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singleRcapture: A Package for Single-Source Capture-Recapture Models

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Abstract

Estimating population size is an important issue in official statistics, social sciences and natural sciences. One way to approach this problem is to use capture-recapture methods, which can be classified according to the number of sources used, the main distinction being between methods based on one source and those based on two or more sources. In this presentation we will introduce the **singleRcapture** R package for fitting SSCR models. The package implements state-of-the-art models as well as some new models proposed by the authors (e.g. extensions of zero-truncated one-inflated and one-inflated zero-truncated models). The software is intended for users interested in estimating the size of populations, particularly those that are difficult to reach or for which information is available from only one source and dual/multiple system estimation cannot be used.

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. 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. 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. 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. 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. 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. 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 is implemented in various open-source software the single-source capture-recapture (SSCR) methods are less available or partially implemented in existing packages. The goal of the paper is to bridge this gap by the **singleRcapture** and **singleRcaptureExtra** packages which implements state-of-the-art methods in SSCR and provides user friendly API which mimics existing R software. In the next subsections we briefly describe the main approach used in SSCR and the available software that tan be used for estimating population size based on SSCR methods.

1.1. 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 $Y_k >$ 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

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

where $I_k := \mathcal{I}_{\mathbb{N}}(Y_k)$, and maximum likelihood estimate of N is obtained after substituting regression estimates for $\mathbb{P}[Y_k > 0|\boldsymbol{x}_k]$ into (1).

The analytic variance estimation is then done by computing two parts of the decomposition due to the law of total variance given by

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

where the first part can be estimated using the multivariate δ method given by

$$\mathbb{E}\left[\operatorname{var}\left[\hat{N}|I_1,\ldots,I_n\right]\right] = \left(\frac{\partial(N|I_1,\ldots,I_N)}{\partial\boldsymbol{\beta}}\right)^\top \operatorname{cov}\left[\boldsymbol{\beta}\right]\left(\frac{\partial(N|I_1,\ldots,I_N)}{\partial\boldsymbol{\beta}}\right)\Bigg|_{\boldsymbol{\beta}=\hat{\boldsymbol{\beta}}}, \tag{3}$$

while the second part of the decomposition in (2) is under the assumption of independence of I_k's and after some omitted simplifications one sees that this is optimally estimated by

$$\operatorname{var}\left(\mathbb{E}(\hat{N}|I_1,\ldots,I_n)\right) = \operatorname{var}\left(\sum_{k=1}^{N}\frac{I_k}{\mathbb{P}(Y_k>0)}\right) \approx \sum_{k=1}^{N_{obs}}\frac{1-\mathbb{P}(Y_k>0)}{\mathbb{P}(Y_k>0)^2}, \tag{4}$$

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

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

where:

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

where z is standardized 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, Bustami, Cruyff, Engbersen, and van Houwelingen 2003).

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

While population size estimation based on two or more source have many implementations in R (cf.) and other languages (cf.) methods for SSCR are only partially covered. For instance, **countreg** or **VGAM** covers selected number of truncated distributions and (pkg for distributions, e.g. distributions3). More advanced methods are not widely available and need to be implemented from scratch. Moreover, estimation of variance or diagnostics are not widely available in open-source software which limits possibilities of easy usage of these methods in comparison to multiple source capture-recapture methods.

Therefore, the goal of the **singleRcapture** is R language is to bridge this gap to provide scientists tool for estimation of population size based on SSCR methods. The package implements state-of-the-art methods such as .... and its extensions (full list of available methods is presented in section ...). The package implements variance estimation based on various methods 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`).

The remaining part of the paper is as follows. In Section @ref(sec-basic-usage) introduces the package main functionalities, covers main S3 methods as well as implemented diagnostics and useful functions. Section @ref(sec-details) provides information on the fitting methods, the `estimatePopsizeFit` function for estimating population size with more control and presents information on the available methods. Section @ref(sec-integration) covers integration with **countreg** and **VGAM** packages through **singleRcaptureExtra** package. The paper ends with conclusions and an appendix that

2. Basic usage

2.1. 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. The most important arguments are:

- `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 `model = ztpoisson(lambdaLink = "log")` the third way is the only one where the user may (but doesn't have to) select a link function.
- `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, controlPopVar` – control parameters for numerical fitting, specifying additional formulas (inflation, dispersion) and population size estimation respectively. We will tackle these arguments separately,
- `offset` – a matrix of offset values with number of columns matching the number of distribution parameters providing offset values to each of linear predictors.

With the `formula, data, model` being the three arguments which must be provided in `estimatePopsize` syntax.

