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

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TODO abstract

Contents

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 evaluation. In this paper, we present our package **fitdistrplus** for the statistical software R [35].

Function `fitdistr` in the R package **MASS** [43] is a well known general-purpose maximum-likelihood fitting routine for the parameter estimation step in R. Other steps of the process may be developed using R [36]. Our first objective by developping package **fitdistrplus** [14] was to provide R users a set of functions dedicated to help the overall process of fitting a univariate parametric distribution to data.

Function `fitdistr` estimates distribution parameters by maximizing the log-likelihood using function `optim`. In some cases, other estimation methods could be prefered, such as maximum goodness-of-fit estimation also commonly called minimum distance estimation, and proposed in package **actuar** with three different goodness-of-fit distances, see [15]. While developping package **fitdistrplus**, our second objective was to extend function `fitdistr` by providing various estimation methods to fit distributions in addition to maximum likelihood. Functions were developped to enable matching moment estimation, matching quantile estimation, and maximum goodness-of-fit estimation (or minimum distance estimation) using eight different distances. Moreover, package **fitdistrplus** offers the possibility to specify a user-supplied function for optimization, useful in cases where optimization techniques not included in function `optim` may be more adequate.

In applied statistics, it is not uncommon to have to fit distributions to censored data. Function `fitdistr` does not enable maximum likelihood estimation from this type data. Some packages deal with censored data, especially survival data [41], 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 [26] 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 packages provide functions to estimate the mode, the moments or the L-moments of a distribution, see the reference manuals of packages **modeest**, **lmomco** and **Lmoments**.

This manuscript reviews the various features of version 1.0-0 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)
```

2 Fitting distributions to continuous non-censored data

For illustrating the use of various functions of package **fitdistrplus** to help the fit of a distribution to continuous data, we use a data set named "ground beef" 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. This data set is used by [13], a quantitative risk assessment published in the international journal of food microbiology journal.

```
> data(groundbeef)
> str(groundbeef)
```

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

2.1 Choice of candidate distributions

Before fitting one or more distributions to a data set, it is generally necessary to choose good candidates among a predefined family of distributions. To help the user in this preliminary task, we developed functions to plot and characterise the empirical distribution.

2.1.1 Graphical display of the observed distribution

First of all, the empirical distribution and density functions may be plotted using the classical R functions `ecdf` and `hist` or using Function `plotdist`. This function provides such plots : the left-hand plot is the histogram (on a density level) and the right-hand plot is the empirical cumulative distribution function (cdf). Below, we give an example for a continuous variables giving in Figure 1.

```
> plotdist(groundbeef$serving)
```

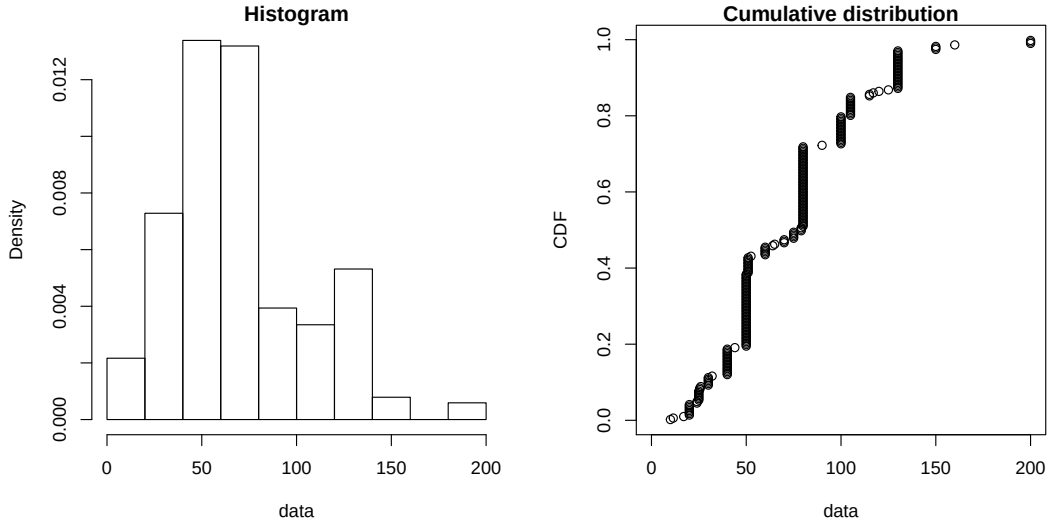


Figure 1: Density and cdf plots of an empirical distribution for a continuous variable (serving size from the "ground beef" data set)

2.1.2 Empirical basis for selecting candidate distributions

In addition to empirical plots, descriptives 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. The concept of skewness relates to deviations from symmetry of the distribution is defined as The normal distribution has a skewness of zero. A positive (resp. negative) skewness indicates that the right (resp. left) tail of the distribution is more extended than the left (resp. right) one. The concept of kurtosis relates to the tail weight. The normal distribution has a kurtosis of 3. Distributions with a higher kurtosis are said to be leptokurtic, with heavier tails, such as the logistic distribution, while distributions with a smaller kurtosis are said platykurtic, with lighter tails, such as the uniform distribution, see

Function `descdist` provides calculations of classical descriptive statistics (minimum, maximum, median, mean, standard deviation) and skewness and Pearsons's 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. Skewness and kurtosis with their corresponding unbiased estimator of a sample $(X_i)_i \overset{\text{i.i.d.}}{\sim} X$ 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.

A skewness-kurtosis plot such as the one proposed by [11] 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 as tools to help the choice of distributions to fit to data. For some distributions (normal, uniform, logistic, exponential for example), there is only one possible value for the skewness and the kurtosis and the distribution is thus represented by a 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. `boot` 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 function `descdist` to describe the distribution of the serving size from the "ground beef" data set and to draw the corresponding skewness-kurtosis plot (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
```

