

# Package ‘preseqR’

August 15, 2017

**Type** Package

**Title** Predicting the Number of Species in a Random Sample

**Version** 3.1.2

**Date** 2017-08-14

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**Description** The relation between the number of species and the number of individuals in a random sample is a classic problem back to Fisher (1943) <doi:10.2307/1411>. We generalize this problem to estimate the number of species represented at least  $r$  times in a random sample. In particular when  $r=1$ , it becomes the classic problem. We use a mixture of Poisson processes to model sampling procedures and apply a nonparametric empirical Bayes approach to obtain an estimator. For more information on 'preseqR', see Deng C, Daley T and Smith AD (2015) <doi:10.1007/s40484-015-0049-7> and Deng C and Smith AD (2016) <arXiv:1607.02804v2>.

**License** GPL-3

**Imports** polynom, graphics, stats

**NeedsCompilation** no

**Repository** CRAN

**Date/Publication** 2017-08-15 06:54:50 UTC

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preseqR-package	<i>An R package for estimating the number of species represented at least <math>r</math> times</i>
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## Description

preseqR provides functions to estimate the number of species represented at least  $r$  times in a random sample based on an initial sample. Functions work through rational function approximations to a modified Good and Toulmin's (1956) non-parametric empirical Bayes power series estimator. The rational function approximation is then boosted to an estimator for the number species represented at least  $r$  times, based on a relation between the number of species represented at least  $r$  times and the number of species represented at least once.

## Details

functions:

ds.mincount.bootstrap

ds.mincount

ztpois.mincount

ztnb.mincount

boneh.mincount

chao.mincount

pois.mincount

nb.mincount

preseqR.ztnb.em

preseqR.simu.hist

preseqR.nonreplace.sampling

preseqR.interpolate.mincount

data: FisherButterflyHist, ShakespeareWordHist

## Author(s)

Chao Deng, Timothy Daley, and Andrew D. Smith

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## References

- Baker, G. A., & Graves-Morris, P. (1996). Pade approximants (Encyclopedia of Mathematics and its Applications vol 59).
- Boneh, S., Boneh, A., & Caron, R. J. (1998). Estimating the prediction function and the number of unseen species in sampling with replacement. *Journal of the American Statistical Association*, 93(441), 372-379.
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- Kalinin V (1965). Functionals related to the poisson distribution and statistical structure of a text. *Articles on Mathematical Statistics and the Theory of Probability* pp. 202-220.

---

boneh.mincount

*Estimating the expected number of species represented r or more times*

---

## Description

The function estimates the expected number of species represented at least r times in a random sample based on the initial sample using a nonparametric approach by Boneh et al. (1998).

## Usage

```
boneh.mincount(n, r=1)
```

**Arguments**

- n** A two-column matrix. The first column is the frequency  $j = 1, 2, \dots$ ; and the second column is  $n_j$ , the number of species with each species represented  $j$  times in the initial sample. The first column must be sorted in an ascending order.
- r** A vector of positive integers. Default is 1.

**Value**

The constructed estimator for the number of species represented at least  $r$  times in a sample. The input of the estimator is a vector of sampling efforts  $t$ , i.e. the relative sample sizes comparing with the initial sample. For example,  $t = 2$  means the sample is twice the size of the initial sample.

**Author(s)**

Chao Deng

**References**

Boneh, S., Boneh, A., & Caron, R. J. (1998). Estimating the prediction function and the number of unseen species in sampling with replacement. *Journal of the American Statistical Association*, 93(441), 372-379.

**Examples**

```
## load library
library(preseqR)

## import data
data(FisherButterflyHist)

## construct the estimator for the number of species
## represented at least once, twice or three times in a sample
boneh.estimator <- boneh.mincount(FisherButterflyHist, r=1:3)

## The number of species represented at least once, twice or three times
## when the sample size is 10 or 20 times of the initial sample
boneh.estimator(c(10, 20))
```

---

chao.mincount

*Estimating the expected number of species represented  $r$  or more times*

---

**Description**

The function estimates the expected number of species represented at least  $r$  times in a random sample based on the initial sample using a nonparametric approach by Chao and Shen (2004).

