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 to 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 modelling the random variable, as well as finding parameter estimates for that distribution. This requires judgment and expertise and generally needs an iterative process of distribution choice, parameter estimation, and quality of fit assessment. In the R ([55]) package MASS ([66]), maximum likelihood estimation is available via the fitdistr function; other steps of the fitting process can be done using other R functions, e.g. [57]. In this paper, we present the R package fitdistrplus ([16]) implementing several methods for fitting univariate parametric distribution. A first objective in 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 likelihood function 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), as proposed in the R package actuar with three different goodness-of-fit distances (see [17]). While developing the fitdistrplus package, a second objective was to consider various estimation methods in addition to maximum likelihood estimation (MLE). Functions were developed 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 [35, 26, 9, 39, 11]. The MASS fitdistr function does not enable maximum likelihood estimation with this type of data. Some packages deal with censored data, especially survival data [64] (see [27, 33] for examples), but those packages generally focused on specific models, enabling the fit of a restricted set of distributions. A third objective was thus to provide R users a function to estimate univariate distribution parameters from right-, left- and interval-censored data.

Few packages on CRAN provide estimation procedures for any user-supplied parametric distribution and support different types of data. The **distrMod** package of [38] provides an object-oriented (S4) implementation of probability models for non-censored data and includes distribution fitting procedures for a given minimization criterion. This package is based on the R-shipped function mle of the **stats4** package producing S4 objects of class "mle" for which generic methods are implemented, e.g. **confint** and **logLik**. In **fitdistrplus**, we choose to use the standard S3 class system for its understanding by most R users. When designing the **fitdistrplus** package, we do not forget to implement generic functions also available for S3 classes. 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 package of the project "Risk Assessment with R" (http://r-forge.r-project.org/projects/riskassessment/). The paper is organized as follows: Section 2 presents 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 [15].

- > library(fitdistrplus)
- > 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 set of distributions. This choice may be guided by the knowledge of stochastic processes governing the modelled variable, or, in the absence of knowledge regarding the underlying process, 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, it is common to start with plots of the empirical distribution function and the histogram, which can be obtained with the plotdist function of the **fitdistrplus** package. This function provides two plots (see Figure 1): the left-hand plot is the histogram (on a density scale) and the right-hand plot the empirical cumulative distribution function (CDF).

> plotdist(groundbeef\$serving)

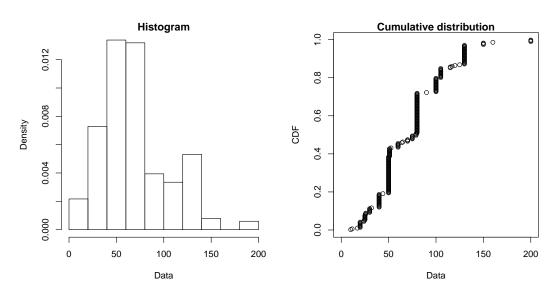


Figure 1: Histogram and CDF plots of an empirical distribution for a continuous variable (serving size from the groundbeef data set) as provided by the plotdist function

In addition to empirical plots, descriptive statistics may help to choose candidates to describe a distribution among a set 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 (e.g. [10]) from a sample $(X_i)_i \stackrel{\text{i.i.d.}}{\sim} X$ 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 classical descriptive statistics (minimum, maximum, median, mean, standard deviation), skewness and kurtosis. By default, unbiased estimations of the three last statistics are provided. Nevertheless,

the argument method can be changed from "unbiased" (default) to "sample" to obtain them without correction for bias. A skewness-kurtosis plot such as the one proposed by [13] 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 nonparametric bootstrap procedure ([18]) can be performed by using the argument boot. Values of skewness and kurtosis are computed on bootstrap samples (constructed by random sampling with replacement from the original data set) and reported on the skewness-kurtosis plot. The properties of the random variable should be considered, notably its expected value, its range, as a complement to the use of the plotdist and descdist. 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

