Fitting parametric univariate distributions to non-censored or censored data using the R package **fitdistrplus**

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The package **fitdistrplus** provides functions for fitting univariate distributions on different types of data (continuous censored or non-censored data and discrete data) and allowing different estimation methods (maximum likelihood, moment matching, quantile matching and maximum goodness-of-fit estimation). Outputs of **fitdist** and **fitdistcens** functions are S3 objects, for which kind generic methods are provided, including **summary**, **plot** and **quantile**. This package also provides various functions to compare the fit of several distributions to a same data set and can handle bootstrap of parameter estimates. Detailed examples are given in food risk assessment, ecotoxicology and insurance contexts.

Keywords: probability distribution fitting, bootstrap, censored data, maximum likelihood, moment matching, quantile matching, maximum goodness-of-fit.

1 Introduction

Fitting distributions to data is a very common task in statistics and consists in choosing a probability distribution that gives a good representation of a statistical variable, as well as finding parameter estimates of that distribution. It requires judgment and expertise and generally needs an iterative process of distribution choice, parameter estimation, and quality of fit assessment. The fitdistr function in the R package MASS ([61]) is a well known general-purpose maximum-likelihood fitting routine for the parameter estimation step in R [50]. Other steps of the process may be developed using R, e.g. [52]. In this paper, we present our R package fitdistrplus ([15]) implementing several methods of fitting univariate parametric distribution. Our first objective by developing this package was to provide R users a set of functions dedicated to help this overall process.

The fitdistr function estimates distribution parameters by maximizing the log-likelihood using the optim function. In some cases, other estimation methods could be prefered, such as maximum goodness-of-fit estimation (also called minimum distance estimation), and proposed in the R package actuar with three different goodness-of-fit distances, see [16]. While developping the fitdistrplus package, our second objective was thus to extend function fitdistr by providing various estimation methods in addition to maximum likelihood estimation (MLE). Functions were developped to enable moment matching estimation (MME), quantile matching estimation (QME), and maximum goodness-of-fit estimation (MGE) using eight different distances. Moreover, the fitdistrplus package offers the possibility to specify a user-supplied function for optimization, useful in cases where classical optimization techniques not included in optim are more adequate.

In applied statistics, it is frequent to have to fit distributions to censored data [32, 24, 9, 35, 10]. The MASS fitdistr function does not enable maximum likelihood estimation with this type data. Some packages deal with censored data, especially survival data [59] (see [25, 30] for examples), but those packages generally focused on specific models, enabling the fit of only one distribution or a restricted family of distributions. Our third objective was thus to provide R users a function to estimate univariate distribution parameters from censored data, whatever the type of censoring.

Few packages on CRAN provide estimation procedures for a general distribution and a general type of data. The **distrMod** package of [34] provides an object-oriented (S4) implementation of probability models and includes distribution fitting procedures for a given minimization criterion. In **fitdistrplus**, we use the standard S3 class system, we believe simpler than the full object-oriented S4 model for most R users. Furthermore, the **distrMod** package does not allow to fit censored data. The mle function of **stats4** package provides a procedure for maximum likelihood estimation whose output has class "mle". Many generic methods are implemented for this type of object, e.g. **confint**, logLik,... When designing the **fitdistrplus** package, we also take this into account. Finally, various other packages provide functions to estimate the mode, the moments or the L-moments of a distribution, see the reference manuals of **modeest**, **lmomco** and **Lmoments** packages.

This manuscript reviews the various features of version 1.0-1 of **fitdistrplus**. The package is available from the Comprehensive R Archive Network at http://cran.r-project.org/package=fitdistrplus. The development version of the package is located at R-forge as one the packages of the project "Risk Assessment with R" (http://r-forge.r-project.org/projects/riskassessment/). The following command will load the package.

> library(fitdistrplus)

The paper is organized as follows: Section 2 present tools for fitting continuous distributions to classic non-censored data. Section 3 deals with other estimation methods and other types of data, before Section 4 concludes.

2 Fitting distributions to continuous non-censored data

2.1 Choice of candidate distributions

For illustrating the use of various functions of the **fitdistrplus** package with continuous non-censored data, we first use a data set named **groundbeef** which is included in our package. This data set contains pointwise values of serving sizes in grams, collected in a French survey, for ground beef patties consumed by children under 5 years old. It was used in a quantitative risk assessment published in the international journal of food microbiology journal [14].

> data(groundbeef)

> str(groundbeef)

'data.frame': 254 obs. of 1 variable: \$ serving: num 30 10 20 24 20 24 40 20 50 30 ...

Before fitting one or more distributions to a data set, it is generally necessary to choose good candidates among a predefined family of distributions. This choice may be guided by the knowledge of stochastic processes governing the modelled variable, but also by the observation of its empirical distribution. To help the user in this choice, we developed functions to plot and characterise the empirical distribution.

First of all, the empirical distribution function and the histogram may be plotted using the classical R functions ecdf and hist, or by using the plotdist function of the **fitdistrplus** package. This function provides two plots (see Figure 1): the left-hand graph is the histogram (on a density level) and the right-hand graph plots the empirical cumulative distribution function (CDF).

> plotdist(groundbeef\$serving)

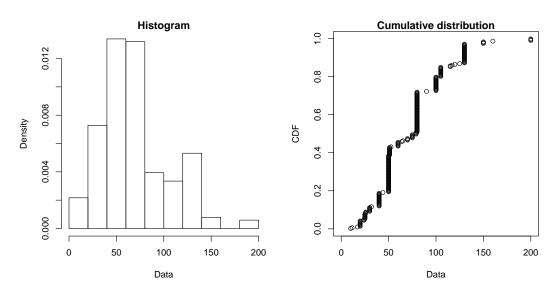


Figure 1: Histogram and CDF plots of an empirical distribution for a continuous variable (serving size from the groundbeef data set)

In addition to empirical plots, descriptive statistics may help to choose good candidates to describe a distribution among a family of parametric distributions. Especially the skewness and kurtosis, linked to the third and fourth moments, are useful for this purpose. A non-zero skewness reveals a lack of symmetry of the empirical distribution, while the kurtosis value quantifies the weight of tails in comparison to the normal distribution for which the kurtosis equals 3.

The skewness and kurtosis and their corresponding unbiased estimator from a sample $(X_i)_i \overset{\text{i.i.d.}}{\sim} X$ with observations $(x_i)_i$ are given by

$$sk(X) = \frac{E[(X - E(X))^3]}{Var(X)^{\frac{3}{2}}} , \ \widehat{sk} = \frac{\sqrt{n(n-1)}}{n-2} \times \frac{m_3}{m_2^{\frac{3}{2}}}, \tag{1}$$

$$kr(X) = \frac{E[(X - E(X))^4]}{Var(X)^2} , \ \widehat{kr} = \frac{n-1}{(n-2)(n-3)}((n+1) \times \frac{m_4}{m_2^2} - 3(n-1)) + 3, \tag{2}$$

where m_2 , m_3 , m_4 denote empirical moments defined by $m_r = \frac{1}{n} \sum_{i=1}^n (x_i - \overline{x})^r$, with x_i the *n* observations of variable x and \overline{x} their mean value.