Example with R code

The package should be installed from CRAN `https://cran.r-project.org/package=singleRcapture` with the usual code:

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

To showcase the main function let us recreate the zero truncated Poisson model from van der Heijden *et al.* (2003) on the same data included in the package under the name `netherlandsimmigrant`:

```
R> library(singleRcapture)
R> head(netherlandsimmigrant)

  capture gender    age        reason       nation
1       1   male <40yrs Other reason North Africa
2       1   male <40yrs Other reason North Africa
3       1   male <40yrs Other reason North Africa
4       1   male <40yrs Other reason         Asia
5       1   male <40yrs Other reason         Asia
6       2   male <40yrs Other reason North Africa
```

This data set contains information about immigrants in four cities (Amsterdam, Rotterdam, The Hague and Utrecht) in Netherlands that have been staying in the country illegally in 1995 and have appeared in police records that year. 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
 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
```

The basic syntax is indeed vary similar to that of `glm` with the output of the summary method being also quite simmilar except for the additional results of the population size estimates:

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

```
Warning in singleRcaptureinternalIRLSmultipar(dependent = y, covariates = X, :
Convergence at halfstepsize
```

```
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 2808.165
95% CI for the population size:
          lowerBound upperBound
normal      7186.449   18194.25
logNormal   8431.277   19718.31
95% CI for the share of observed population:
          lowerBound upperBound
```

```
normal     10.332933   26.16035
logNormal   9.534288   22.29793
```

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 (see table bellow):

```
R> table(netherlandsimmigrant$capture)


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

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 one should

```
R> set.seed(123456)
R> modelInflated <- estimatePopsize(
+     formula = capture ~ nation,
+     model   = oiztgeom(omegaLink = "cloglog"),
+     data    = netherlandsimmigrant,
+     controlModel = controlModel(
+         omegaFormula = ~ gender + age
+     ),
+     popVar = "bootstrap",
+     controlPopVar = controlPopVar(bootType = "semiparametric")
+ )

Warning in estimatePopsize.default(formula = capture ~ nation, model = oiztgeom(omegaLink
NOTE: Second derivative test failing does not
        necessarily mean that the maximum of score function that was found
        numericaly is invalid since R^k is not a bounded space.
Additionally in one inflated and hurdle models second derivative test often fails even on

Warning in estimatePopsize.default(formula = capture ~ nation, model =
oiztgeom(omegaLink = "cloglog"), : Switching from observed information matrix
to Fisher information matrix because hessian of log-likelihood is not negative
define.

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.     Max.
-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
0 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
```

Methods

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

Point estimate: 12690.35
Variance: 7885790
95% confidence intervals:
          lowerBound upperBound
normal      7186.449   18194.25
logNormal   8431.277   19718.31
```

the `popEst` object is of the `popSizeEstResults` class and `list` type and 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.

```
R> dfb <- dfbeta(basicModel)
R> apply(dfb, 2, quantile)

       (Intercept)    gendermale     age>40yrs    nationAsia nationNorth Africa
0%   -0.0099087522 -0.0905349870 -0.0200100686 -9.555875e-02      -9.660498e-02
25%  -0.0015325874 -0.0007770048  0.0001792918 -5.288544e-04      -8.417624e-04
50%   0.0001906118 -0.0002829978  0.0003789034  6.642632e-05      -1.768274e-04
75%   0.0005208531  0.0010171840  0.0006909682  1.199821e-04       8.674555e-05
100%  0.0866193889  0.0221346454  0.1600608767  1.799137e-01       3.125955e-02
     nationRest of Africa nationSurinam  nationTurkey
0%          -9.449682e-02 -9.313832e-02 -9.619821e-02
25%         -2.436010e-04 -6.484354e-05 -2.199798e-04
50%          2.984337e-05  2.101820e-05  7.918083e-05
75%          8.278833e-05  3.676223e-05  1.427685e-04
100%         1.097872e-01  9.933828e-01  3.209798e-01

R> dfp <- dfpopsize(basicModel, dfbeta = dfb)
R> summary(dfp)

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

2.2. Marginal frequencies

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

```
R> margFreq <- marginalFreq(basicModel)
R> summary(margFreq, df = 1, dropl5 = "group")
```

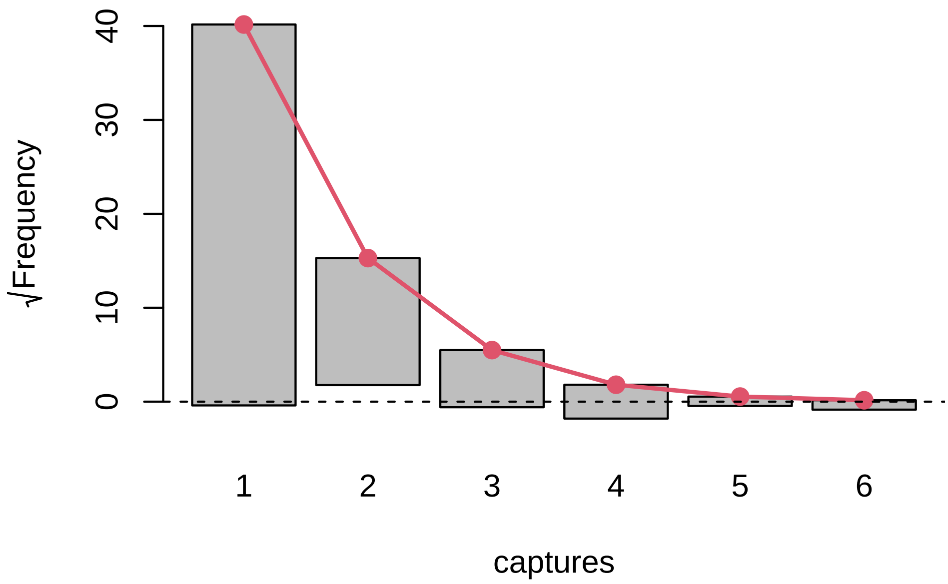
```
Test for Goodness of fit of a regression model:

                 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
```

where the `dropl5` 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.