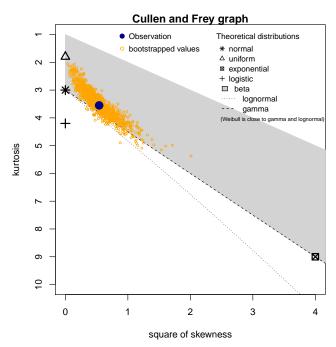


Figure 2: Skewness-kurtosis plot for a continuous variable (serving size from the groundbeef data set) as provided by the descdist function

2.2 Fit of distributions by maximum likelihood estimation

Once selected, one or more parametric distributions $f(.|\theta)$ (with parameter $\theta \in \mathbb{R}^d$) 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 likelihood function defined as:

$$L(\theta) = \prod_{i=1}^{n} f(x_i | \theta)$$
(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 an S3 object of class "fitdist" for which print, summary and plot functions are provided. The fit of a distribution using fitdist assumes that the corresponding d, p, q functions (standing respectively for the density, the distribution and the quantile functions) are defined. Classical distributions are already defined in that way in the stats package, e.g. dnorm, pnorm and qnorm for the normal distribution (see ?Distributions). Others may be found in various packages (see the CRAN task view: Probability Distributions). Distributions not found in any package must be implemented by the user as d, p, q functions. In the call to fitdist, a distribution has to be specified via the argument dist either by the character string corresponding to its common root name used in the names of d, p, q functions (e.g. "norm" for the normal distribution) or by the density function itself from which the root name is extracted (e.g. dnorm 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 Bayesian 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
shape
         2.186
                    0.1046
        83.348
                    2.5269
scale
Loglikelihood:
                -1255
                               2514
                                       BIC:
                                             2522
                         AIC:
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 ([13]) presented on Figures 3 and 4:

- 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).

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 (see the reference manual [16] for details).

Unlike the generic plot function, the denscomp, cdfcomp, qqcomp and ppcomp functions enable to draw separately each of these four plots, in order to compare the empirical distribution and multiple parametric 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 optionally further arguments to customize the plot (see the reference manual [16] for lists of arguments that may be specific to 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"))
```

The density plot and the CDF plot may be considered as the basic 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 correctly describes the center of the distribution, but the Weibull and gamma distributions could be prefered for their better description of the right tail of the empirical distribution, especially if this tail is important in the use of the fitted distribution, as it is in the context of food risk assessment.

The data set named endosulfan is now used to illustrate other features of the fitdistrplus 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 [29]).

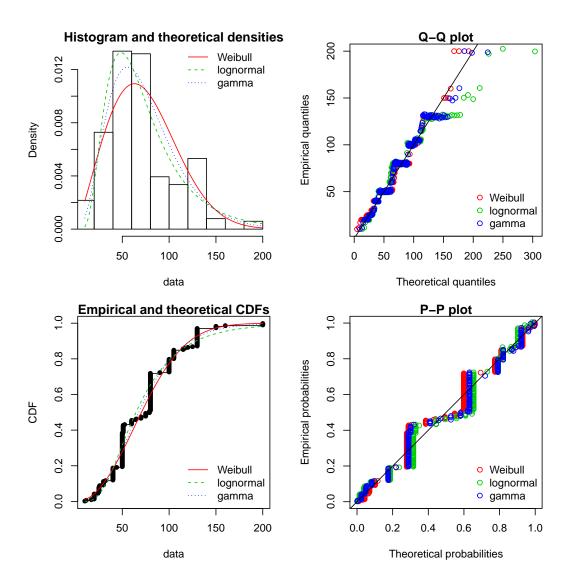


Figure 3: Four Goodness-of-fit plots for various distributions fitted to continuous data (Weibull, gamma and lognormal distributions fitted to serving sizes from the groundbeef data set) as provided by functions denscomp, qqcomp, cdfcomp and ppcomp

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 ([49]). 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. The two-parameter Pareto distribution and the three-parameter Burr distribution (which is an extension of both the loglogistic and the Pareto distributions) have been fitted. Pareto and Burr distributions are provided in the package actuar. Until here, we did not have to define starting values (in the optimization process) as reasonable starting values are implicitly defined within the fitdist function for most of the distributions defined in R (see ?fitdist for details). For other distributions like the Pareto and the Burr distribution, initial values for the distribution parameters have to be supplied in the argument start as a named list with initial values for each parameter (as they appear in the d, p, q functions). Having defined reasonable starting values¹, various distributions can be fitted and graphically compared. On this example, the function cdfcomp can be used to report CDF values in a logscale so as to emphasize discrepancies on the tail of interest while defining an HC5 value.

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 [16] for examples).