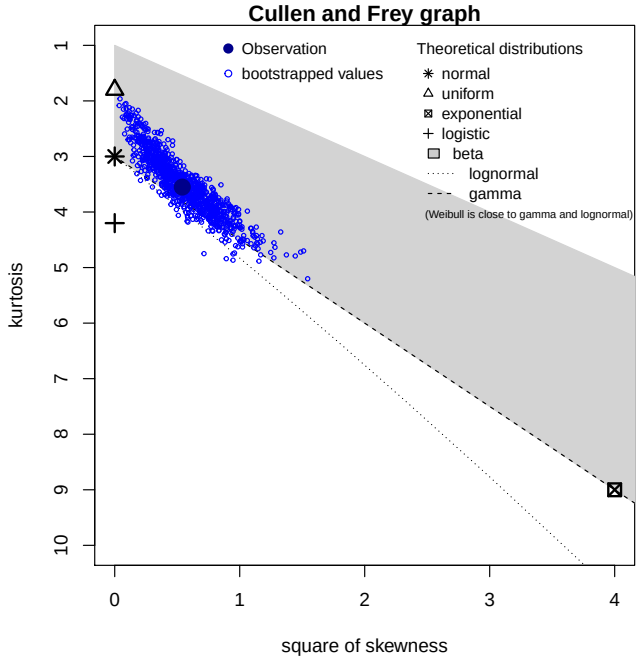


Figure 2: Skewness-kurtosis plot for a continuous variable (serving size from the `groundbeef` data set)

2.2 Fit of a distribution by maximum likelihood estimation

2.2.1 Parameter estimation

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

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

with x_i the n observations of variable x and f the density function of the parametric distribution. The other proposed estimation methods are described in Section 4.1.

Function `fitdist` 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 (see Figure 3 in Section 2.2.2). The parametric distribution must be a classically defined R distributions, with at least d, p and q functions respectively for the density, cumulative distribution and quantile functions (for example `dnorm`, `pnorm` and `qnorm` for the normal distribution). The name of the fitted distribution is specified in the first argument by its classical abbreviation used as the second part of d, p and q functions (for example `"norm"` for the normal distribution). Numerical results returned by Function `fitdist` are parameter estimates with estimated standard errors computed from the estimate of the Hessian matrix at the maximum likelihood solution, correlation matrix between parameter estimates, the loglikelihood, the Akaike and the Schwarz information criteria (so called AIC and BIC). Below is a call to function `fitdist` to fit a Weibull distribution to the serving size in the "ground beef" data set.

```
> fw <- fitdist(groundbeef$serving, "weibull")
> summary(fw)

Fitting of the distribution ' weibull ' by maximum likelihood
Parameters :
      estimate Std. Error
shape    2.186     0.1046
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
```

For some distributions (see the help of `fitdist` for details), it is necessary to specify initial values for the distribution parameters in the argument `start` when using the maximum likelihood method. `start` must be a named list of parameters initial values. The names of the parameters in `start` must correspond exactly to their definition in R or in a user-supplied R code. Function `plotdist` (see Section 2.2.2), which can plot any parametric distribution with specified parameter values in argument `para` may help to find correct initial values for the distribution parameters in non trivial cases, by iterative calls if necessary (see the reference manual [14] for examples).