2.3. Plots

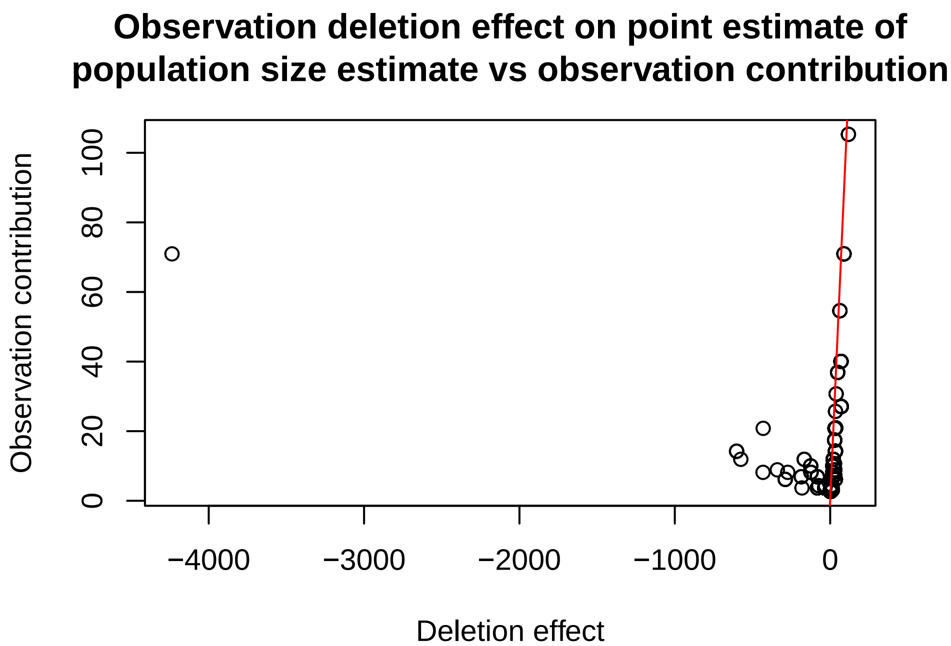
The `singleRStaticCountData` class has a `plot` method implementing several types of quick demonstrative plots such as the rootogram Kleiber and Zeileis (2016) for comparing the fitted and marginal frequencies which we can get with the syntax:

```
R> plot(basicModel, plotType = "rootogram")
```



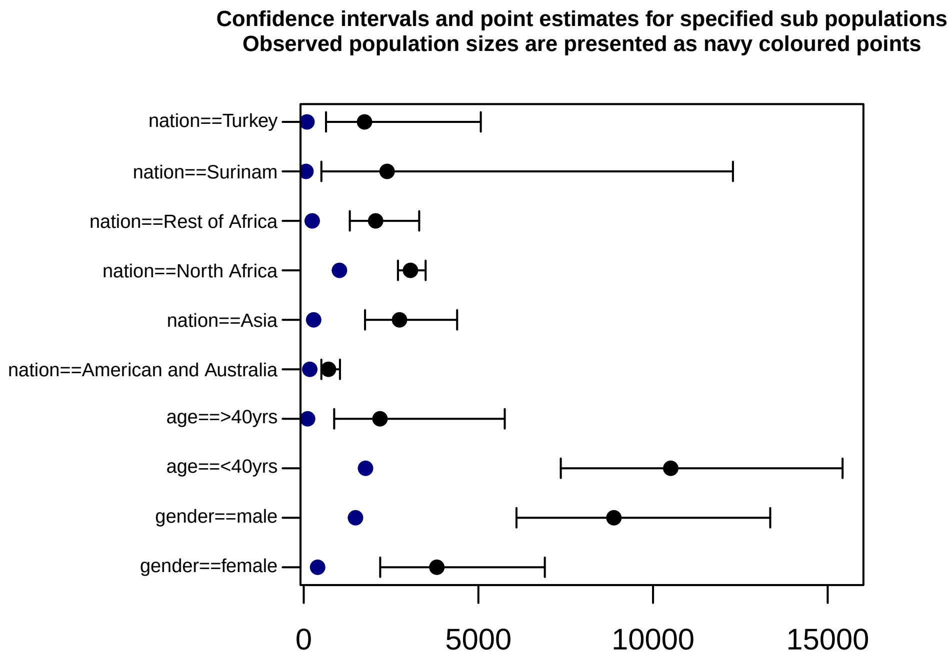
The comparison of deletion effect on population size estimate and inverse probability weights:

```
R> plot(basicModel, plotType = "dfpopContr", dfpop = dfp)
```



and the plot that showcases stratified stimates:

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



the information which was supplied to the plot function above comes from the `stratifyPopsize` method:

```
R> stratifyPopsize(basicModel)

   Observed  Estimated ObservedPercentage  StdError normalLowerBound
1       398  3811.0911          10.443203 1153.9733       1549.34513
2      1482  8879.2594          16.690581 1812.0790       5327.64991
3      1769 10506.8971          16.836560 2017.2284       6553.20200
4       111  2183.4535           5.083690 1132.4502        -36.10819
5       173   708.3688          24.422308  132.8183        448.04969
6       284  2742.3147          10.356215  655.0929       1458.35623
7      1023  3055.2033          33.483860  201.2387       2660.78263
8       243  2058.1533          11.806701  493.2612       1091.37903
9        64  2386.4513           2.681806 2380.1835      -2278.62266
10       93  1739.8592           5.345260 1008.1794       -236.13602
   normalUpperBound logNormalLowerBound logNormalUpperBound
1         6072.8372           2189.0443            6902.133
2        12430.8689           6090.7762           13354.880
3        14460.5922           7359.4155           15426.455
4         4403.0151            872.0130            5754.876
5          968.6878            504.6086            1037.331
6         4026.2732           1755.2548            4391.590
7         3449.6240           2697.4900            3489.333
8         3024.9276           1318.7466            3305.786
9         7051.5252            505.2457           12287.983
10        3715.8544            638.0497            5068.959
                     name confLevel
1          gender==female      0.05
2            gender==male      0.05
3             age==<40yrs      0.05
4             age==>40yrs      0.05
```

```
5  nation==American and Australia      0.05
6                     nation==Asia      0.05
7             nation==North Africa      0.05
8           nation==Rest of Africa      0.05
9                  nation==Surinam      0.05
10                  nation==Turkey      0.05
```

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:

```
R> ?plot.singleRStaticCountData
```

The `stratifyPopsize` *method*

As previously showcased the `stratifyPopsize` may be used to estimate the population sizes for different stratas using the same fitted regression model as previously computed using the call to the `estimatePopsize` function. The method for `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.

The full call is of the type:

```
R> library(sandwich)

Warning: package 'sandwich' was built under R version 4.3.3

R> stratifyPopsize(
+   object  = basicModel,
+   stratas = ~ gender / (nation + age),
+   alpha   = rep(c(.1, .2, .3, .4, .5),
+                 length.out = 18),
+   cov     = vcovHC(basicModel, type = "HC4")
+ )

   Observed Estimated ObservedPercentage   StdError normalLowerBound
1       398 3811.0911          10.443203 1282.09956       1702.22504
2      1482 8879.2594          16.690581 1999.39209       6316.93533
3        67  328.8780          20.372297   84.81957        240.96814
4       106  379.4908          27.932167   83.91530        308.86588
5        62  775.9054           7.990665  303.01257        571.52651
6       222 1966.4093          11.289613  603.18021        974.26616
7       169  644.0545          26.240014  116.46407        494.79982
8       854 2411.1488          35.418801  172.33202       2232.53812
9        65  682.1776           9.528310  218.28791        498.46186
10      178 1375.9757          12.936275  369.03697       1127.06403
11       20  931.4677           2.147149  985.54139       -689.60358
12       44 1454.9835           3.024089 1520.27163       -493.32295
13       15  448.6079           3.343677  300.30767        137.35901
14       78 1291.2513           6.040652  733.06058        674.29194
15      378 3169.8263          11.924944  937.42614       2537.54198
16     1391 7337.0708          18.958520 1313.47160       5176.60226
17       20  641.2648           3.118836  453.82492         59.66481
18       91 1542.1886           5.900705  887.97851        621.85804
   normalUpperBound logNormalLowerBound logNormalUpperBound
```

```
1         5919.9573           2275.6416           6602.1612
2        11441.5835           6745.5675          11877.8858
3          416.7878            255.7692            430.3013
4          450.1157            318.4739            458.0301
5          980.2842            604.5269           1001.4205
6         2958.5525           1225.6476           3253.9046
7          793.3092            517.5628            816.4495
8         2589.7594           2242.8856           2599.7970
9          865.8933            527.2996            888.9423
10        1624.8873           1155.7975           1645.7331
11        2552.5391            234.3583           3895.6296
12        3403.2900            502.1052           4389.8894
13         759.8568            241.6446            844.5624
14        1908.2106            836.6593           2018.2367
15        3802.1106           2617.4717           3858.4164
16        9497.5393           5543.4798           9905.3720
17        1222.8649            288.7316           1456.2658
18        2462.5192            899.8794           2694.5381
                                          name confLevel
1                                gender==female       0.1
2                                  gender==male       0.2
3  genderfemale:nationAmerican and Australia       0.3
4    gendermale:nationAmerican and Australia       0.4
5                        genderfemale:nationAsia       0.5
6                          gendermale:nationAsia       0.1
7                genderfemale:nationNorth Africa       0.2
8                  gendermale:nationNorth Africa       0.3
9              genderfemale:nationRest of Africa       0.4
10               gendermale:nationRest of Africa       0.5
11                    genderfemale:nationSurinam       0.1
12                      gendermale:nationSurinam       0.2
13                     genderfemale:nationTurkey       0.3
14                       gendermale:nationTurkey       0.4
15                        genderfemale:age<40yrs       0.5
16                          gendermale:age<40yrs       0.1
17                        genderfemale:age>40yrs       0.2
18                          gendermale:age>40yrs       0.3
```

where we 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,
- a logical vector with number of entries equal to number of rows in the dataset in which case only one strata will be created,
- a (named) list where each element is a logical vector, names of the list will be used to specify names variable in returned object,
- 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,
- 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).