```
> 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(shape1=0.3, shape2=1, rate=1))
> cdfcomp(list(fendo.ln, fendo.ll, fendo.P, fendo.B), xlogscale = TRUE,
+ ylogscale = TRUE,legendtext = c("lognormal","loglogistic","Pareto","Burr"))
```

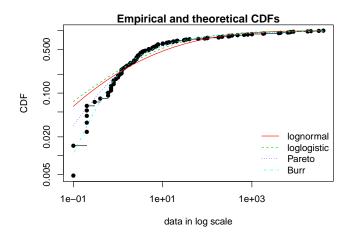


Figure 4: CDF plot to compare the fit of four distributions to acute toxicity values of various organisms for the organochlorine pesticide endosulfan (endosulfan data set) as provided by the cdfcomp function, with CDF values in a logscale to emphasize discrepancies on the left tail

None of the fitted distribution correctly describes the right tail observed in the data set, but as shown in Figure 4, 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.

The computation of different goodness-of-fit statistics is proposed in the **fitdistrplus** package in order to further compare fitted distributions. 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 [14]. 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 [14].

```
> 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-mie-inorm	2-mre-rrogis	3-mie-pareto	4-mie-burr
Aikake's	${\tt Information}$	${\tt Criterion}$	1069	1069	1048	1046
Bayesian	Information	Criterion	1074	1075	1053	1054

Table 1: Goodness-of-fit statistics as defined by Stephens [14].

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	$n \int_{-\infty}^{\infty} \frac{(F_n(x) - F(x))^2}{F(x)(1 - F(x))} dx$	$-n - \frac{1}{n} \sum_{i=1}^{n} ((2i-1)(\log(F(x_i)) + \log(1 - F(x_{n+1-i}))))$
(AD)		<i>t</i> -1

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. [13, 67]. 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. Keeping in mind that the weighting of each CDF quadratic difference depends on the parametric distribution in its definition (see Table 1), Anderson-Darling statistics computed for several distributions fitted on a same data set are 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 (i.e. parameter number). 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 (AIC, BIC) seems thus also interesting, especially to discourage overfitting.

In the previous example, all the goodness-of-fit statistics based on the CDF distance are in favor of the Burr distribution, the only one characterized by three parameters, while AIC and BIC values respectively give 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 [16] for examples).

2.3 Uncertainty in parameter estimates

The uncertainty in the parameters of the fitted distribution may be estimated by parametric or nonparametric bootstraps using the boodist function for non-censored data, see [18]. 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. When inferior to the whole number of iterations (due to lack of convergence of the optimization algorithm for some bootstrapped data sets), the number of iterations for which the estimation 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 0.09755 0.3642 shape2 1.5861 1.03452 2.9930 rate 1.4923 0.68657 2.8278
```

The estimation method converged only for 1000 among 1001 iterations