For a pedagogic purpose, here is a fit of a user-supplied distribution. We fit the Gumbel distribution (also named the extreme value distribution) on the `groundbeef` data set.

```
> dgumbel<-function(x,a,b) 1/b*exp((a-x)/b)*exp(-exp((a-x)/b))
> pgumbel<-function(q,a,b) exp(-exp((a-q)/b))
> qgumbel<-function(p,a,b) a-b*log(-log(p))
> summary(fitdist(groundbeef$serving, "gumbel", start=list(a=5, b=10)))

Fitting of the distribution ' gumbel ' by maximum likelihood
Parameters :
  estimate Std. Error
a    56.95      1.924
b    29.08      1.432
Loglikelihood:  -1256   AIC:  2515   BIC:  2523
Correlation matrix:
       a      b
a 1.0000 0.3167
b 0.3167 1.0000
```

2.2.2 Goodness-of-fit plots

The plot of an object of class `"fitdist"` corresponding to the fit of a continuous distribution to non-censored data, provides four goodness-of-fit plots : a draw of pdf curve and histogram together (density plot), an cdf plot of both empirical and theoretical distributions, a Q-Q plot (plot of the quantiles of the theoretical fitted distribution (x-axis) against the empirical quantiles of the data (y-axis)) and a P-P plot (i.e. for each value of the data set, plot of the cumulative density function of the fitted distribution (x-axis) against the empirical cumulative density function (y-axis)) are also given [11]. For all these four plots, the probability plotting position is defined as recommended by Blom [5], by a call to Function `ppoints` from the **stats** package with its default arguments. 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, let us look at the plot of the previous fit of a Weibull distribution to the `groundbeef` data set (Figure 3). The fit is not perfect, especially in the center of the distribution, but seems correct when looking at the tails.

```
> plot(fw)
```

2.2.3 Plots to compare multiple fits

Functions `denscomp`, `cdfcomp`, `qqcomp` and `ppcomp`, enable the visual comparison of the empirical and various theoretical distributions fitted on a same data set, using one of the four plots provided by `plotdist`. 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 [14] for lists of arguments that may be changed for each plot), as in the following example comparing the fit of Weibull, lognormal and gamma distributions to `groundbeef` data set. On Figure 4, we compare density, quantile, distribution and probability functions.

```
> 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"),
+   xlab="serving sizes (g)", lwd=2)
> qqcomp(list(fw,fln,fg), legendtext=c("Weibull", "lognormal", "gamma"),
+         xlab="theo. quantiles", lwd=2, line01=FALSE, fitcol=2:4, ylim=c(0,300))
> cdfcomp(list(fw,fln,fg), legendtext=c("Weibull", "lognormal", "gamma"),
+   xlab="serving sizes (g)", lwd=2)
> ppcomp(list(fw,fln,fg), legendtext=c("Weibull", "lognormal", "gamma"),
+   xlab="theo. prob.", lwd=2, line01=FALSE, fitcol=2:4)
```

COMMENT THEM, ESPECIALLY THE QQPLOT !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!! TODO