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

3. Detailed information

3.1. Fitting method

As previously showcased 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 $\boldsymbol{X}_{\text{vlm}}$ at call to `estimatePopsize`. In the context of the models implemented in **singleRcapture** this matrix can be written as:

$$\boldsymbol{X}_{vlm} = \begin{pmatrix} \boldsymbol{X}_1 & \boldsymbol{0} & \dots & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{X}_2 & \dots & \boldsymbol{0} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{0} & \boldsymbol{0} & \dots & \boldsymbol{X}_p \end{pmatrix} \tag{5}$$

where each $\boldsymbol{X}_i$ corresponds to a model matrix associated with user specified formula.

In the context of multi-parameter families we have a matrix of linear predictors $\boldsymbol{\eta}$ 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 $\boldsymbol{\eta}_{(k)}$ is the k'th row of $\boldsymbol{\eta}$, while in the usual IRLS they are scalars $\mathbb{E}\left[-\frac{\partial^2\ell}{\partial\eta_k^2}\right]$ which is often just $-\frac{\partial^2\ell}{\partial\eta^2}$.

1. Initialize with `iter`$\leftarrow 1, \boldsymbol{\eta} \leftarrow$`start` $, \boldsymbol{W} \leftarrow I, \ell \leftarrow \ell(\boldsymbol{\beta})$.
2. Store values from the previous step: $\ell_{-} \leftarrow \ell, \boldsymbol{W}_{-} \leftarrow \boldsymbol{W}, \boldsymbol{\beta}_{-} \leftarrow \boldsymbol{\beta}$ (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: $\boldsymbol{\beta} \leftarrow \left(\boldsymbol{X}_{\text{vlm}}\boldsymbol{W}\boldsymbol{X}_{\text{vlm}}\right)^{-1}\boldsymbol{X}_{\text{vlm}}\boldsymbol{W}\boldsymbol{Z}$.
4. If $\ell(\boldsymbol{\beta}) < \ell(\boldsymbol{\beta}_{-})$ try selecting the smallest value h such that for $\boldsymbol{\beta}_h \leftarrow 2^{-h}\left(\boldsymbol{\beta} + \boldsymbol{\beta}_{-}\right)$ the inequality $\ell(\boldsymbol{\beta}_h) > \ell(\boldsymbol{\beta}_{-})$ holds if this is successful $\boldsymbol{\beta} \leftarrow \boldsymbol{\beta}_h$ else stop the algorithm.
5. If convergence is achieved or `iter` is higher than `maxiter` end algorithm, else `iter`$\leftarrow$ 1+`iter` and return to step 2.

3.2. The `estimatePopsizeFit` function

```
R> X <- matrix(data = 0, nrow = 2 * NROW(farmsubmission), ncol = 7)
R> X[1:NROW(farmsubmission), 1:4] <- model.matrix(
+ ~ 1 + log_size + log_distance + C_TYPE,
+ farmsubmission
+ )
R> X[-(1:NROW(farmsubmission)), 5:7] <- X[1:NROW(farmsubmission), c(1, 3, 4)]
R> # this attribute tells the function which elements of the design matrix
R> # correspond to which linear predictor
R> attr(X, "hwm") <- c(4, 3)
R> start <- glm.fit(# get starting points
+   y = farmsubmission$TOTAL_SUB,
+   x = X[1:NROW(farmsubmission), 1:4],
+   family = poisson()
+ )$coefficients
R> res <- estimatePopsizeFit(
+   y            = farmsubmission$TOTAL_SUB,
+   X            = X,
+   method       = "IRLS",
+   priorWeights = 1,
+   family       = ztoigeom(),
+   control      = controlMethod(silent = TRUE),
+   coefStart    = c(start, 0, 0, 0),
+   etaStart     = matrix(X %*% c(start, 0, 0, 0), ncol = 2),
+   offset       = cbind(rep(0, NROW(farmsubmission)),
+                        rep(0, NROW(farmsubmission)))
+ )# extract results
R> ll <- ztoigeom()$makeMinusLogLike(y = farmsubmission$TOTAL_SUB, X = X)
R> print(c(res$beta, -ll(res$beta), res$iter))

[1] -2.784523e+00  6.170270e-01 -6.455925e-02  5.346108e-01 -3.174491e+00
[6]  1.280589e-01 -1.086452e+00 -1.727876e+04  1.500000e+01

R> # Compare with optim call
R> res2 <- estimatePopsizeFit(
+   y = farmsubmission$TOTAL_SUB,
+   X = X,
+   method = "optim",
+   priorWeights = 1,
+   family = ztoigeom(),
+   coefStart = c(start, 0, 0, 0),
+   control = controlMethod(silent = TRUE),
+   offset = cbind(rep(0, NROW(farmsubmission)), rep(0, NROW(farmsubmission)))
+ )# extract results
R> c(res2$beta, -ll(res2$beta), res2$iter)


-2.640779e+00  6.258275e-01 -8.293688e-02  5.324707e-01 -1.243731e-01
```

```
                                          function        gradient
-1.629884e-01 -1.105502e+00 -1.728034e+04  1.002000e+03          NA
```