**Usage**

```
chao.mincount(n, r=1, k=10)
```

**Arguments**

**n** A two-column matrix. The first column is the frequency  $j = 1, 2, \dots$ ; and the second column is  $n_j$ , the number of species with each species represented  $j$  times in the initial sample. The first column must be sorted in an ascending order.

**r** A vector of positive integers. Default is 1.

**k** A cutoff for common species. Default is 10.

**Value**

The constructed estimator for the number of species represented at least  $r$  times in a sample. The input of the estimator is a vector of sampling efforts  $t$ , i.e. the relative sample sizes comparing with the initial sample. For example,  $t = 2$  means the sample is twice the size of the initial sample.

**Author(s)**

Chao Deng

**References**

Chao, A., & Shen, T. J. (2004). Nonparametric prediction in species sampling. *Journal of agricultural, biological, and environmental statistics*, 9(3), 253-269.

**Examples**

```
## load library
library(preseqR)

## import data
data(FisherButterflyHist)

## construct the estimator for the number of species
## represented at least once, twice or three times in a sample
chao.estimator <- chao.mincount(FisherButterflyHist, r=1:3)

## The number of species represented at least once, twice or three times
## when the sample size is 10 or 20 times of the initial sample
chao.estimator(c(10, 20))
```

---

Dickens

*Dickens' vocabulary*


---

### Description

Words frequencies of a collection of Charles Dickens from Project Gutenberg

### Details

A two-column matrix. The first column is the frequency  $j = 1, 2, \dots$ ; and the second column is  $n_j$ , the number of unique words appeared  $j$  times in a collection of Charles Dickens.

### References

<http://zipfr.r-forge.r-project.org/>

### Examples

```
##load library
library(preseqR)

##load data
data(Dickens)
```

---

ds.mincount

*Estimating the expected number of species represented r or more times*


---

### Description

The function estimates the expected number of species represented at least  $r$  times in a random sample based on the initial sample.

### Usage

```
ds.mincount(n, r=1, mt=20)
```

### Arguments

n	A two-column matrix. The first column is the frequency $j = 1, 2, \dots$ ; and the second column is $n_j$ , the number of species with each species represented $j$ times in the initial sample. The first column must be sorted in an ascending order.
mt	An positive integer constraining possible rational function approximations. Default is 20.
r	A vector of positive integers. Default is 1.

## Details

The difference between this function and `ds.mincount.bootstrap` is that no bootstrapping for the initial sample. Therefore the function could be less stable than estimates by bootstrap. However, this function is much faster. In general, we recommend `ds.mincount.bootstrap` for estimating the expected number of species represented at least  $r$  times in a sample.

See `ds.mincount.bootstrap` for more information.

## Value

`FUN` The constructed estimator for the number of species represented at least  $r$  times in a sample. The input of the estimator is a vector of sampling efforts  $t$ , i.e. the relative sample sizes comparing with the initial sample. For example,  $t = 2$  means the sample is twice the size of the initial sample.

`FUN.elements` A list of two components for the estimator. The estimator can be expressed as

$$\hat{E}(S_r(t)) = \sum_{i=1}^l c_i \left( \frac{t}{t - x_i} \right)^r.$$

`PF.elements` contains both coefficients  $c_i$  and roots  $x_i$ .

`M` The number of terms used when applying rational function approximation to the power series of the average discovery rate.

`M.adjust` The number of terms in the estimator, equal to 1

## Author(s)

Chao Deng

## References

Kalinin V (1965). Functionals related to the poisson distribution and statistical structure of a text. *Articles on Mathematical Statistics and the Theory of Probability* pp. 202-220.

Daley, T., & Smith, A. D. (2013). Predicting the molecular complexity of sequencing libraries. *Nature methods*, 10(4), 325-327.

## Examples

```
## load library
library(preseqR)

## import data
data(ShakespeareWordHist)

## construct the estimator for the number of unique word
## represented at least once, twice or twenty times in a sample
estimator = ds.mincount(ShakespeareWordHist, r=c(1,2,20))

## print the elements of the estimator
estimator$FUN.elements
```

```
## The number of unique words represented at least once, twice or twenty times
## when the sample size is 10 or 20 times of the initial sample
estimator$FUN(c(10, 20))
```

---

ds.mincount.bootstrap *Estimating the number of species represented r or more times*

---

## Description

The function estimates the expected number of species represented at least  $r$  times in a random sample based on the initial sample. The initial sample is bootstrapped to improve the stability of estimates.