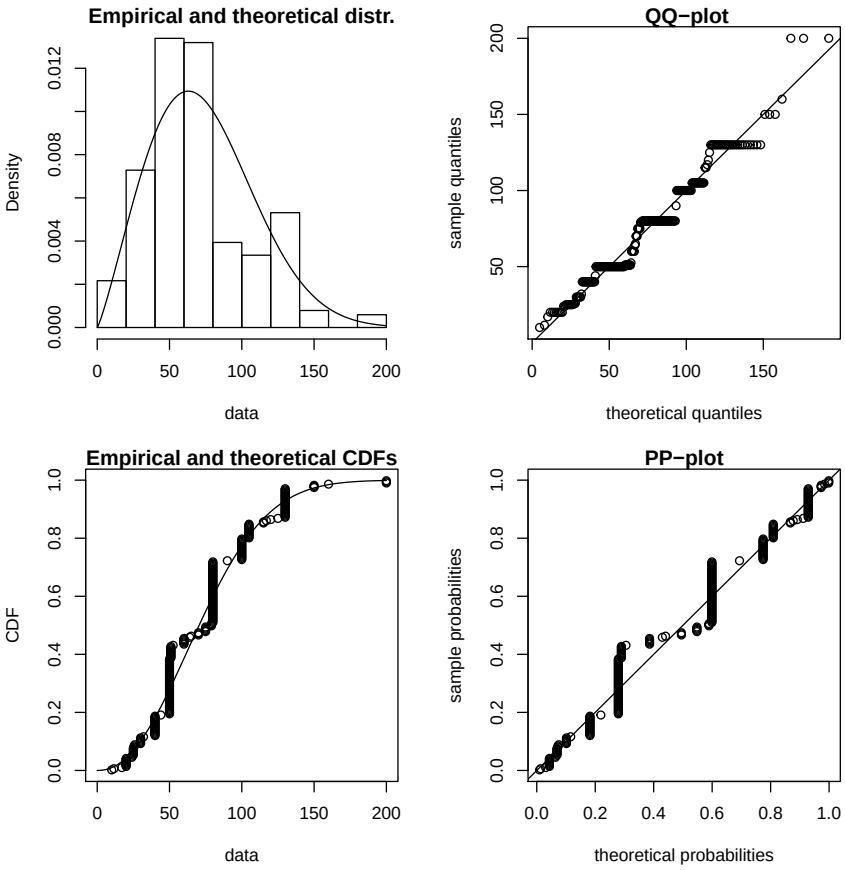


Figure 3: Plot of the fit of a continuous distribution (a Weibull distribution fitted to serving sizes from the `groundbeef` data set)

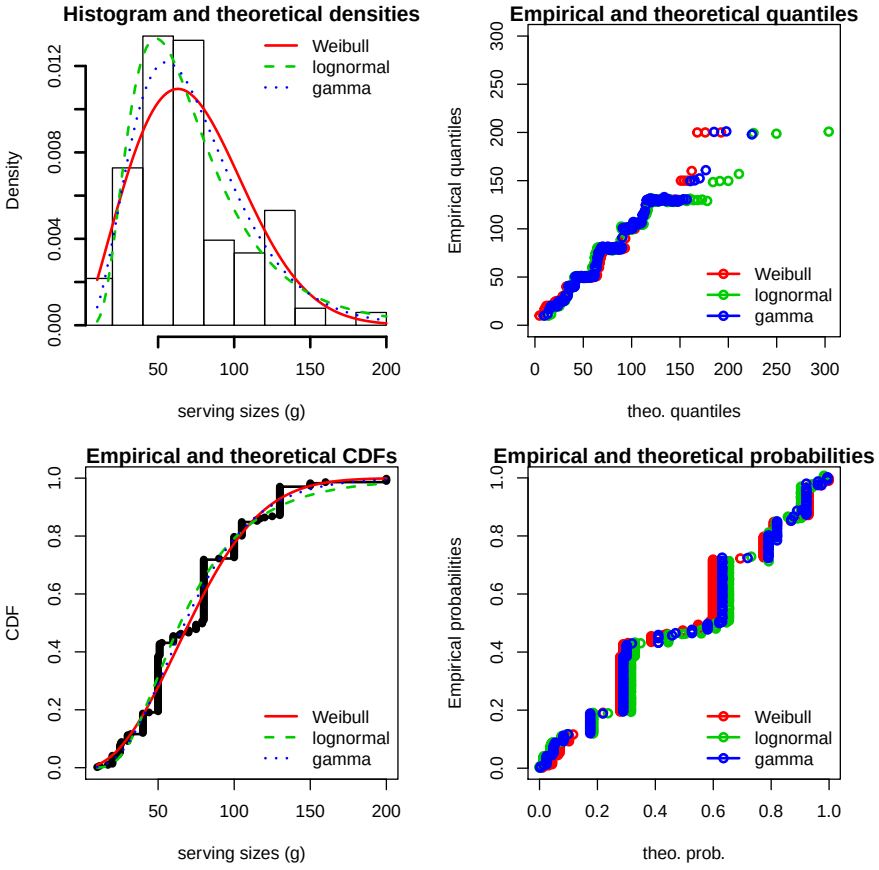


Figure 4: Comparison of CDF plots of various distributions fitted on continuous data (Weibull, gamma and lognormal distributions fitted to serving sizes from the "ground beef" data set)

2.2.4 Measures of goodness-of-fit

The purpose of goodness-of-fit statistics aims to measure the distance beetween the cumulative distribution function F defined from the fitted parametric distribution with the empirical distribution function F_n based on the data. When fitting continuous distributions, three goodness-of-fit statistics are classicaly considered: Cramer-von Mises, Kolmogorov-Smirnov and Anderson-Darling statistics. They can be computed using the function `gofstat` as defined by Stephens [12]. Table 1 gives the definition and their empirical estimate.

check formula in Table 1 TODO

Table 1: Goodness-of-fit statistics as defined by Stephens [12].