The descdist function provides calculations of classical descriptive statistics (minimum, maximum, median, mean, standard deviation), skewness and kurtosis. By default, unbiased estimations of the three last statistics are provided. But, the argument method may be used to obtain them without correction for bias. A skewness-kurtosis plot such as the one proposed by [12] is provided by the function descdist for the empirical distribution (see Figure 2 for the groundbeef data set). On this plot, values for common distributions are displayed in order to help the choice of distributions to fit to data. For some distributions (normal, uniform, logistic, exponential), there is only one possible value for the skewness and the kurtosis. Thus, the distribution is represented by a single point on the plot. For other distributions, areas of possible values are represented, consisting in lines (as for gamma and lognormal distributions), or larger areas (as for beta distribution).

Skewness and kurtosis are known not to be robust. In order to take into account the uncertainty of the estimated values of kurtosis and skewness from data, a bootstrap procedure can be performed by fixing the argument boot to an integer above 10. Bootstrap samples of the same size of the original data set are then constructed by random sampling with replacement from that original data set. Values of skewness and kurtosis are computed on that bootstrap samples and reported on the skewness-kurtosis plot. Below is a call to the descdist function to describe the distribution of the serving size from the groundbeef data set and to draw the corresponding skewness-kurtosis plot (see Figure 2). Looking at the results on this example with a positive skewness and a kurtosis not far from 3, the fit of three common right-skewed distributions could be considered, Weibull, gamma and lognormal distributions.

> descdist(groundbeef\$serving, boot=1000)

summary statistics

min: 10 max: 200

median: 79 mean: 73.65

estimated sd: 35.88

estimated skewness: 0.7353 estimated kurtosis: 3.551

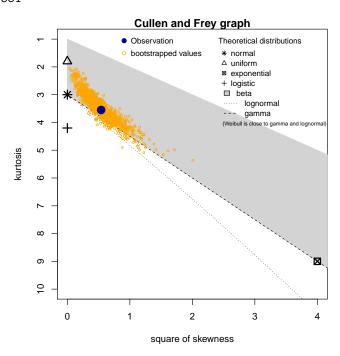


Figure 2: Skewness-kurtosis plot for a continuous variable (serving size from the groundbeef data set)

Together with the use of the plotdist and descdist functions to characterize the empirical distribution, the properties of the modeled variable should be considered, especially its range. Having chosen good candidates for the distribution, we turn to the fit of distributions and comparison of goodness-of-fits.

2.2 Fit of distributions by maximum likelihood estimation

Once selected, one or more parametric distributions $f(.|\theta)$ may be fitted to the data set, one at a time, using the fitdist function. Under the i.i.d. sample assumption, distribution parameters θ are by default estimated by maximizing the

$$L(\theta) = \prod_{i=1}^{n} f(x_i | \theta)$$
 (3)

with x_i the *n* observations of variable *X* and $f(.|\theta)$ the density function of the parametric distribution. The other proposed estimation methods are described in Section 3.1.

The fitdist function returns the results of the fit of any parametric distribution to a data set as an S3 class object that may be easily printed, summarized or plotted. In order to be used in fitdist, a distribution dist must be defined by the d, p, q functions, standing respectively for the density, the cumulative distribution and the quantile functions, e.g. dnorm, pnorm and qnorm for the normal distribution. The name of the fitted distribution is specified in the first argument by its classical abbreviation dist used in the d, p, q functions, e.g. "norm" for the normal distribution. Numerical results returned by the fitdist function are (1) the parameter estimates, (2) the estimated standard errors (computed from the estimate of the Hessian matrix at the maximum likelihood solution), (3) the loglikelihood, (4) Akaike and Schwarz information criteria (the so-called AIC and BIC), and (5) the correlation matrix between parameter estimates. Below is a call to the fitdist function to fit a Weibull distribution to the serving size from the groundbeef data set.

```
> fw <- fitdist(groundbeef$serving, "weibull")</pre>
> summary(fw)
Fitting of the distribution 'weibull 'by maximum likelihood
Parameters :
      estimate Std. Error
         2.186
                   0.1046
shape
scale
        83.348
                   2.5269
Loglikelihood: -1255
                        AIC: 2514
                                     BIC:
                                            2522
Correlation matrix:
       shape scale
shape 1.0000 0.3218
scale 0.3218 1.0000
```

The plot of an object of class "fitdist" provides four classical goodness-of-fit plots [12]:

- a density plot representing the density function of the fitted distribution along with the histogram of the empirical distribution,
- a CDF plot of both the empirical distribution and the fitted distribution,
- a Q-Q plot representing the empirical quantiles (y-axis) against the theoretical quantiles (x-axis)
- a P-P plot representing the empirical distribution function evaluated at each data point (y-axis) against the fitted distribution function (x-axis).

Unlike plot.fitdist, the denscomp, cdfcomp, qqcomp and ppcomp functions enable to separately plot each of these four plots, in order to compare the empirical and multiple theoretical distributions fitted on a same data set. These functions must be called with a first argument corresponding to a list of objects of class fitdist, and optionaly further arguments to customize the plot (see the reference manual [15] for lists of arguments that may be changed for each plot). In the following example, we compare the fit of a Weibull, a lognormal and a gamma distributions to the groundbeef data set (Figure 3).

```
> fg <- fitdist(groundbeef$serving,"gamma")
> fln <- fitdist(groundbeef$serving,"lnorm")
> par(mfrow=c(2, 2))
> denscomp(list(fw,fln,fg), legendtext=c("Weibull", "lognormal", "gamma"))
> qqcomp(list(fw,fln,fg), legendtext=c("Weibull", "lognormal", "gamma"))
> cdfcomp(list(fw,fln,fg), legendtext=c("Weibull", "lognormal", "gamma"))
> ppcomp(list(fw,fln,fg), legendtext=c("Weibull", "lognormal", "gamma"))
```

For CDF, Q-Q and P-P plots, the probability plotting position is defined by default using the Hazen's rule, with probability points of the empirical distribution defined as (1:n - 0.5)/n, as recommended by Blom [6]. This plotting position can be easily changed using the arguments use.ppoints and a.ppoints. When use.ppoints = TRUE, the argument a.ppoints is passed to the ppoints function from the stats package to define the probability points of the empirical distribution as (1:n - a.ppoints)/(n - 2a.ppoints + 1). When use.ppoints = FALSE, the probability points are simply defined as 1:n / n.