3.3. Avaiable models

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

```
R> ?ztpoisson
```

Here we limit ourselves to just listing the family functions:

- Zero-truncated and zero-one-truncated Poisson, geometric, NB type II regression where the untruncated distribution is parameterized as:

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

- 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:

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

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

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

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

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

- Generalized Chao's and Zelterman's 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 $\text{logit}(p)=\ln(\lambda/2)$ for poisson parameter λ,

$$\hat{N}=N_{obs}+\sum_{k=1}^{\boldsymbol{f}_1+\boldsymbol{f}_2}\left(2\exp\left(\boldsymbol{x}_k\hat{\boldsymbol{\beta}}\right)+2\exp\left(2\boldsymbol{x}_k\hat{\boldsymbol{\beta}}\right)\right)^{-1}, \qquad \text{(Chao's estimator)}$$

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

- Alternative approaches to modelling one-inflation that mimic hurdle models where the first type zero truncated hurdle model (ztHurdle) is defined as:

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

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

- The Hurdle zero truncarted (Hurdlezt) is defined as:

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

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

Key takeaways of different models

- The dispersion parameter α in the negative binomial 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 negative binomial 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 (to the best of the knowledge of the authors) the interpretation of α being heterogeneous 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 (negative binomial with $\alpha = 1$) is singled out in the package and often considered in the literature due to inherent computational issues with negative binomial 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) negative binomial model.

- The extra mass ω in the inflated models is an important addition to the researcher's toolbox in SSCR 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 theoritical 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 situationally the Hurdle zero truncated models seem to be more numerically stable.
- Although interpretation of regression parameters tends to be somewhat overlooked in SSCR studies we should point out that interpretation of of the ω inflation parameter is more convenient that the interpretation of the π probability parameter. 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" quite close to one another.

3.4. Structure of a family function

- `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 $\boldsymbol{y}$ vector and $\boldsymbol{X}_{vlm}$ 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 $\mathbb{E}[Y|Y>0], \mathrm{var}[Y|Y>0]$ or $\mathbb{E}[Y], \mathrm{var}[Y]$ 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 $\mathrm{cov}(\hat{\boldsymbol{\beta}})$ and $\boldsymbol{X_{vlm}}$ 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 predictors.
- `getStart` – Expression for generating starting points.

3.5. Bootstrap algorithms

There are three types of bootstrap algorithms which the user may specify in `controlPopVar` controls with `bootType` argument which has three possible values `"parametric", "semiparametric", "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 semiparametric 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:

1. Draw the sample size $N'_{obs} \sim \mathrm{Be}\left(N', \frac{N'-N_{obs}}{N'}\right)$, where $N' = \lfloor\hat{N}\rfloor + b\left(\lfloor\hat{N}\rfloor - \hat{N}\right)$.
2. Draw N'_{obs} units from the data uniformly without replacement.
3. Obtain new population size estimate using bootstrap data.
4. Repeat $1-3$ 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:

1. Draw the number of covariates equal to $\lfloor\hat{N}\rfloor + b\left(\lfloor\hat{N}\rfloor - \hat{N}\right)$ proportional to the estimated contribution $(\mathbb{P}\left[Y_k > 0|\boldsymbol{x}_k\right])^{-1}$ with replacement.
2. Using the fitted model and regression coefficients $\hat{\boldsymbol{\beta}}$ 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 based on the truncated data.
5. Repeat $1-4$ B times.

Note however 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 semiparametric bootstrap. The parametric bootstrap algorithm is the default in **singleRcapture**.

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, foreach, parallel** packages.
- `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.

4. Integration with the VGAM, countreg packages

The **singleRcaptureExtra** extensions 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 controll 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, Vidal-Diez, Lerdsuwansri, Viwatwongkasem, and Arnold (2013):

```
R> library(VGAM)

Warning: package 'VGAM' was built under R version 4.3.3

Loading required package: stats4

Loading required package: splines

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
+   )
+ )
```

can be acomplished with the following syntax simple syntax:

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

Compare with a simmilar linear model from base **singleRcapture**:

```
R> modelBase <- estimatePopsize(
+   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.      Max.
-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)              -1.77609    0.45894  -3.870 0.000109 ***
log_size                  0.49391    0.02521  19.594  < 2e-16 ***
log_distance             -0.14106    0.04098  -3.442 0.000578 ***
C_TYPEDairy              -1.68591    0.55327  -3.047 0.002310 **
log_size:C_TYPEDairy      0.26504    0.03495   7.583 3.37e-14 ***
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
normal      35448.14   42305.85
```

```
logNormal   35661.32   42530.37
95% CI for the share of observed population:
          lowerBound upperBound
normal      28.44996   33.95382
logNormal   28.29978   33.75085

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
logNormal   29.24274   34.62823

-------------------------------
-- 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:   1

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                                       1
(Intercept):2                                       1
s(log_size, df = 3)                                 1     1.8     51.949
s(log_distance, df = 2)                             1     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
```

5. Conclusions

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A. Implementing custom singleRcapture family function

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

$$\mathbb{P}[Y=y|\lambda,\pi]=\begin{cases}1-\frac{1}{2}\lambda-\frac{1}{2}\pi & \text{when: } y=0\\ \frac{1}{2}\pi & \text{when: } y=1\\ \frac{1}{2}\lambda & \text{when: } y=2,\end{cases} \tag{6}$$