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

```
> gofstat(fw)

Kolmogorov-Smirnov statistic:  0.1397
Cramer-von Mises statistic:  0.6841
Anderson-Darling statistic:  3.574

> gofstat(fln)

Kolmogorov-Smirnov statistic:  0.1493
Cramer-von Mises statistic:  0.8277
Anderson-Darling statistic:  4.544

> gofstat(fg)

Kolmogorov-Smirnov statistic:  0.1281
Cramer-von Mises statistic:  0.6934
Anderson-Darling statistic:  3.566
```

As giving more weight to distribution tails, Anderson-Darling statistics is of special interest where it is important to place equal emphasis on fitting a distribution at the tails as well as the main body, as it is often the case in risk assessment [11, 44]. Nevertheless, this statistics should be used cautiously when comparing fits of various distributions, keeping in mind that the weighting of each cdf quadratic difference is dependent of the theoretical distribution.

Even if specifically recommended for discrete distributions, the Chi-squared statistic may also be used for continuous distributions (see Section 3.1.4 and the reference manual [14] for examples).

ADD A PART ON THE DRAWBACKS OF EACH GOFSTAT AND THE PREFERABLE USE OF AIC AND BIC TO COMPARE FITS ESPECIALLY WHEN THE NUMBER OF PARAMETERS CHARACTERIZING THE DISTRIBUTIONS DIFFERS TODO

2.2.5 Goodness-of-fit tests

TO BE REMOVED AT LEAST IN THE JSS VERSION TODO

For continuous distributions, an approximate Kolmogorov-Smirnov test is performed by assuming the distribution parameters known. The critical value defined by Stephens [12] for a completely specified distribution is used to reject or not the distribution at the significance level 0.05. Because of this approximation, the result of the test (decision of rejection of the distribution or not) is returned only for datasets with more than 30 observations. Note that this approximate test may be too conservative.

For datasets with more than 5 observations and for continuous distributions for which the test is described by Stephens [12] for maximum likelihood estimations (exponential, Cauchy, gamma and Weibull), the Cramer-von Mises and Anderson-darling tests are performed as described by Stephens [12]. Those tests take into account the fact that the parameters are not known but estimated from the data. The result is the decision to reject or not the distribution at the significance level 0.05. Both tests are available only for maximum likelihood estimations.

When the Chi-squared statistic is computed (for discrete or optionnaly continuous distributions), and if the degree of freedom (nb of cells - nb of parameters - 1) of the corresponding distribution is strictly positive, the p-value of the Chi-squared test is returned.

The results of the tests are not printed, unless the argument `print.test` is set to `TRUE`. We chose not to print their results by default, as goodness-of-fit tests are often misused. As for any null-hypothesis significance test, the non reject of the null hypothesis dose not imply its acceptation. However, this misinterpretation of p-values is very common and comes from the wrong assumption that absence of evidence is evidence of absence [2]. On the contrary, in some cases, especially on very big datasets, even if the null hypothesis is rejected, a fitted distribution may be chosen as the best one among simple distributions to describe an empirical distribution, if the goodness-of-fit plots do not show strong differences between empirical and theoretical distributions.

3 Fitting distributions to other types of data

3.1 The case of discrete data

The `toxocara` data set corresponds to the observation of a discrete variable, the number of *Toxocara cati* parasites present in digestive tract, on a random sample of feral cats living on Kerguelen island ([18]). We will use it in order 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 0 ...
```

3.1.1 Graphical display of the observed distribution

In some cases a discrete variable may be plotted as a continuous one, for example for a large data set from a binomial distribution converging to a normal one, but Function `plotdist` also proposes specific plots in density and in cdf for discrete variables (Figure 5):