The density plot and the CDF plot are the most classical goodness-of-fits plots. The two other plots are complementary and can be very informative in some cases. The Q-Q plot emphasizes the lack-of-fit at the distribution tails while the P-P plot emphasizes the lack-of-fit at the distribution center. As an example in Figure 3, none of the three fitted distributions describes the center of the distribution rather better than the two others, but the Weibull

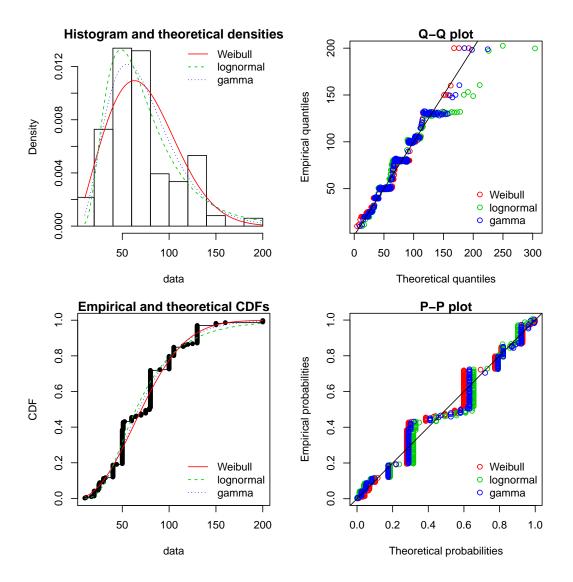


Figure 3: Four Goodness-of-fit plots for various distributions fitted on continuous data (Weibull, gamma and lognormal distributions fitted to serving sizes from the groundbeef data set)

and gamma distributions should be preferred for their better description of the right tail of the empirical distribution, especially if the weight of this tail is important in the use of the fitted distribution, as it is in the context of food risk assessment.

To illustrate other features of the **fitdistrplus** package, we will now use another data set named **endosulfan**, which is included in our package. This data set contains acute toxicity values for the organochlorine pesticide endosulfan (geometric mean of LC50 ou EC50 values in $\mu g.L^{-1}$), tested on Australian and non-Australian laboratory-species (arthropods, fish or nonarthropod invertebrates, see [27]).

```
> data(endosulfan)
> str(endosulfan)
```

```
'data.frame': 104 obs. of 3 variables:

$ ATV : num 0.6 2.8 182.2 0.8 478 ...

$ Australian: Factor w/ 2 levels "no","yes": 2 2 2 2 2 2 2 2 2 1 ...

$ group : Factor w/ 3 levels "Arthropods","Fish",..: 1 1 1 1 1 1 1 1 1 1 ...
```

In ecotoxicology, a lognormal or a loglogistic distribution is often fitted to such a data set in order to characterize the species sensitivity distribution (SSD) for a pollutant. A low percentile of the fitted distribution, generally the 5% percentile, is calculated and named the hazardous concentration 5% (HC5). It is interpreted as the value of the pollutant concentration protecting 95% of the species. But the fit of a lognormal or a loglogistic distribution to the whole endosulfan data set is rather bad, especially due to a minority of very high values. We can try to fit this data set by the Pareto distribution or the three-parameter Burr distribution which is an extension of both the loglogistic and the Pareto distribution. Pareto and Burr distributions are provided in package actuar. Until here, we did not have to implicity define starting values (in the optimization process) as reasonable starting values are defined within function fitdist for most of the distributions defined in R packages (see the help of fitdist for details). For other distributions like the Pareto and the Burr distribution, we have to supply initial values for the distribution parameters

in the argument start when using the maximum likelihood method. start must be a named list with initial values for each parameter (as they appear in the d, p, q functions). Having defined reasonable starting values¹, we can fit various distributions and graphically compare their fits. On this example, the use of functions cdfcomp and qqcomp is especially interesting to evaluate the goodness-of-fit on the tail of interest while defining an HC5 value.

```
> ATV <-endosulfan$ATV
> fendo.ln <- fitdist(ATV, "lnorm")
> library(actuar)
> fendo.ll <- fitdist(ATV, "llogis", start=list(shape=1, scale=500))
> fendo.P <- fitdist(ATV, "pareto", start=list(shape=1, scale=500))
> fendo.B <- fitdist(ATV, "burr", start=list(shape=0.3, shape=0.3, shape=0.3, shape=0.3)
> par(mfrow=c(1, 2))
> cdfcomp(list(fendo.ln, fendo.ll, fendo.P, fendo.B), xlogscale=TRUE,
+ legendtext = c("lognormal", "loglogistic", "Pareto", "Burr"))
> qqcomp(list(fendo.ln, fendo.ll, fendo.P, fendo.B), xlogscale=TRUE, ylogscale=TRUE,
+ legendtext = c("lognormal", "loglogistic", "Pareto", "Burr"))
```

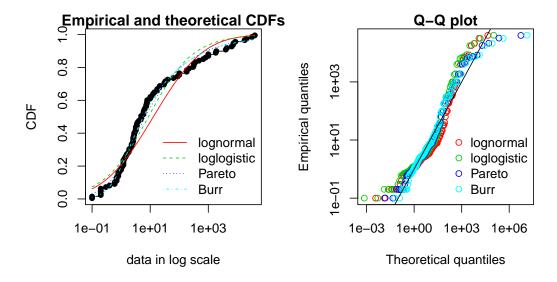


Figure 4: CDF and Q-Q plots to compare the fit of four distributions to acute toxicity values of various organisms for the organochlorine pesticide endosulfan (endosulfan data set)

We can see in Figure 4 that none of the fitted distribution correctly describes the right tail observed in the data set. But the left tail seems to be better described by the Burr distribution. Its use could then be considered to estimate the HC5 value as the 5% quantile of the distribution. This can be easily done using the quantile generic function defined for an object of class "fitdist". Below is this calculation together with the calculation of the empirical quantile for comparison.

To go further in the comparison of various distributions, we propose the calculation of different goodness-of-fit statistics in our package. The purpose of goodness-of-fit statistics aims to measure the distance between the fitted parametric distribution and the empirical distribution: e.g. the distance between the fitted cumulative distribution function F and the empirical distribution function F_n . When fitting continuous distributions, three goodness-of-fit statistics are classically considered: Cramer-von Mises, Kolmogorov-Smirnov and Anderson-Darling statistics. Naming x_i the n observations of a continuous variable X arranged in an ascending order, Table 1 gives the definition and the empirical estimate of the three considered goodness-of-fit statistics.

They can be computed using the function gofstat as defined by Stephens [13].

¹The plotdist function can plot any parametric distribution with specified parameter values in argument para. It can thus help to find correct initial values for the distribution parameters in non trivial cases, by iterative calls if necessary (see the reference manual [15] for examples).