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"),
+                              piLink     = c("logit", "cloglog", "probit"),
+                              ...) {
+   if (missing(lambdaLink)) lambdaLink <- "logit"
+   if (missing(piLink))         piLink <- "logit"
+
+   links <- list()
+   attr(links, "linkNames") <- c(lambdaLink, piLink)
+
+   lambdaLink <- switch(lambdaLink,
+     "logit"   = singleRcapture:::singleRinternallogitLink,
+     "cloglog" = singleRcapture:::singleRinternalcloglogLink,
+     "probit"  = singleRcapture:::singleRinternalprobitLink
+   )
+
+   piLink <- switch(piLink,
+     "logit"   = singleRcapture:::singleRinternallogitLink,
+     "cloglog" = singleRcapture:::singleRinternalcloglogLink,
+     "probit"  = singleRcapture:::singleRinternalprobitLink
+   )
+
+   links[1:2] <- c(lambdaLink, piLink)
+
+   mu.eta <- function(eta, type = "trunc", deriv = FALSE, ...) {
```

```
+     pi     <-     piLink(eta[, 2], inverse = TRUE) / 2
+     lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2
+
+     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", ...) {
+     pi     <-     piLink(eta[, 2], inverse = TRUE) / 2
+     lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2
+
+     switch (type,
+     "nontrunc" = pi * (1 - pi) + 4 * lambda * (1 - lambda - pi),
+     "trunc" = lambda * (1 - lambda) / (pi + lambda)
+     )
+   }
+
+   Wfun <- function(prior, y, eta, ...) {
+     pi     <-     piLink(eta[, 2], inverse = TRUE) / 2
+     lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2
+
+     G01 <- ((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 <- G00 * prior * (piLink(eta[, 2], inverse = TRUE, deriv = 1) ^ 2) / 4
+
+     G11 <- ((lambda + pi) ^ (-2)) - (((lambda + pi) * lambda) ^ -1)
+     G11 <- G11 * prior * (lambdaLink(eta[, 1], inverse = TRUE, deriv = 1) ^ 2) / 4
+
+     matrix(
+       -c(G11, # lambda
+          G01, # mixed
+          G01, # mixed
```

```
+         G00  # pi
+       ),
+       dimnames = list(rownames(eta), c("lambda", "mixed", "mixed", "pi")),
+       ncol = 4
+     )
+   }
+
+   funcZ <- function(eta, weight, y, prior, ...) {
+     pi     <-     piLink(eta[, 2], inverse = TRUE) / 2
+     lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2
+
+     weight <- weight / prior
+
+     G0 <- (2 - y) / pi     - ((lambda + pi) ^ -1)
+     G1 <- (y - 1) / lambda - ((lambda + pi) ^ -1)
+
+     G1 <- G1 * lambdaLink(eta[, 1], inverse = TRUE, deriv = 1) / 2
+     G0 <- G0 *     piLink(eta[, 2], inverse = TRUE, deriv = 1) / 2
+
+     uMatrix <- matrix(c(G1, G0), ncol = 2)
+
+     weight <- lapply(X = 1:nrow(weight), FUN = function (x) {
+       matrix(as.numeric(weight[x, ]), ncol = 2)
+     })
+
+     pseudoResid <- sapply(X = 1:length(weight), FUN = function (x) {
+       #xx <- chol2inv(chol(weight[[x]])) # less computationally demanding
+       xx <- solve(weight[[x]]) # more stable
+       xx %*% uMatrix[x, ]
+     })
+     pseudoResid <- t(pseudoResid)
+     dimnames(pseudoResid) <- dimnames(eta)
+     pseudoResid
+   }
+
+   minusLogLike <- function(y, X, offset,
+                            weight    = 1,
+                            NbyK      = FALSE,
+                            vectorDer = FALSE,
+                            deriv     = 0,
+                            ...) {
+     y <- as.numeric(y)
+     if (is.null(weight)) {
+       weight <- 1
+     }
+     if (missing(offset)) {
+       offset <- 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 # to make it conform to how switch in R works, i.e. indexing begins with 1
+
+     switch (deriv,
+       function(beta) {
+         eta <- matrix(as.matrix(X) %*% beta, ncol = 2) + offset
+         pi     <-     piLink(eta[, 2], inverse = TRUE) / 2
+         lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2
```