```
> plotdist(toxocara$number, discrete = TRUE)
```

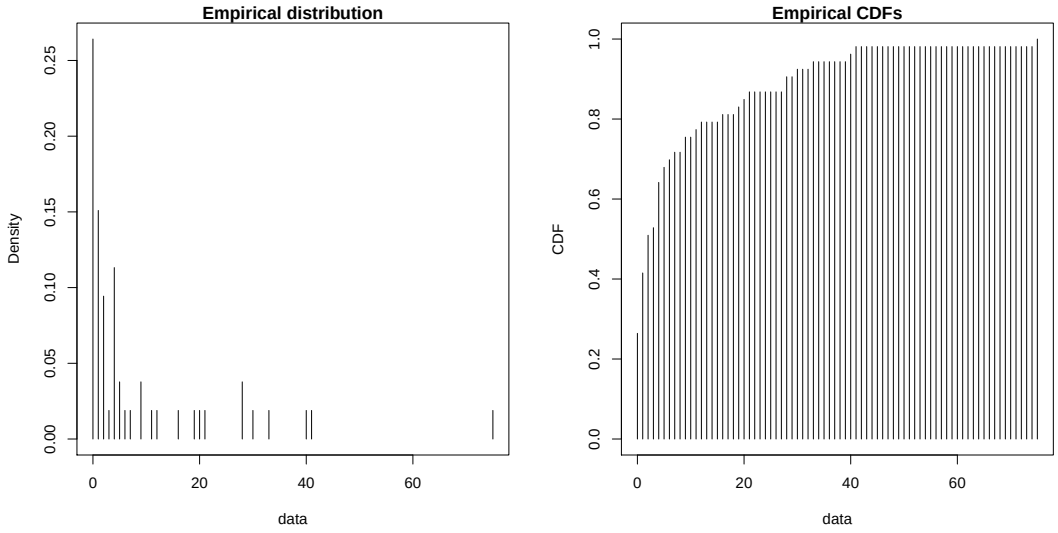


Figure 5: Density and cdf plots of an empirical distribution for a discrete variable (number of *Toxocara cati* parasites from the `toxocara` data set)

As for continuous non-censored data (see Section 2.1.2) Function `descdist` can be used, but with the argument `discrete` fixed to `TRUE`. This function will especially compute skewness and kurtosis values, and plot them in a skewness-kurtosis plot with skewness and kurtosis values or set of values of Poisson and negative binomial together with values for the normal distribution, to which discrete distributions may converge.

3.1.2 Maximum likelihood estimation

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 may be easily fitted and AIC values compared, in this case giving the preference to the negative binomial distribution, with a much smaller AIC value.

```
> fp <- fitdist(toxocara$number, "pois")
> summary(fp)
```

```
Fitting of the distribution ' pois ' by maximum likelihood
Parameters :
       estimate Std. Error
lambda    8.679     0.4047
Loglikelihood:  -507.5   AIC:  1017   BIC:  1019
```

```
> fnb <- fitdist(toxocara$number, "nbinom")
> summary(fnb)
```

```
Fitting of the distribution ' nbinom ' by maximum likelihood
Parameters :
     estimate Std. Error
size   0.3971    0.08289
mu     8.6803    1.93501
Loglikelihood:  -159.3   AIC:  322.7   BIC:  326.6
Correlation matrix:
           size         mu
size  1.0000000 -0.0001039
mu   -0.0001039  1.0000000
```

3.1.3 Goodness-of-fit plot

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 cdf. As an exemple, let us look at the plot of the previous fit of a negative binomial distribution to the `toxocara` data set.

```
> plot(fnb, col="blue")
```

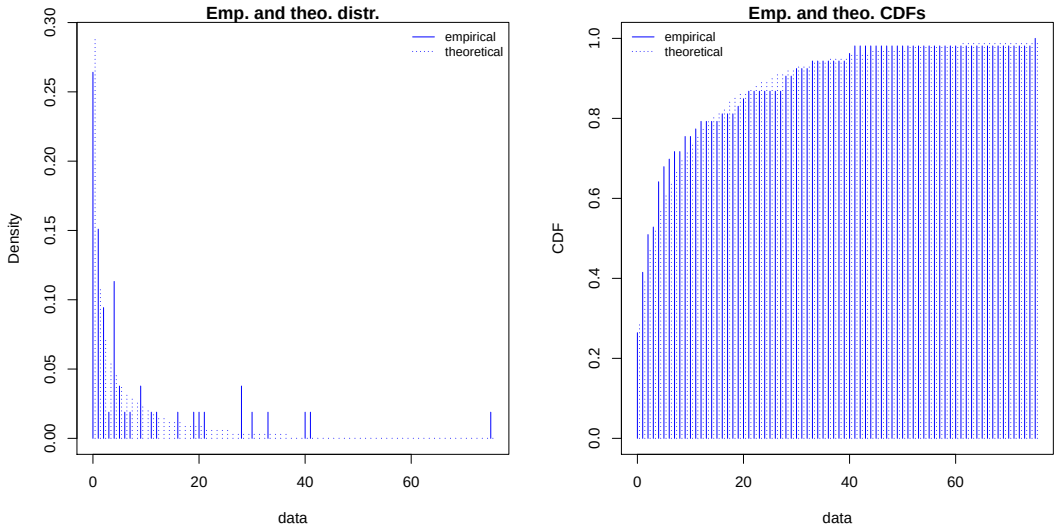


Figure 6: Plot of the fit of a discrete distribution (a negative binomial distribution fitted to numbers of *Toxocara cati* parasites from the `toxocara` data set)

3.1.4 Measures of goodness-of-fit

When fitting discrete distributions, the Chi-squared statistic is computed by Function `gofstat` 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 dataset. 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 dataset [44]. Using this default option with the fit of a negative binomial distribution to `toxocara` data set gives following results :