Table 1: Goodness-of-fit statistics as defined by Stephens [13].

| Statistic | General formula | Computational formula |
|--------------------|---|--|
| Kolmogorov-Smirnov | $\sup F_n(x) - F(x) $ | $\max(D^+, D^-)$ with |
| (KS) | | $D^{+} = \max_{i=1,\dots,n} \left(\frac{i}{n} - F(x_i) \right); D^{-} = \max_{i=1,\dots,n} \left(F(x_i) - \frac{i-1}{n} \right)$ |
| Cramer-von Mises | $n \int_{-\infty}^{\infty} (F_n(x) - F(x))^2 dx$ | $\frac{1}{12n} + \sum_{i=1}^{n} \left(F(x_i) - \frac{2i-1}{2n} \right)^2$ |
| (CvM) | | <i>i</i> =1 |
| Anderson-Darling | $n \int_{-\infty}^{\infty} \frac{(F_n(x) - F(x))^2}{F(x)(1 - F(x))} dx$ | $-n - \frac{1}{n} \sum_{i=1}^{n} \left((2i - 1)(\log(F(x_i)) + \log(1 - F(x_{n+1-i}))) \right)$ |
| (AD) | | <i>i</i> –1 |

> gofstat(list(fendo.ln, fendo.ll, fendo.P, fendo.B))

Goodness-of-fit statistics

| | 1-mle-Inorm | 2-mle-llogis | 3-mle-pareto | 4-mle-burr |
|------------------------------|-------------|--------------|--------------|------------|
| Kolmogorov-Smirnov statistic | 0.1672 | 0.1196 | 0.08488 | 0.06155 |
| Cramer-von Mises statistic | 0.6374 | 0.3827 | 0.13926 | 0.06803 |
| Anderson-Darling statistic | 3.4721 | 2.8316 | 0.89206 | 0.52393 |

Goodness-of-fit criteria

| | | 1-mle-lnorm | 2-mle-llogis | 3-mle-pareto | 4-mle-burr |
|------------------------|-----------|-------------|--------------|--------------|------------|
| Aikake's Information (| Criterion | 1069 | 1069 | 1048 | 1046 |
| Bayesian Information C | Criterion | 1074 | 1075 | 1053 | 1054 |

As giving more weight to distribution tails, Anderson-Darling statistics is of special interest when it matters to equally emphasize the tails as well as the main body of a distribution. This is often the case in risk assessment, e.g. [12, 62]. For this reason, this statistics is often used to select the best distribution among those fitted. Nevertheless, this statistics should be used cautiously when comparing fits of various distributions. We must keep in mind that the weighting of each CDF quadratic difference depends on the theoretical distribution in its definition, see Table 1. Anderson-Darling statistics computed for several distributions fitted on a same data set are thus theoretically difficult to compare. Moreover, such a statistic, as Cramer-von Mises and Kolmogorov-Smirnov ones, does not take into account the complexity of the model. It is not a problem when compared distributions are characterized by the same number of parameters, but it could systematically promote the selection of the more complex distributions in the other case. Looking at classical penalized criteria based on the loglikehood seems thus also interesting, especially to discourage overfitting.

In the previous example, all the goodness-of-fit statistics based on the cdf distance encourage the choice of the Burr distribution, the only one characterized by three parameters, while Akaike and Schwarz information criteria (so called AIC and BIC) respectively gives the preference to the Burr distribution or the Pareto distribution. The choice between these two distributions seems thus less obvious and could be discussed. Even if specifically recommended for discrete distributions, the Chi-squared statistic may also be used for continuous distributions (see Section 3.3 and the reference manual [15] for examples).

2.3 Uncertainty in parameter estimates

The uncertainty in the parameters of the fitted distribution may be simulated by parametric or nonparametric bootstraps using the boodist function for non-censored data. This function returns the bootstrapped values of parameters in a S3 class object which may be plotted to visualize the bootstrap region. The medians and the 95 percent confidence intervals of parameters (2.5 and 97.5 percentiles) are printed in the summary. If inferior to the whole number of iterations, the number of iterations for which the function converges is also printed in the summary.

The plot of an object of class "bootdist" consists in a scatterplot or a matrix of scatterplots of the bootstrapped values of parameters providing a representation of the joint uncertainty distribution of the fitted parameters (see Figure 5). Below is an example of the use of the bootdist function with the previous fit of the Burr distribution to the endosulfan data set.

```
> bendo.B <- bootdist(fendo.B, niter=1001)</pre>
```

> summary(bendo.B)

```
Parametric bootstrap medians and 95% percentile CI Median 2.5% 97.5% shape1 0.1998 0.09871 0.3652 shape2 1.5847 1.03291 2.9930 rate 1.4955 0.67666 2.8278
```

> plot(bendo.B)

Bootstrapped values of parameters

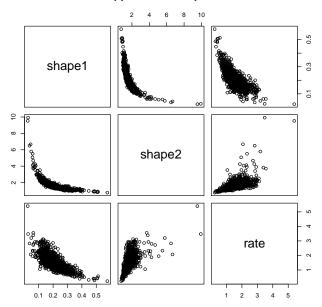


Figure 5: Bootstrappped values of parameters for a fit of the Burr distribution characterized by three parameters (example on the endosulfan data set)

Bootstrap samples of parameter estimates are useful especially to calculate confidence intervals on each parameter of the fitted distribution from the marginal distribution of the bootstraped values. It is also interesting to look at the joint distribution of the bootstraped values in a scatterplot (or a matrix of scatterplots if the number of parameters exceeds two) in order to understand the potential structural correlation between parameters (see Figure 5).

The use of the whole bootstrap sample is also of interest in the risk assessment field. Its use enables the characterization of uncertainty in distribution parameters. It can be directly used within a second-order Monte Carlo simulation framework, especially within the package $\mathbf{mc2d}$ ([48]). One could refer to Pouillot *et al.* ([45]) for an introduction to the use of $\mathbf{mc2d}$ and **fitdistrplus** packages in the context of quantitative risk assessment.

Bootstrap can also be used to calculate confidence intervals on quantiles of the fitted distribution. For this purpose, a generic quantile function is provided for class bootdist. By default 95% bootstrap confidence intervals of quantiles are provided. Going back to the previous example from ecotoxicolgy, this function can be used to estimate the uncertainty associated to the HC5 estimation, for example from the previously fitted Burr distribution to the endosulfan data set.

The estimation method converged only for 1000 among 1001 bootstrap iterations.

3 Advanced topics

3.1 Alternative methods for parameter estimation

Despite maximum likelihood estimation is the default estimation proposed by fitdist, other classical estimation methods can be handled to estimate parameters for non-censored data. Thus, this subsection focuses on alternative estimation methods.

One of the alternative for continuous distributions is the maximum goodness-of-fit estimation method also called minimum distance estimation method. In this package this method is proposed with eight different distances: the three classical distances defined in Table 1, or one of the variants of the Anderson-Darling distance proposed by [37] and defined in Table 2. The right-tail AD gives more weight only to the right tail, the left-tail AD gives more weight only to the left tail. Either of the tails, or both of them, can receive even larger weights by using second order Anderson-Darling Statistics.