## Usage

```
ds.mincount.bootstrap(n, r=1, mt=20, times=100)
```

## Arguments

n	A two-column matrix. The first column is the frequency $j = 1, 2, \dots$ ; and the second column is $n_j$ , the number of species with each species represented $j$ times in the initial sample. The first column must be sorted in an ascending order.
mt	An positive integer constraining possible rational function approximations. Default is 20.
r	A vector of positive integers. Default is 1.
times	An positive integer representing the minimum required number of successful estimation. Default is 100. See detail below.

## Details

Under a mixture of Poisson models, the expected number of species represented at least  $r$  times in a random sample can be expressed as higher derivatives of the expected number of species represented at least once. We first use rational function approximations to the modified Good and Toulmin's (1956) non-parametric empirical Bayes power series to estimate the average discovery rate. By differentiating the rational function approximation, we obtain an estimator for the number of species represented at least  $r$  times in a random sample.

## Value

FUN.nobootstrap	The estimator constructed based on the initial sample by the function. No bootstrap procedure is involved.
FUN.bootstrap	The bootstrap samples from an initial sample are used to construct estimators. The median value of these estimators are estimates of the number of species represented at least $r$ times in a sample.
var	The estimated variance for the estimator FUN.nobootstrap by bootstrap.



**Author(s)**

Chao Deng

**References**

- Efron, B., & Tibshirani, R. J. (1994). An introduction to the bootstrap. CRC press.
- Kalinin V (1965). Functionals related to the poisson distribution and statistical structure of a text. Articles on Mathematical Statistics and the Theory of Probability pp. 202-220.
- Daley, T., & Smith, A. D. (2013). Predicting the molecular complexity of sequencing libraries. Nature methods, 10(4), 325-327.

**Examples**

```
## load library
#library(preseqR)

## import data
#data(FisherButterflyHist)

## estimate the number of species captured at least once, twice or 20 times
## as a function of the number of individuals

# result = ds.mincount.bootstrap(FisherButterflyHist, r=c(1,2, 20), times=10)

## estimates of the number of unique words appeared at least once, twice or three
## times when the sample size 10 times the size of the initial sample

## estimates by the function ds.mincount
# result$FUN.nobootstrap$FUN(10)

## estimates by the bootstrapped estimator
# result$FUN.bootstrap(10)
```

---

`fisher.alpha`*Estimating the parameter alpha in the logseries estimator*

---

**Description**

The function estimates the parameter alpha in the logseries estimator by Fisher, R. A., et al. (1943) based on a sample.

**Usage**`fisher.alpha(n)`

**Arguments**

`n` A two-column matrix. The first column is the frequency  $j = 1, 2, \dots$ ; and the second column is  $n_j$ , the number of species with each species represented  $j$  times in the initial sample. The first column must be sorted in an ascending order.

**Value**

A double, the estimated value of the parameter alpha

**Author(s)**

Chao Deng

**References**

Fisher, R., Corbet, A., & Williams, C. (1943). The Relation Between the Number of Species and the Number of Individuals in a Random Sample of an Animal Population. *Journal of Animal Ecology*, 12(1), 42-58. doi:10.2307/1411

**Examples**

```
## load library
library(preseqR)

## import data
data(WillButterfly)

## estimating alpha
fisher.alpha <- fisher.alpha(WillButterfly)
```

---

<code>fisher.mincount</code>	<i>Estimating the expected number of species represented <math>r</math> or more times</i>
------------------------------	---

---

**Description**

The function estimates the expected number of species represented at least  $r$  times in a random sample based on the initial sample using a parametric approach by Fisher, R. A., et al. (1943).

**Usage**

```
fisher.mincount(n, r=1)
```

**Arguments**

- n** A two-column matrix. The first column is the frequency  $j = 1, 2, \dots$ ; and the second column is  $n_j$ , the number of species with each species represented  $j$  times in the initial sample. The first column must be sorted in an ascending order.
- r** A vector of positive integers. Default is 1.

**Value**

The constructed estimator for the number of species represented at least  $r$  times in a sample. The input of the estimator is a vector of sampling efforts  $t$ , i.e. the relative sample sizes comparing with the initial sample. For example,  $t = 2$  means the sample is twice the size of the initial sample.

