.03277732 0.32746933

4. Use estimatePopsizeFit function to fit the model assuming 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(),
                 = controlMethod(silent = TRUE),
   control
                = c(start, 0, 0, 0),
   coefStart
                 = matrix(X %*% c(start, 0, 0, 0), ncol = 2),
  etaStart
                 = cbind(rep(0, NROW(farmsubmission)),
+
   offset
                         rep(0, NROW(farmsubmission)))
+ )
```

5. Compare our results with those from 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
1
      -2.7845
                  -2.5971
2
       0.6170
                   0.6163
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
      15.0000
                1696.0000
```

The default maxiter parameter for "optim" fitting is 1000, here we needed to increase it since the optim did not converge in 1000 steps and still "gets stuck" in at a plateau resulting as we see indicating by lower log-likelihood value as compared to the standard "IRLS".

The situation above is rather typical, although we conducted no formal numerical analyses it seems that when one attempts to model more than one parameter of the distribution as covariate dependent <code>optim</code> 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 on 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:
	$\ell(\boldsymbol{\beta}), \frac{\partial \ell}{\partial \boldsymbol{\beta}}, \frac{\partial^2 \ell}{\partial \boldsymbol{\beta}^\top \partial \boldsymbol{\beta}}$
	functions from y vector and X_{vlm} the argument deriv with possible values in $c(0, 1, 2)$ provides which derivative to return with the default 0 being just the minus log-likelihood
links	List with link functions
mu.eta, variance	Functions of linear predictors that return expected value and variance. There is a 'type' argument with 2 possible values "trunc" and "nontrunc" that specifies whether to return $\mathbb{E}[Y Y>0]$, var $[Y Y>0]$ or $\mathbb{E}[Y]$, var $[Y]$ respectively, also the deriv argument with values in c(0, 1, 2) is used for indicating the derivative with respect to the linear predictors with is used for providing standard error in predict method
family	Character that specifies name of the model
valideta, validmu	For now only returns true. In near future will be used to check whether applied linear predictors are valid (i.e. are transformed into some elements of parameter space the subjected to inverse link function)
funcZ, Wfun	Functions that create pseudo residuals and working weights used in IRLS algorithm
devResids	Function that given the linear predictors prior weights vector and response vector returns deviance residuals
pointEst, popVar	Functions that given prior weights linear predictors and in the later case also estimation of $cov(\hat{\beta})$ and X_{vlm} matrix return point estimate for population size and analytic estimation of its variance. There is a additional boolean parameter contr in the former function that if set to true returns contribution of each unit
etaNames	Names of linear predictors
densityFunction	A function that given linear predictors returns value of PMF at values x . Additional argument type specifies whether to return $\mathbb{P}[Y Y>0]$ or $\mathbb{P}[Y]$
simulate	A function that generates values of dependent vector given linear pre- dictors
getStart	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"),</pre>
                                          = c("logit", "cloglog", "probit"),
                                piLink
                                ...) {
    if (missing(lambdaLink)) lambdaLink <- "logit"</pre>
   if (missing(piLink)) piLink <- "logit"</pre>
   links <- list()</pre>
   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 link up to third order:
R> singleRcapture:::singleRinternalcloglogLink
function (x, inverse = FALSE, deriv = 0)
{
   deriv <- deriv + 1
   if (isFALSE(inverse)) {
```

one might of course include code for computing them manually.

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