```
+         -sum(weight * ((2 - y) * log(pi) + (y - 1) * log(lambda) - log(pi + lambda)))
+       },
+       function(beta) {
+         eta <- matrix(as.matrix(X) %*% beta, ncol = 2) + offset
+         pi     <-     piLink(eta[, 2], inverse = TRUE) / 2
+         lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2
+
+         G0 <- (2 - y) / pi     - ((lambda + pi) ^ -1)
+         G1 <- (y - 1) / lambda - ((lambda + pi) ^ -1)
+
+         G1 <- G1 * weight * lambdaLink(eta[, 1], inverse = TRUE, deriv = 1) / 2
+         G0 <- G0 * weight *     piLink(eta[, 2], inverse = TRUE, deriv = 1) / 2
+
+         if (NbyK) {
+           XX <- 1:(attr(X, "hwm")[1])
+           return(cbind(as.data.frame(X[1:nrow(eta), XX]) * G1, as.data.frame(X[-(1:nrow(eta)), -XX]) *
+         }
+         if (vectorDer) {
+           return(cbind(G1, G0))
+         }
+
+         as.numeric(c(G1, G0) %*% X)
+       },
+       function (beta) {
+         lambdaPredNumber <- attr(X, "hwm")[1]
+         eta <- matrix(as.matrix(X) %*% beta, ncol = 2) + offset
+         pi     <-     piLink(eta[, 2], inverse = TRUE) / 2
+         lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2
+
+         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 <- ((lambda + pi) ^ (-2)) - (2 - y) / (pi ^ 2)
+
+         G00 <- 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 <- t(as.data.frame(X[1:(nrow(X) / 2), 1:lambdaPredNumber]) *
+         G01 * (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 <- ((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] *
+         (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
```

```
+         res[1:lambdaPredNumber, 1:lambdaPredNumber] <- G11
+         res[1:lambdaPredNumber, -(1:lambdaPredNumber)] <- t(G01)
+         res[-(1:lambdaPredNumber), 1:lambdaPredNumber] <- G01
+
+         res
+       }
+     )
+   }
+
+   validmu <- function(mu) {
+     (sum(!is.finite(mu)) == 0) && all(0 < mu) && all(2 > mu)
+   }
+
+   # this is optional
+   devResids <- function(y, eta, wt, ...) {
+     0
+   }
+
+   pointEst <- function (pw, eta, contr = FALSE, ...) {
+     pi     <-     piLink(eta[, 2], inverse = TRUE) / 2
+     lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2
+     N <- pw / (lambda + pi)
+     if(!contr) {
+       N <- sum(N)
+     }
+     N
+   }
+
+   popVar <- function (pw, eta, cov, Xvlm, ...) {
+     pi     <-     piLink(eta[, 2], inverse = TRUE) / 2
+     lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2
+
+     bigTheta1 <- -pw / (pi + lambda) ^ 2 # w.r to pi
+     bigTheta1 <- bigTheta1 * piLink(eta[, 2], inverse = TRUE, deriv = 1) / 2
+     bigTheta2 <- -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)
+
+     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"
+     pi     <-     piLink(eta[, 2], inverse = TRUE) / 2
+     lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2
+
+     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) {
+     pi     <-     piLink(eta[, 2], inverse = TRUE) / 2
+     lambda <- lambdaLink(eta[, 1], inverse = TRUE) / 2
+     CDF <- function(x) {
+       ifelse(x == Inf, 1,
+       ifelse(x < 0, 0,
+       ifelse(x < 1, 1 - pi - lambda,
+       ifelse(x < 2, 1 - lambda, 1))))
+     }
+     lb <- CDF(lower)
+     ub <- CDF(upper)
+     p_u <- stats::runif(n, lb, ub)
+     sims <- rep(0, n)
+     cond <- CDF(sims) <= p_u
+     while (any(cond)) {
+       sims[cond] <- sims[cond] + 1
+       cond <- CDF(sims) <= p_u
+     }
+     sims
+   }
+
+   getStart <- expression(
+     if (method == "IRLS") {
+       etaStart <- cbind(
+         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))
+       } else {
+         coefStart <- rep(init[1] / attr(Xvlm, "hwm")[1], attr(Xvlm, "hwm")[1])
+       }
+       if ("(Intercept):pi" %in% colnames(Xvlm)) {
+         coefStart <- c(coefStart, init[2], rep(0, attr(Xvlm, "hwm")[2] - 1))
+       } else {
+         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(
+         mean       = "pi / 2 + lambda",
+         variance   = paste0("(pi / 2) * (1 - pi / 2) + 2 * lambda * (1 - lambda / 2 - pi / 2)"),
+         popSizeEst = "(1 - (pi + lambda) / 2) ^ -1",
+         meanTr     = "1 + lambda / (pi + lambda)",
+         varianceTr = paste0("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(
+     myFamilyFunction(lambdaLink = "logit", piLink = "logit"),
+     nsim = 1000, eta = matrix(0, nrow = 1000, ncol = 2),
+     truncated = FALSE
+ )
R> mm <- estimatePopsize(
+     formula = Y ~ 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
normal      848.2127   1123.787
logNormal   866.3167   1144.053
95% CI for the share of observed population:
          lowerBound upperBound
normal      43.86951   58.12221
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)) {
        res <- switch(deriv, log(-log(1 - x)), -1/((1 - x) *
            log(1 - x)), -(1 + log(1 - x))/((x - 1)^2 * log(1 -
            x)^2), (2 * log(1 - x)^2 + 3 * log(1 - x) + 2)/(log(1 -
            x)^3 * (x - 1)^3))
    }
    else {
        res <- switch(deriv, 1 - exp(-exp(x)), exp(x - exp(x)),
            (1 - exp(x)) * exp(x - exp(x)), (exp(2 * x) - 3 *
```

```
                exp(x) + 1) * exp(x - exp(x)))
    }
    res
}
<bytecode: 0x1112b4e90>
<environment: namespace:singleRcapture>
```

one might of course include code for computing them manually.

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