**Author(s)**

Chao Deng

**References**

Fisher, R., Corbet, A., & Williams, C. (1943). The Relation Between the Number of Species and the Number of Individuals in a Random Sample of an Animal Population. *Journal of Animal Ecology*, 12(1), 42-58. doi:10.2307/1411

**Examples**

```
## load library
library(preseqR)

## import data
data(WillButterfly)

## construct the estimator for the number of species
## represented at least once, twice or three times in a sample
fisher.estimator <- fisher.mincount(WillButterfly, r=1:3)

## The number of species represented at least once, twice or three times
## when the sample size is 10 times of the initial sample
fisher.estimator(10)
```

---

FisherButterflyHist *Fisher's butterfly data*

---

**Description**

Frequencies data of butterflies collected in the Malay peninsula was from Fisher, R. A., Corbet, A. S., & Williams, C. B. (1943).

**Details**

A two-column matrix. The first column is the frequency  $j = 1, 2, \dots$ ; and the second column is  $n_j$ , the number of butterflies captured  $j$  times in the sample.

**References**

Fisher, R. A., Corbet, A. S., and Williams, C. B. ,1943, The Relation Between the Number of Species and the Number of Individuals in a Random Sample of an Animal Population, Journal of Animal Ecology, 12, 42-58, Table 1,2.

**Examples**

```
##load library
library(preseqR)

##load data
data(FisherButterflyHist)
```

---

```
preseqR.interpolate.mincount
```

*Interpolating the number of species represented r or more times*

---

**Description**

Interpolating the expected number of species represented at least r times in a random sample based on an initial sample.

**Usage**

```
preseqR.interpolate.mincount(ss, n, r=1)
```

**Arguments**

ss	An positive double equal to the step size between samples.
n	A two-column matrix. The first column is the frequency $j = 1, 2, \dots$ ; and the second column is $n_j$ , the number of species with each species represented $j$ times in the initial sample. The first column must be sorted in an ascending order.
r	A positive integer.

**Details**

Assume that a random sample (subsample) follows a multivariant hypergeometric distribution given an initial sample. The expected number of unique species represented at least r times in the subsample is then calculated by an expended version of the formula in Heck Jr, KL. et al. (1975).

**Value**

A two-column matrix for the number of species represented at least  $r$  times in a random sample. The first column is the size of the random sample; the second column is the expected number of species represented at least  $r$  times in the sample.

NULL if failed.

**Author(s)**

Chao Deng

**References**

Heck Jr, K. L., van Belle, G., & Simberloff, D. (1975). Explicit calculation of the rarefaction diversity measurement and the determination of sufficient sample size. *Ecology*, 1459-1461.

**Examples**

```
## load library
library(preseqR)

## import data
data(ShakespeareWordHist)

## The expected number of species represented twice or more in a random sample
## The step size is 1e5; the initial sample is "ShakespeareWordHist"
preseqR.interpolate.mincount(n=ShakespeareWordHist, ss=1e5, r=2)
```

---

```
preseqR.nonreplace.sampling
```

*Sampling without replacement*

---

**Description**

Generating a histogram by subsampling without replacement.

**Usage**

```
preseqR.nonreplace.sampling(size, n)
```

**Arguments**

size	An positive integer representing the size of the subsample.
n	A two-column matrix. The first column is the frequency $j = 1, 2, \dots$ ; and the second column is $n_j$ , the number of species with each species represented $j$ times in the initial sample. The first column must be sorted in an ascending order.

**Details**

The function `sample()` in R is used to implement the function. We wrap the `sample()` function in a way that both input and output are histograms.

**Value**

A two-column matrix as a subsample. The first column is the frequency  $j = 1, 2, \dots$ ; and the second column is  $n_j$ , the number of species with each species represented  $j$  times in the subsample.

**Author(s)**

Chao Deng

**References**

<https://stat.ethz.ch/R-manual/R-patched/library/base/html/sample.html>

**Examples**

```
## load library
library(preseqR)

## import data
data(FisherButterflyHist)

## generate a subsample of size 1000.
preseqR.nonreplace.sampling(size=1000, FisherButterflyHist)
```

---

preseqR.simu.hist      *Simulating a histogram*

---

**Description**

Generating a histogram based on a Poisson mixture model.