| | C 1.C 1 | O 1 1 1 1 |
|------------------|--|---|
| Statistic | General formula | Computational formula |
| Right-tail AD | $\int_{-\infty}^{\infty} \frac{(F_n(x) - F(x))^2}{1 - F(x)} dx$ | $\frac{n}{2} - 2\sum_{i} F(x_i) - \frac{1}{n}\sum_{i} ((2i-1)ln(1 - F(x_{n+1-i})))$ |
| (ADR) | . , | |
| Left-tail AD | $\int_{-\infty}^{\infty} \frac{(F_n(x) - F(x))^2}{(F(x))} dx$ | $-\frac{3n}{2} + 2\sum_{i} F(x_i) - \frac{1}{n}\sum_{i} ((2i-1)ln(F(x_i)))$ |
| (ADL) | (- (-// | |
| Right-tail AD | $ad2r = \int_{-\infty}^{\infty} \frac{(F_n(x) - F(x))^2}{(1 - F(x))^2} dx$ | $ad2r = 2\sum_{i} ln(1 - F(x_i)) + \frac{1}{n}\sum_{i} \frac{2i - 1}{1 - F(x_{n+1-i})}$ |
| 2nd order (AD2R) | | (/ |
| Left-tail AD | $ad2l = \int_{-\infty}^{\infty} \frac{(F_n(x) - F(x))^2}{(F(x))^2} dx$ | $ad2l = 2\sum_{i} ln(F(x_i)) + \frac{1}{n}\sum_{i} \frac{2i-1}{F(x_i)}$ |
| 2nd order (AD2L) | | |
| AD 2nd order | ad2r + ad2l | ad2r + ad2l |
| (AD2) | | |

Table 2: Modified Anderson-Darling statistics as defined by Luceno [37].

To fit a distribution by maximum goodness-of-fit estimation, one needs to fix the argument method to "mge" in the call to fitdist and to specify the argument gof coding for the chosen goodness-of-fit distance. This function is intended to be used only with continuous non-censored data.

Maximum goodness-of-fit estimation may be useful to give more weight to data at one tail of the distribution. Let us go back to the previous example from ecotoxicology. Instead of trying to find a less classical distribution to correctly fit the empirical distribution especially on its left tail, one could consider the fit of the classical lognormal distribution, but minimizing a goodness-of-fit distance giving more weight to the left tail of the empirical distribution, so as to correctly estimate the 5% percentile. In the following example of endosulfan data set, we use left tail Anderson-Darling distances of first or second order (see Figure 6).

```
> fendo.ln.ADL <- fitdist(ATV,"lnorm",method="mge",gof="ADL")
> fendo.ln.AD2L <- fitdist(ATV,"lnorm",method="mge",gof="AD2L")
> cdfcomp(list(fendo.ln, fendo.ln.ADL, fendo.ln.AD2L),
+ xlogscale = TRUE, main = "",
+ legendtext = c("MLE",
+ "Left-tail AD", "Left-tail AD 2nd order"),cex=0.7,
+ xlegend = "bottomright")
```

Comparing the 5% percentiles (HC5) calculated using these three fits to the one calculated from the MLE fit of the Burr distribution, we can observe, on this example, that fitting the lognormal distribution by maximizing left tail Anderson-Darling distances of first or second order enables to approach the value obtained by fitting the Burr distribution by MLE.

```
> ( HC5.estimates <- cbind(empirical = as.numeric(quantile(ATV, probs = 0.05)),
+ Burr = as.numeric(quantile(fendo.B,probs = 0.05)$quantiles),
+ lognormal_MLE = as.numeric(quantile(fendo.ln,probs = 0.05)$quantiles),
+ lognormal_AD2 = as.numeric(quantile(fendo.ln.ADL,probs = 0.05)$quantiles),
+ lognormal_AD2L = as.numeric(quantile(fendo.ln.AD2L,probs = 0.05)$quantiles)) )
empirical Burr lognormal_MLE lognormal_AD2 lognormal_AD2L
[1,] 0.2 0.2939 0.07259 0.1959 0.2588</pre>
```

Another method commonly used to fit parametric distribution is the moment matching estimation (MME). It consists in finding the value of the parameter θ that equalizes the first theoretical raw moments of the parametric

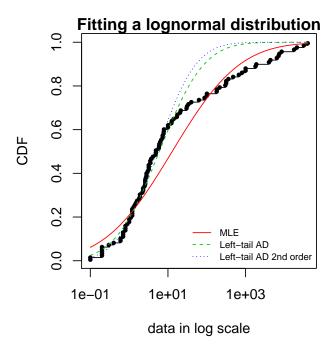


Figure 6: Comparison of a lognormal distribution fitted by MLE and by MGE using two different goodness-of-fit distances: left-tail Anderson-Darling and left-tail Anderson Darling of seond order (example on the endosulfan data set)

distribution to the empirical moments (Equation 4)

$$E(X^k|\theta) = \frac{1}{n} \sum_{i=1}^n x_i^k,$$
 (4)

for k = 1, ..., p, with p the number of parameters to estimate and x_i the n observations of variable X. For moments of order greater or equal than 2, it may also be relevant to match centered moments as given by Equation (5).

$$E((X - E(X))^{k}|\theta) = \frac{1}{n} \sum_{i=1}^{n} (x_{i} - \bar{x}_{n})^{k}$$
(5)

This method can be performed by setting the argument method to "mme" in the call to fitdist. The estimate is computed by a closed-form formula for the following distributions: normal, lognormal, exponential, Poisson, gamma, logistic, negative binomial, geometric, beta and uniform distributions (i.e. base R distributions). In this case, for distributions characterized by one parameter (geometric, Poisson and exponential), this parameter is simply estimated by matching theoretical and observed means, and for distributions characterized by two parameters, these parameters are estimated by matching theoretical and observed means and variances (see e.g. [62]). Otherwise, for not so-common distributions, the equation of moments is solved numerically using the optim function by minimizing the sum of squared differences between observed and theoretical moments (see the fitdistrplus reference manual [15] for technical details).

To illustrate this method, we use a classical data set from the Danish insurance industry published in [40]. In **fitdistrplus**, the data set is stored in **danishuni** for the univariate version.

mettre deux mots sur les objectifs par rapport a ce type de jeu de donnees pour qu'on comprenne tes choix de lois, NA Dire alors d'emblee qu'on va s'interesser plus a cette queue de distribution a droite et pourquoi

```
> data(danishuni)
```

> str(danishuni)

```
'data.frame': 2167 obs. of 2 variables:

$ Date: Date, format: "1980-01-03" "1980-01-04" ...

$ Loss: num 1.68 2.09 1.73 1.78 4.61 ...
```

We can first fit a lognormal distribution on danishuni data set by matching moments using a closed-form formula. By comparison to the lognormal distribution fitted by maximum likelihood, we observe on the left part of Figure 7 that the moment matching estimation is far more conservative than the maximum likelihood estimation (overestimate the right tail of the distribution)

pour moi le terme conservative utilise ainsi n'est pas habituel. Est-ce classique en stat independamment du domaine d'application? Si non il faut le modifier ou l'expliquer mieux. Et je ne suis pas convaincue de comprendre quel ajustement tu preferes au final ici. Faudrait aussi a mon sens commentez les ajustements

10

```
TODO
```

```
> fdanish.ln.MLE <- fitdist(danishuni$Loss, "lnorm")
> fdanish.ln.MME <- fitdist(danishuni$Loss, "lnorm", method="mme", order=1:2)
> cdfcomp(list(fdanish.ln.MLE, fdanish.ln.MME),
+ legend=c("lognormal MLE", "lognormal MME"), main="Fitting a lognormal distribution",
+ xlogscale=TRUE, datapch="*")
```

In a second time we can fit a Pareto type II distribution. Explique pourquoi ce choix. Quel interet? Qu'en attends-tu?