```
> gofstat(fnb)
```

```
Chi-squared statistic:  7.486
```

Among its returned values, Function `gofstat` provides a table with observed and theoretical counts used for the Chi-squared calculations:

```
> gofstat(fnb)$chisqtable

Chi-squared statistic:  7.486
      obscounts theocounts
<= 0     14.000     15.295
<= 1      8.000      5.809
<= 3      6.000      6.845
<= 4      6.000      2.408
<= 9      6.000      7.835
<= 21     6.000      8.271
> 21      7.000      6.537
```

3.2 The special case of censored data

Censored data may contain left censored, right censored and interval censored values, with several lower and upper bounds. 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.

The `smokedfish` data set, included in the package, corresponds to the observation of a continuous censored variable, the *Listeria monocytogenes* microbial concentration, on a random sample of smoked fish distributed on the Belgian market in the period 2005 to 2007 ([7]). Censored data are coded within 2 columns named left and right, describing each observed value of *Listeria monocytogenes* concentration (in $CFU.g^{-1}$) 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 noncensored observations.

```
> data(smokedfish)
> str(smokedfish)

'data.frame':        103 obs. of  2 variables:
 $ left : num  NA NA NA NA NA NA NA NA NA NA ...
 $ right: num  0.04 0.04 0.04 0.04 0.04 0.04 0.04 0.04 0.04 0.04 ...
```

3.2.1 Graphical display of the observed distribution

Using censored data such as those coded in the `smokedfish` data set, the empirical distribution may be plotted using the `plotdistcens` function. By default, this function uses the EM approach of Turnbull [42] to compute the overall empirical cdf curve with confidence intervals, by calls to `survfit` and `plot.survfit` functions from the **survival** package. Let us see such a plot for `smokedfish` data set after classical transformation of microbial counts in decimal logarithm (Figure 7).

```
> log10C <- data.frame(left=log10(smokedfish$left), right=log10(smokedfish$right))
> plotdistcens(log10C)
```

3.2.2 Maximum likelihood estimation

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

$$L(\theta) = \prod_{i=1}^{N_{nonC}} f(x_i|\theta) \times \prod_{j=1}^{N_{leftC}} F(x_j^{upper}|\theta) \times \prod_{k=1}^{N_{rightC}} (1 - F(x_k^{lower}|\theta)) \times \prod_{m=1}^{N_{intC}} (F(x_m^{upper}|\theta) - F(x_j^{lower}|\theta)) \qquad (4)$$

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`, it 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. For "smokedfish" data set, a normal distribution may be fitted to log transformed data as commonly done for microbial count data.

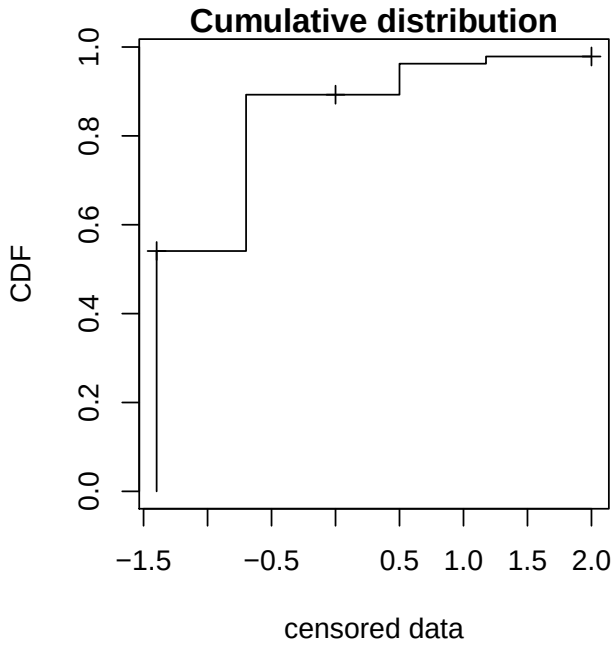


Figure 7: CDF plot of censored data (microbial counts from the `smokedfish` data set)

```
> flog10Cn <- fitdistcens(log10C, "norm")
> summary(flog10Cn)