```
> plot(bendo.B)
```

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 $\mathbf{mc2d}$ ([53]). One could refer to Pouillot and Delignette-Muller ([50]) for an introduction to the use of $\mathbf{mc2d}$ and $\mathbf{fitdistrplus}$ packages in the context of quantitative risk assessment.

Bootstrapped values of parameters

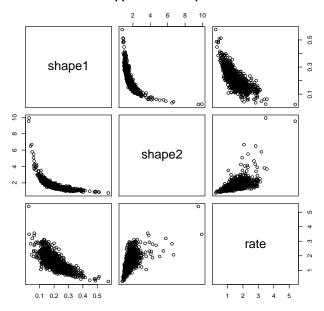


Figure 5: Bootstrappped values of parameters for a fit of the Burr distribution characterized by three parameters (example on the endosulfan data set) as provided by the plot of an object of class "bootdist"

The bootstrap method 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% percentiles 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

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 [14, 17]. 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 [41] and defined in Table 2. The right-tail AD gives more weight 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.

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. Going 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

Table 2: Modified Anderson-Darling statistics as defined by Luceno [41].

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)		

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, ylogscale = TRUE,
+ main = "Fitting a lognormal distribution",xlegend = "bottomright",
+ legendtext = c("MLE","Left-tail AD", "Left-tail AD 2nd order"))
```

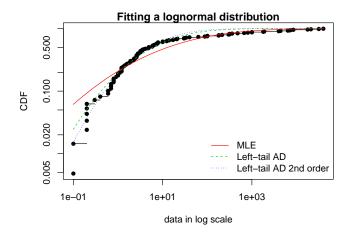


Figure 6: Comparison of a lognormal distribution fitted by MLE and by MGE using two different goodness-of-fit distances: left-tail Anderson-Darling and left-tail Anderson Darling of seond order (example on the endosulfan data set) as provided by the cdfcomp function, with CDF values in a logscale to emphasize discrepancies on the left tail

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

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, ..., d, with d 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. 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. [67]). For other 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 [16] for technical details).

A classical data set from the Danish insurance industry published in [44] is used to illustrate this method. In **fitdistrplus**, the data set is stored in **danishuni** for the univariate version and contains the losse amounts collected at Copenhagen Reinsurance between 1980 and 1990. In actuarial science, it is standard to consider positive heavy-tailed distribution and have a special focus on the right-tail of the distribution. In this numerical experiment, the lognormal distribution is first considered and then the Pareto type II distribution ([36]).