We use the implementation of the **actuar** package providing moments and limited expected value for that distribution (in addition to d, p, q and r functions, see [23]). Fitting a heavy-tailed distribution for which the first and the second moments do not exist for certain values of the shape parameter requires some cautiousness. This is carried out by providing for the optimization process a lower and an upper bound for each parameter. Our call below immediately calls the L-BFGS-B optimization method in optim, since this quasi-Newton allows box constraints². Note that we have to pass a function for computing the empirical raw moment to fitdist, since the user may choose either (4) and (5).

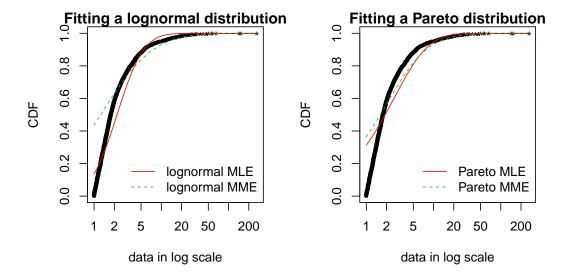


Figure 7: Comparison between MME and MLE when fitting a lognormal or a Pareto distribution to loss data from the danishuni data set

Faudrait peut-etre conclure sur l'interet de la methode des moments. Ou au contraire une remarque de prudence par rapport a cette methode qui est parfois la seule utilisee dans certains logiciels. Enfin il faut conclure quelque chose en tout cas. Voici un essai ci-dessous mais tu as certainement d'autres choses a dire et/ou un autre point de vue

We can see on Figure 7 that matching moments and maximum likelihood fits are far less distant for the Pareto distribution than for the lognormal distribution on this data set. Maximum likelihood and moment matching are certainly the most commonly used method for fitting distributions. But one should keep in mind that these two methods may give very different results. When choosing the matching moment method, the user should be aware of its great sensitivity to outliers. This may be seen as an advantage in our example if the objective is to better describe the right tail of the distribution, but it may be seen as a drawback if the objective is different.

Fitting of a parametric distribution may also be done by matching theoretical quantiles of the parametric distributions (for specified probabilities) against the empirical quantiles. Equation (6) below is thus very similar to Equations (4) and (5)

$$F^{-1}(p^k|\theta) = Q_{n,p_k} \tag{6}$$

 $^{^2\}mathrm{That}$ is what the B stands for.

for k = 1, ..., p, with p the number of parameters to estimate (dimension of θ if there is no fixed parameters) and Q_{n,p_k} the empirical quantiles calculated from data for specified probabilities p_k .

Quantile matching is performed by setting the argument method to "qme" in the call to fitdist and adding an argument probs defining the probabilities for which the quantile matching is performed. The length of this vector must be equal to the number of parameters to estimate. Empirical quantiles are computed using the quantile function of the stats package using the type argument equal to 7 by default, but the type of quantile can be easily changed by using the qty argument in the call to the qme function. The quantile matching is carried out numerically, by minimizing the sum of squared differences between observed and theoretical quantiles.

```
> fdanish.ln.QME1 <- fitdist(danishuni$Loss, "lnorm", method="qme", probs=c(1/3, 2/3))
> fdanish.ln.QME2 <- fitdist(danishuni$Loss, "lnorm", method="qme", probs=c(3/4, 4/5))
> cdfcomp(list(fdanish.ln.MLE, fdanish.ln.QME1, fdanish.ln.QME2),
+ legend=c("MLE", "QME(1/3, 2/3)", "QME(3/4, 4/5)"), main="Fitting a lognormal distribution",
+ xlogscale=TRUE, datapch="*")
```

Above is an example of fitting of a lognormal distribution to danishuni data set by matching probabilities ($p_1 = 1/3, p_2 = 2/3$) and ($p_1 = 3/4, p_2 = 4/5$). As expected, the second QME fit is more conservative when looking at the tail of the distributions. Compared to the maximum likelihood estimation, the second QME fit is also more conservative, whereas the first QME fit is less conservative. The quantile matching estimation is of particular interest when we need a focus around particular quantiles, e.g. p = 99.5% in the Solvency II insurance context or p = 5% for the HC5 estimation in the ecotoxicology context.

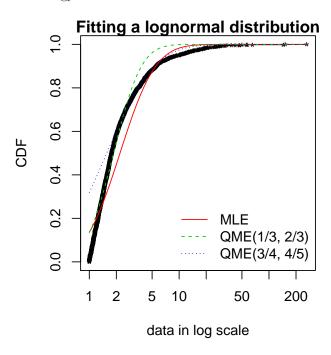


Figure 8: Comparison between QME and MLE when fitting a lognormal distribution to loss data from the danishuni data set

3.2 Customization of the optimization algorithm

Each time a numerical minimization (or maximization) is carried out using fitdist, the optim function of the stats package is used by default with the "Nelder-Mead" method for distributions characterized by more than one parameter and the "BFGS" method for distributions characterized by only one parameter. Sometimes the default algorithm fails to converge. It is then interesting to change some options of the optim function or to use another optimization function than optim to maximize the likelihood or to minimize a squared difference. The argument optim.method can be used in the call to fitdist or fitdistcens. It will internally be passed to mledist and to optim (see the help page of optim from the package stats for details about the different algorithms available proposed by optim).

Below are examples of fits of a gamma distribution $\mathcal{G}(\alpha,\lambda)$ to the **groundbeef** data set with various algorithms. Note that the conjugate gradient algorithm ("CG") needs far more iterations to converge (around 2500 iterations) compared to other algorithms (converging in less than 100 iterations).

```
> data(groundbeef)
> fNM <- fitdist(groundbeef$serving, "gamma", optim.method="Nelder-Mead")
> fBFGS <- fitdist(groundbeef$serving, "gamma", optim.method="BFGS")
> fSANN <- fitdist(groundbeef$serving, "gamma", optim.method="SANN")</pre>
```

```
> fCG <- try(fitdist(groundbeef$serving, "gamma", optim.method="CG", control=list(maxit=10000)))
> if(class(fCG) == "try-error")
+ fCG <- list(estimate=NA)</pre>
```

It is also possible to use another function than optim to maximize the likelihood. This optimization function must be specified by the argument custom.optim in the call to fitdist. But before that, it may be necessary to customize this optimization function to meet the following requirements. (1) custom.optim function must have (at least) the following arguments: fn for the function to be optimized and par for the initialized parameters. (2) custom.optim should carry out a MINIMIZATION and must return (at least) the following components: par for the estimate, convergence for the convergence code, value for fn(par) and hessian. Below is an example of code written to wrap the genoud function from the rgenoud package in order to respect our optimization "template". The rgenoud package implements the genetic (stochastic) algorithm.

```
> mygenoud <- function(fn, par, ...)
+ {
+    require(rgenoud)
+    res <- genoud(fn, starting.values=par, ...)
+    standardres <- c(res, convergence=0)
+    return(standardres)
+ }</pre>
```