**Usage**

```
preseqR.simu.hist(L=1e8, N, FUN)
```

**Arguments**

L	A positive integer, the number of species in a population.
N	A positive interger, the simulated sample size.
FUN	An RNG generating non negative real number.

## Details

The function uses a compound Poisson model to generate a sample of size  $n$ . It assumes for each species the number of individuals captured in a sample follows a Poisson process. The Poisson rates among species are generated by a given function FUN per unit of sampling effort. Under this statistical assumption, for a given sample size  $N$ , the number of individuals in the sample for each species follow a multinomial distributions.

The function FUN must take an argument indicating the number of random numbers generated and return a vector of generated numbers.

## Value

A two-column matrix. The first column is the frequency  $j = 1, 2, \dots$ ; and the second column is  $n_j$ , the number of species with each species represented  $j$  times in the initial sample. The first column must be sorted in an ascending order.

## Author(s)

Chao Deng

## Examples

```
## load library
library(preseqR)
## construct a RNG
f <- function(n) {
  rgamma(n, shape=0.5, scale=1)
}

preseqR.simu.hist(L=1e5, N=1, f)
```

---

preseqR.ztnb.em

*Fitting a zero-truncated negative binomial distribution*

---

## Description

This function fits a zero-truncated negative binomial (ZTNB) distribution to the initial sample. Since the species with zero observations are missed in the sample, an EM algorithm is used to estimate the parameters assuming the number of individuals for each species follows a Negative Binomial distribution with the zero counts as a missing latent data.

## Usage

```
preseqR.ztnb.em(n, size = SIZE.INIT, mu = MU.INIT)
```

**Arguments**

n	A two-column matrix. The first column is the frequency $j = 1, 2, \dots$ ; and the second column is $n_j$ , the number of species with each species represented $j$ times in the initial sample. The first column must be sorted in an ascending order.
size	A positive double setting the initial value of the parameter size in a negative binomial distribution for the EM algorithm. Default value is 1.
mu	A positive double setting the initial value of the parameter mu in a negative binomial distribution for the EM algorithm. Default value is 0.5.

**Details**

See the supplement of Daley and Smith (2013).

**Value**

size	The estimate of the parameter size in the negative binomial.
mu	The estimate of the parameter mu in the negative binomial.
loglik	Log-likelihood under estimated ZTNB.

**Author(s)**

Chao Deng

**Examples**

```
## load library
library(preseqR)

## import data
data(FisherButterflyHist)

## print the parameters of a fitting negative binomial distribution
preseqR.ztnb.em(FisherButterflyHist)
```

---

ShakespeareWordHist    *Shakespeare's word type frequencies*

---

**Description**

The Shakespeare's word type frequencies data was from Efron, B., & Thisted, R. (1976).

**Details**

A two-column matrix. The first column is the frequency  $j = 1, 2, \dots$ ; and the second column is  $n_j$ , the number of unique words appeared  $j$  times in Shakespeare's work.



**References**

Efron, B., & Thisted, R. (1976). Estimating the number of unseen species: How many words did Shakespeare know?. *Biometrika*, 63(3), 435-447.

**Examples**

```
##load library
library(preseqR)

##load data
data(ShakespeareWordHist)
```

---

Twitter

*Social network*

---

**Description**

Following relationships of Twitter's social network

**Details**

A two-column matrix. The first column is the frequency  $j = 1, 2, \dots$ ; and the second column is  $n_j$ , the number of users with  $j$  followers.

**References**

Zafarani R, Liu H (2009) Social computing data repository at ASU.

**Examples**

```
##load library
library(preseqR)

##load data
data(Twitter)
```

---

WillButterfly

*Fisher's butterfly data*

---

**Description**

Frequencies data of butterflies collected in the Malay peninsula was from Fisher, R. A., Corbet, A. S., & Williams, C. B. (1943).

**Details**

A two-column matrix. The first column is the frequency  $j = 1, 2, \dots$ ; and the second column is  $n_j$ , the number of butterflies captured  $j$  times in the sample.

**References**

Fisher, R. A., Corbet, A. S., and Williams, C. B. ,1943, The Relation Between the Number of Species and the Number of Individuals in a Random Sample of an Animal Population, Journal of Animal Ecology, 12, 42-58, Table 3.