The lognormal distribution on danishuni data set is fitted by matching moments implemented as a closed-form formula. On the left-hand graph of Figure 7, we compare the fitted distribution function between MME and MLE method. The moment matching estimation provides a more cautious estimation of the insurance risk as the MME-fitted distribution function (resp. MLE-fitted) underestimates (overestimates) the empirical distribution function for large values of claim amounts.

```
> 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 ...

> 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, a Pareto type-II distribution, which gives more weight to the right-tail of the distribution, is fitted. As the lognormal distribution, the Pareto type-II has two parameters, which allows a fair comparison.

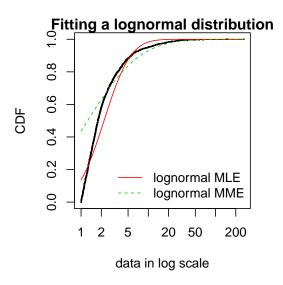
We use the implementation of the **actuar** package providing raw and centered moments for that distribution (in addition to d, p, q and r functions, see [25]). Fitting a heavy-tailed distribution for which the first and the second moments do not exist for certain values of the shape parameter requires 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 a function (called memp in our example) for computing the empirical raw moment to fitdist has to be passed, since the user may choose either Equation (4) or (5).

²That is what the B stands for

Goodness-of-fit statistics

	I-mre-rnorm	z-mie-pareto	2-mme-rnorm	4-mme-pareco	
Kolmogorov-Smirnov statistic	0.1375	0.3124	0.4368	0.3638	
Cramer-von Mises statistic	14.7911	37.7166	88.9503	53.0783	
Anderson-Darling statistic	87.1933	208.3139	416.2567	272.4729	
Coodnoss-of-fit critoria					

		1-mle-lnorm	2-mle-pareto	3-mme-lnorm
${\tt Information}$	${\tt Criterion}$	8120	9250	9792
${\tt Information}$	${\tt Criterion}$	8131	9261	9803
		4-mme-pareto)	
${\tt Information}$	${\tt Criterion}$	9398	5	
${\tt Information}$	${\tt Criterion}$	9407	7	
	Information Information	Information Criterion Information Criterion Information Criterion Information Criterion	Information Criterion 8120 Information Criterion 8131 4-mme-pareto Information Criterion 9398	Information Criterion 8131 9261 4-mme-pareto Information Criterion 9395



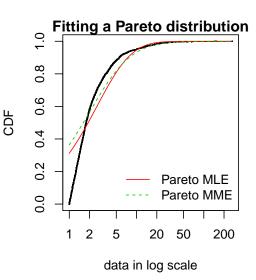


Figure 7: Comparison between MME and MLE when fitting a lognormal or a Pareto distribution to loss data from the danishuni data set

As shown on Figure 7, matching moments and maximum likelihood fits are far less distant (when looking at the right-tail) for the Pareto distribution than for the lognormal distribution on this data set. Furthermore for these two distributions, the MME method better fits the right-tail of the distribution, which seems logical since empirical moments are influenced by large observed values. In the previous traces, we give the values of goodness-of-fit statistics. Whatever the statistic considered, the MLE-fitted lognormal always provides the best fit to the observed data.

Maximum likelihood and moment matching estimations are certainly the most commonly used method for fitting distributions. Keeping in mind that these two methods may produce very different results, the user should be aware of its great sensitivity to outliers when choosing the matching moment estimation (MME). 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)

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

for $k = 1, \ldots, d$, with d 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 estimation 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 (as the vector of moment orders for MME). Empirical quantiles are computed using the quantile function of the stats package using type=7 by default (see ?quantile and [30]). 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(8/10, 9/10)) cdfcomp(list(fdanish.ln.MLE, fdanish.ln.QME1, fdanish.ln.QME2), legend=c("MLE", "QME(1/3, 2/3)", "QME(8/10, 9/10)"), 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 ($p_1 = 8/10, p_2 = 9/10$). As expected, the second QME fit gives more weight to the right-tail of the distribution, despite we do not choose the Pareto type-II distribution. 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.

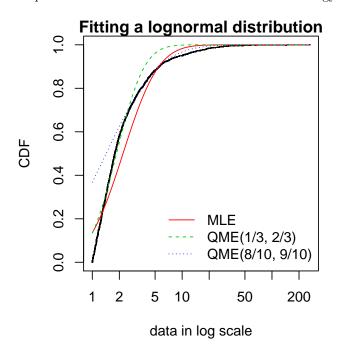


Figure 8: Comparison between QME and MLE when fitting a lognormal distribution to loss data from the danishuni data set

3.2 Customization of the optimization algorithm

Each time a numerical minimization (or maximization) is carried out in the fitdistrplus package, 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 ?optim for details about the different algorithms available).

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$serving, "gamma", optim.method="SANN")
> fCG <- try(fitdist(groundbeef$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 by specifying by the argument custom.optim in the call to fitdist. It may be necessary to customize this optimization function to meet the following requirements. (1) custom.optim function must have 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 the following components: par for the estimate, convergence for the convergence code, value=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)</pre>
```

```
+ 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 $(\hat{\alpha}, \hat{\lambda})$ by the different algorithms: shape α and rate λ parameters are relatively similar on this example, roughly 4.00 and 0.05, respectively.

```
> 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 3.97131 4.12891 4.00834
rate 0.05442 0.05742 0.05392 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 left-censored data. Observations only known to be above a limit of quantification are right-censored data. Results known to lie between two bounds are 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 with survival data [35]. 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 [35, 26].

Censored data can thus contain left-censored, right-censored and interval-censored values, with several lower and upper bounds. 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 for 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 [34]).

```
> data(salinity)
> str(salinity)

'data.frame': 108 obs. of 2 variables:
$ left : num 20 20 20 20 20 21.5 15 20 23.7 25 ...
$ right: num NA NA NA NA NA 21.5 30 25 23.7 NA ...
```

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 [65] 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)
```

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

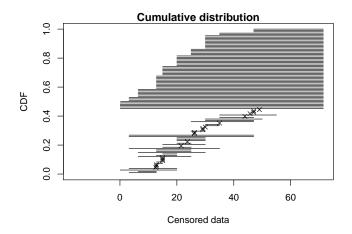


Figure 9: Simple plot of censored raw data (72-hour acute salinity tolerance of riverine macro-invertebrates from the salinity data set) as ordered points and intervals

 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 ([35, 26]).

As fitdist, fitdistcens returns the results of the fit of any parametric distribution to a data set as a 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 [16] 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 a manual iterative use if necessary.