The customized optimization function can then be passed as the argument custom.optim in the call to fitdist or fitdistcens. The following code can for example be used to fit a gamma distribution to the groundbeef data set. Note that in this example various arguments are also passed from fitdist to genoud: nvars, Domains, boundary.enforcement, print.level and hessian. The code below compares all the parameter estimates by the different algorithms: shape and rate parameters are relatively similar on this example.

```
> fgenoud <- mledist(groundbeef$serving, "gamma", custom.optim= mygenoud, nvars=2, 
+ max.generations=10, Domains=cbind(c(0,0), c(10,10)), boundary.enforcement=1, 
+ hessian=TRUE, print.level=0, P9=10) 
> cbind(NM = fNM$estimate, 
+ BFGS = fBFGS$estimate, 
+ SANN = fSANN$estimate, 
+ CG = fCG$estimate, 
+ fgenoud = fgenoud$estimate) 
NM BFGS SANN CG fgenoud 
shape 4.00825 4.22848 4.03305 4.12891 4.00834 
rate 0.05442 0.05742 0.05457 0.05607 0.05443
```

3.3 Fitting distributions to other types of data

Analytical methods often lead to semi-quantitative results which are referred to as censored data. Observations only known to be under a limit of detection are called left censored data. Observations only known to be above a limit of quantification are called right censored data. Results known to lie between two bounds are called interval censored data. These two bounds may correspond to a limit of detection and a limit of quantification, or more generally to uncertainty bounds around the observation. Right censored data are also commonly encountered among survival data. A data set may thus contain right, left, or interval censored data, or may be a mixture of these categories, possibly with different upper and lower bounds. Censored data are sometimes excluded from the data analysis or replaced by a fixed value, which in both cases may lead to biased results. A more recommended approach to correctly model such data is based upon maximum likelihood [32, 24]. We chose this approach in our package.

Censored data can thus contain left censored, right censored and interval censored values, with several lower and upper bounds. Before using the **fitdistrplus** package, such data must be coded into a dataframe with two columns, respectively named left and right, describing each observed value as an interval. The left column contains either NA for left censored observations, the left bound of the interval censored observations, or the observed value for non-censored observations. The right column contains either NA for right censored observations, the right bound of the interval for interval censored observations, or the observed value for non-censored observations. To illustrate the use of package **fitdistrplus** to fit distributions to censored continuous data, we use another data set from ecotoxicology, included in our package and named **salinity**. This data set contains acute salinity tolerance (LC50 values in electrical conductivity, $mS.cm^{-1}$) of riverine macro-invertebrates taxa from the southern Murray-Darling Basin in Central Victoria, Australia (see [31]).

Using censored data such as those coded in the salinity data set, the empirical distribution can be plotted using the plotdistcens function. By default, this function uses the Expectation-Maximization approach of Turnbull [60] to compute the overall empirical cdf curve with optional confidence intervals, by calls to survfit and plot.survfit functions from the survival package (Figure 10 shows the Turnbull plot of data together with two fitted distributions). A less rigorous but sometimes more illustrative plot to see the real nature of censored data can be obtained by fixing the argument Turnbull to FALSE in the call to plotdistcens (see Figure 9 for an example and the help page of Function plotdistcens for details).

> plotdistcens(salinity, Turnbull = FALSE)

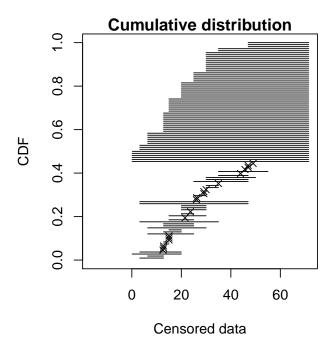


Figure 9: Simple plot of censored data (72-hour acute salinity tolerance of riverine macro-invertebrates from the salinity data set) as ordered points and intervals

As for non censored data, one or more parametric distributions can be fitted to the censored data set, one at a time, but using in this case the **fitdistcens** function. This function estimates the vector of distribution parameters θ by maximizing the likelihood for censored data defined as:

$$L(\theta) = \prod_{i=1}^{N_{nonC}} f(x_i|\theta) \times \prod_{j=1}^{N_{leftC}} F(x_j^{upper}|\theta) \times \prod_{k=1}^{N_{rightC}} (1 - F(x_k^{lower}|\theta)) \times \prod_{m=1}^{N_{intC}} (F(x_m^{upper}|\theta) - F(x_j^{lower}|\theta))$$
(7)

with x_i the N_{nonC} non-censored observations, x_j^{upper} upper values defining the N_{leftC} left-censored observations, x_k^{lower} lower values defining the N_{rightC} right-censored observations, $[x_m^{lower}; x_m^{upper}]$ the intervals defining the N_{intC} interval-censored observations, and F the cumulative distribution function of the parametric distribution.

As fitdist, fitdistcens returns the results of the fit of any parametric distribution to a data set as an S3 class object that can be easily printed, summarized or plotted. For the salinity data set, a lognormal distribution or a loglogistic can be fitted as commonly done in ecotoxicology for such data. As with fitdist, for some distributions (see [15] for details), it is necessary to specify initial values for the distribution parameters in the argument start. The plotdistcens function can help to find correct initial values for the distribution parameters in non trivial cases, by an manual iterative use if necessary.

```
meanlog sdlog
         1.0000 0.2938
meanlog
sdlog
         0.2938 1.0000
> summary(fsal.11)
FITTING OF THE DISTRIBUTION ' llogis ' BY MAXIMUM LIKELIHOOD ON CENSORED DATA
PARAMETERS
      estimate Std. Error
shape
         3.421
                   0.4158
        29.930
scale
                    1.9447
Loglikelihood:
                -140.1
                          AIC:
                                284.1
                                        BIC:
                                               289.5
Correlation matrix:
        shape
                scale
shape 1.0000 -0.2022
scale -0.2022
              1.0000
```

Computations of goodness-of-fit statistics have not yet been developed for fits using censored data but the quality of fit can be judged using Akaike and Schwarz information criteria (AIC and BIC) and the goodness-of-fit CDF plot, respectively provided when summarizing or plotting an object of class "fitdistcens". Function cdfcompcens can also be used to compare the fit of various distributions to the same censored data set. Its call is similar to the one of cdfcomp. Below is an example of comparison of the two fitted distributions to the salinity data set (see Figure 10).

```
> cdfcompcens(list(fsal.ln, fsal.ll),
+ legendtext=c("lognormal", "loglogistic "))
```

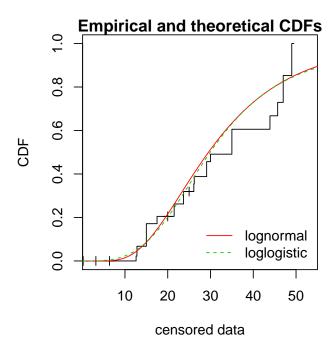


Figure 10: Goodness-of-fit CDF plot for fits of a lognormal and a loglogistic distribution to censored data: LC50 values from the salinity data set

Function bootdistcens is the equivalent of bootdist for censored data, except that it only proposes nonparametric bootstrap, as it is not obvious to simulate censoring within a parametric bootstrap resampling procedure. The generic function quantile can also be applied, as for continuous non-censored data, to an object of class "fitdistcens" or "bootdistcens".