**Examples**

```
##load library
library(preseqR)

##load data
data(WillButterfly)
```

---

ztnb.mincount

*Estimating the expected number of species represented r or more times*


---

**Description**

The function estimates the expected number of species represented at least r times in a random sample based on the initial sample using zero truncated negative binomial model.

**Usage**

```
ztnb.mincount(n, r=1, size=SIZE.INIT, mu=MU.INIT)
```

**Arguments**

n	A two-column matrix. The first column is the frequency $j = 1, 2, \dots$ ; and the second column is $n_j$ , the number of species with each species represented $j$ times in the initial sample. The first column must be sorted in an ascending order.
r	A vector of positive integers. Default is 1.
size	A positive double setting the initial value of the parameter size in a negative binomial distribution for the EM algorithm. Default value is 1.
mu	A positive double setting the initial value of the parameter mu in a negative binomial distribution for the EM algorithm. Default value is 0.5.

## Details

The statistical assumption is that for each species the number of individuals in a sample follows a Poisson distribution. The Poisson rate  $\lambda$  obeys a latent gamma distribution. So the random variable  $X$ , which is the number of species represented  $x$  ( $x > 0$ ) times, follows a zero-truncated negative binomial distribution. The unknown parameters are estimated by the function `preseqR.ztnb.em`. Based on the estimated distribution, we calculate the expected number of species in a random sample. Details of the estimation procedure see supplement of Daley T. and Smith AD. (2013).

## Value

The constructed estimator for the number of species represented at least  $r$  times in a sample. The input of the estimator is a vector of sampling efforts  $t$ , i.e. the relative sample sizes comparing with the initial sample. For example,  $t = 2$  means the sample is twice the size of the initial sample.

## Author(s)

Chao Deng

## References

Daley, T., & Smith, A. D. (2013). Predicting the molecular complexity of sequencing libraries. *Nature methods*, 10(4), 325-327.

## See Also

[preseqR.ztnb.em](#)

## Examples

```
## load library
library(preseqR)

## import data
data(FisherButterflyHist)

## construct the estimator for the number of species
## represented at least once, twice or three times in a sample
ztnb.estimator <- ztnb.mincount(FisherButterflyHist, r=1:3)

## The number of species represented at least once, twice or three times
## when the sample size is 10 or 20 times of the initial sample
ztnb.estimator(c(10, 20))
```

---

ztpois.mincount	<i>Estimating the expected number of species represented <math>r</math> or more times</i>
-----------------	---

---

### Description

The function estimates the expected number of species represented at least  $r$  times in a random sample based on the initial sample using zero truncated Poisson distributino.

### Usage

```
ztpois.mincount(n, r=1)
```

### Arguments

$n$	A two-column matrix. The first column is the frequency $j = 1, 2, \dots$ ; and the second column is $n_j$ , the number of species with each species represented $j$ times in the initial sample. The first column must be sorted in an ascending order.
$r$	A vector of positive integers. Default is 1.

### Details

The statistical assumption is that for each species the number of individuals in a sample follows a Poisson distribution. The Poisson rate  $\lambda$  is the same among all species. So the random variable  $X$ , which is the number of species represented  $x$  ( $x > 0$ ) times, follows a zero-truncated Poisson distribution. The unknown parameters are estimated by Cohen (1960). Based on the estimated distribution, we calculate the expected number of species in a random sample.

### Value

The constructed estimator for the number of species represneted at least  $r$  times in a sample. The input of the estimator is a vector of sampling efforts  $t$ , i.e. the relative sample sizes comparing with the initial sample. For example,  $t = 2$  means the sample is twice the size of the initial sample.

### Author(s)

Chao Deng

### References

Cohen Jr, A. C. (1960). Estimating the parameters of a modified Poisson distribution. Journal of the American Statistical Association, 55(289), 139-143.

**Examples**

```
## load library
library(preseqR)

## import data
data(FisherButterflyHist)

## construct the estimator for the number of species
## represented at least once, twice or three times in a sample
ztpois.estimator <- ztpois.mincount(FisherButterflyHist, r=1:3)

## The number of species represented at least once, twice or three times
## when the sample size is 10 or 20 times of the initial sample
ztpois.estimator(c(10, 20))
```

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