```
> fsal.ln <- fitdistcens(salinity, "lnorm")
> fsal.11 <- fitdistcens(salinity, "llogis", start=list(shape=5, scale=40))
> summary(fsal.ln)
FITTING OF THE DISTRIBUTION ' lnorm ' BY MAXIMUM LIKELIHOOD ON CENSORED DATA
PARAMETERS
        estimate Std. Error
          3.3854
                    0.06487
meanlog
sdlog
          0.4961
                    0.05455
Loglikelihood: -139.1
                         AIC:
                               282.1
                                        BIC:
                                              287.5
Correlation matrix:
        meanlog sdlog
meanlog 1.0000 0.2938
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
                   1.9447
Loglikelihood:
                -140.1
                         ATC:
                               284.1
                                        BTC:
                                              289.5
Correlation matrix:
        shape
                scale
shape 1.0000 -0.2022
scale -0.2022 1.0000
```

To our knowledge, 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's Bayesian 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 "))
```

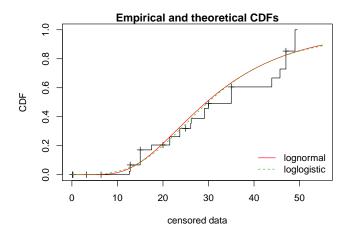


Figure 10: Goodness-of-fit CDF plot for fits of a lognormal and a loglogistic distribution to censored data: LC50 values from the salinity data set

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 accommodate 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 ([21]). 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 binomial 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
mu
       8.6803
                  1.93501
```

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).

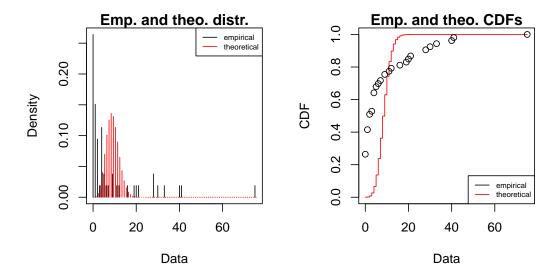


Figure 11: Plot of the fit of a discrete distribution (Poisson distribution fitted to numbers of *Toxocara cati* parasites from the toxocara data set)

> plot(ftoxo.P)

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

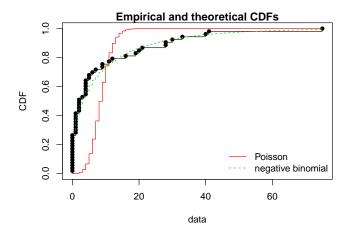


Figure 12: Comparison of the fits of a negative binomial and a Poisson distribution to numbers of *Toxocara cati* parasites from the toxocara data set)

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 [67]. 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))
```

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:

<= 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-mle-pois	2-mle-nbinom
Aikake's	${\tt Information}$	${\tt Criterion}$	1017	322.7
Bayesian	Information	Criterion	1019	326.6

4 Conclusion

The R package fitdistrplus allows to easily fit distributions. 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 [38, 31, 59, 68, 37, 43, 46, 60, 61, 24, 42], for MLE fits and goodness-of-fit statistics in [23, 62, 3, 5, 7, 48, 51], for MLE fits and bootstrap in [12, 45, 47, 63, 28], for MLE fits, bootstrap and goodness-of-fit statistics in [56], for MME fit in [40], for censored MLE and bootstrap in [39, 54, 32, 11, 52], for graphic analysing in [2, 58], for grouped-data fitting methods in [22] and more generally in [20, 9, 8, 1, 19, 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.

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