In addition to the fit of distributions to censored or non censored continuous data, our package can also accomodate discrete variables, such as count numbers, using the functions developed for continuous non-censored data. These functions will provide somewhat different graphs and statistics, taking into account the discrete type of the modeled variable. The discrete nature of the variable is automatically recognized when a classical distribution is fitted to data (binomial, negative binomial, geometric, hypergeometric and Poisson distributions) but must be indicated by fixing argument discrete to TRUE in the call to functions in other cases. The toxocara data set included in the package corresponds to the observation of such a discrete variable. It reports numbers of *Toxocara cati* parasites present in digestive tract, from a random sampling of feral cats living on Kerguelen island ([19]). We use it to illustrate the case of discrete data.

```
> data(toxocara)
> str(toxocara)
'data.frame': 53 obs. of 1 variable:
$ number: int 0 0 0 0 0 0 0 0 0 ...
```

The fit of a discrete distribution to discrete data by maximum likelihood estimation requires the same procedure as for continuous non-censored data. As an example, using the toxocara data set, Poisson and negative distributions can be easily fitted.

```
> (ftoxo.P <- fitdist(toxocara$number, "pois"))</pre>
Fitting of the distribution 'pois 'by maximum likelihood
Parameters:
       estimate Std. Error
          8 679
                     0 4047
lambda
> (ftoxo.nb <- fitdist(toxocara$number, "nbinom"))</pre>
Fitting of the distribution 'nbinom 'by maximum likelihood
Parameters:
     estimate Std. Error
size
       0.3971
                  0.08289
       8.6803
                  1.93501
mu
```

For discrete distributions, the plot of an object of class "fitdist" simply provides two goodness-of-fit plots comparing empirical and theoretical distributions in pdf and in cd f(Figure 11). Function cdfcomp can also be used to compare several plots to the same data set, as follows for the previous fits (Figure 12).

> plot(ftoxo.P)

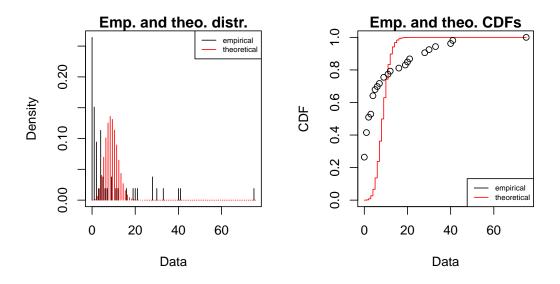


Figure 11: Plot of the fit of a discrete distribution (Poisson distribution fitted to numbers of *Toxocara cati* parasites from the toxocara data set)

> cdfcomp(list(ftoxo.P,ftoxo.nb),legendtext=c("Poisson", "negative binomial"))

When fitting discrete distributions, the Chi-squared statistic is computed by the gofstat function using cells defined by the argument chisqbreaks or cells automatically defined from the data in order to reach roughly the same number of observations per cell, roughly equal to the argument meancount, or sligthly more if there are some ties. The choice to define cells from the empirical distribution (data), and not from the theoretical distribution, was done to enable the comparison of Chi-squared values obtained with different distributions fitted on a same data set. If arguments chisqbreaks and meancount are both omitted, meancount is fixed in order to obtain roughly $(4n)^{2/5}$ cells, with n the length of the data set [62]. Using this default option with the fits of the Poisson and the negative binomial distribution to toxocara data set are compared as follows, giving the preference to the negative binomial distribution, from both Chi-squared statistics and information criteria:

> gofstat(list(ftoxo.P,ftoxo.nb))

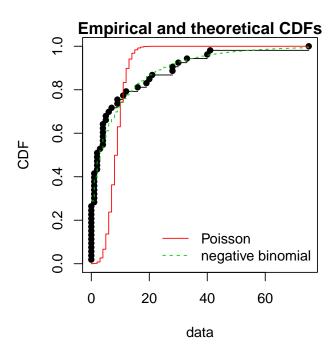


Figure 12: Comparison of the fits of a negative binomial and a Poisson distribution to numbers of *Toxocara cati* parasites from the toxocara data set)

Chi-squared statistic: 31257 7.486

Degree of freedom of the Chi-squared distribution: 5 4

Chi-squared p-value: 0 0.1123

the p-value may be wrong with some theoretical counts < 5

Chi-squared table:

| | obscounts | theo | 1-mle-pois | theo | 2-mle-nbinom |
|-------|-----------|------|------------|------|--------------|
| <= 0 | 14 | | 0.009014 | | 15.295 |
| <= 1 | 8 | | 0.078237 | | 5.809 |
| <= 3 | 6 | | 1.321767 | | 6.845 |
| <= 4 | 6 | | 2.131298 | | 2.408 |
| <= 9 | 6 | | 29.827829 | | 7.835 |
| <= 21 | 6 | | 19.626224 | | 8.271 |
| > 21 | 7 | | 0.005631 | | 6.537 |

Goodness-of-fit criteria

| | | | 1-mre-pois | 2-mie-nbinom |
|----------|---------------------|-------------------|------------|--------------|
| Aikake's | ${\tt Information}$ | ${\tt Criterion}$ | 1017 | 322.7 |
| Bayesian | Information | Criterion | 1019 | 326.6 |

4 Conclusion

In this paper, we present the R statistical package **fitdistrplus** for distribution fitting and demonstrate its use and usefulness. Our main objective while developing this package was to provide tools for helping R users to fit distributions to data. We have been encouraged to pursue our work by feedbacks from users of our package in various areas as food or environmental risk assessment, epidemiology, ecology, molecular biology, genomics, bioinformatics, hydraulics, mechanics, financial and actuarial mathematics or operations research. Indeed, this package is already used a lot by practionners and academics for simple MLE fits in [34, 28, 54, 63, 33, 39, 42, 55, 56, 22, 38], for MLE fits and goodness-of-fit statistics in [21, 57, 3, 5, 7, 44, 46], for MLE fits and bootstrap in [11, 41, 43, 58, 26], for MLE fits, bootstrap and goodness-of-fit statistics in [51], for MME fit in [36], for censored MLE and bootstrap in [35, 49, 29, 10, 47], for graphic analysing in [2, 53], for grouped-data fitting methods in [20] and more generally in [18, 9, 8, 1, 17, 4]. Many extensions of this package are planned in the future: we target to extend to censored data some methods for the moment only available for non-censored data, especially concerning goodness-of-fit evaluation and fitting methods. We will also enlarge the choice of fitting methods for non-censored data, by proposing new goodness-of-fit distances (e.g. distances based on quantiles) for maximum goodness-of-fit estimation and new types of moments (e.g. limited expected values) for moment matching estimation. At last, we will consider the case of multivariate distribution fitting.

5 Acknowledgments

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