FITTING OF THE DISTRIBUTION ' norm ' BY MAXIMUM LIKELIHOOD ON CENSORED DATA
PARAMETERS
     estimate Std. Error
mean   -1.575     0.2014
sd      1.539     0.2118
Loglikelihood:  -87.11   AIC:  178.2   BIC:  183.5
Correlation matrix:
        mean      sd
mean  1.0000 -0.4325
sd   -0.4325  1.0000
```

As with `fitdist`, for some distributions (see [14] 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.

3.2.3 Goodness-of-fit plot

Only one goodness-of-fit plot is provided for censored data, corresponding to the theoretical cumulative distribution function added to the plot of censored data presented in Section 3.2.1. The `cdfcompcens` function can be used to compare the fit of various distributions to the same censored data set. Its call is similar to the one `cdfcomp`. Below is an example of comparison of two fitted distribution to `smokedfish` data set (see Figure 8).

```
> flog10Cl <- fitdistcens(log10C, "logis")
> cdfcompcens(list(flog10Cn, flog10Cl),
+     legendtext=c("normal distribution", "logistic distribution"),
+     xlab="bacterial concentration (log10[CFU/g])", ylab="F")
```

Computations of goodness of fit statistics have not yet been developed for fits using censored data, so the quality of fit may only be estimated from the loglikelihood and the goodness-of-fit CDF plot.

4 Advanced topics

4.1 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. We use a classical data set from the Danish insurance industry published in [31]. In **fitdistrplus**, the data set is stored in `danishuni` and `danishmulti` for univariate and multivariate versions, respectively.

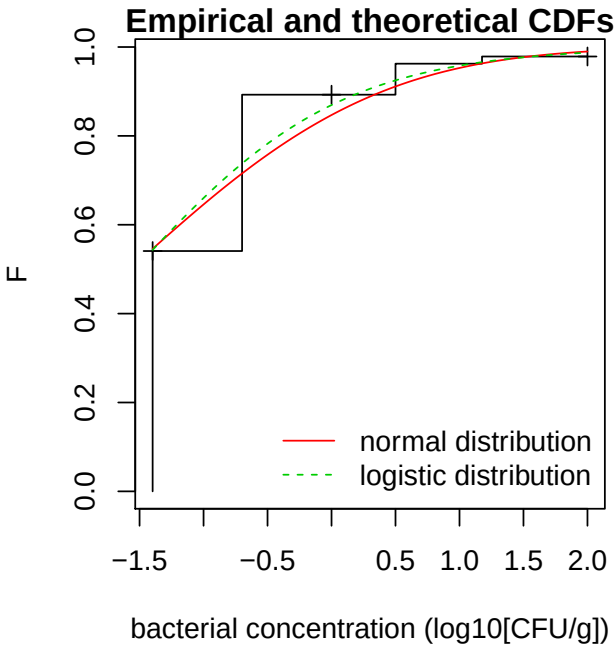


Figure 8: Goodness-of-fit CDF plots for fits of continuous distributions on censored data (Comparison of lognormal and loglogistic distributions fitted to microbial counts from the `smokedfish` data set)

4.1.1 Maximum goodness-of-fit estimation

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 [29] 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.

Table 2: Modified Anderson-Darling statistics as defined by Luceno [29].

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

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 variables and distributions. Below an example of estimation on the `danishuni` data set with the three classical goodness-of-fit distances. We compare the fitting methods with the distribution function.

```
> data(danishuni)
> flndanishAD <- fitdist(danishuni$Loss, "lnorm", method="mge", gof="AD")
> flndanishAD2L <- fitdist(danishuni$Loss, "lnorm", method="mge", gof="AD2L")
> flndanishKS <- fitdist(danishuni$Loss, "lnorm", method="mge", gof="KS")
> flndanishCvM <- fitdist(danishuni$Loss, "lnorm", method="mge", gof="CvM")
> flndanishMLE <- fitdist(danishuni$Loss, "lnorm", method="mle")
> cdfcomp(list(flndanishAD, flndanishAD2L, flndanishKS, flndanishCvM, flndanishMLE),
```

```
+         legend=c("AD", "AD2L", "KS", "CvM", "MLE"), main="Fitting lognormal distribution",
+         xlogscale=TRUE, datapch="*")
```

As plotted 9, the lognormal distribution is not appropriate to model heavy-tailed datae, but this is not the purpose here. The second-order Anderson-Darling distance provides the least conservative fit for high quantiles, whereas the (classic) Anderson-Darling distance is the most conservative fit among goodness-of-fit distances.

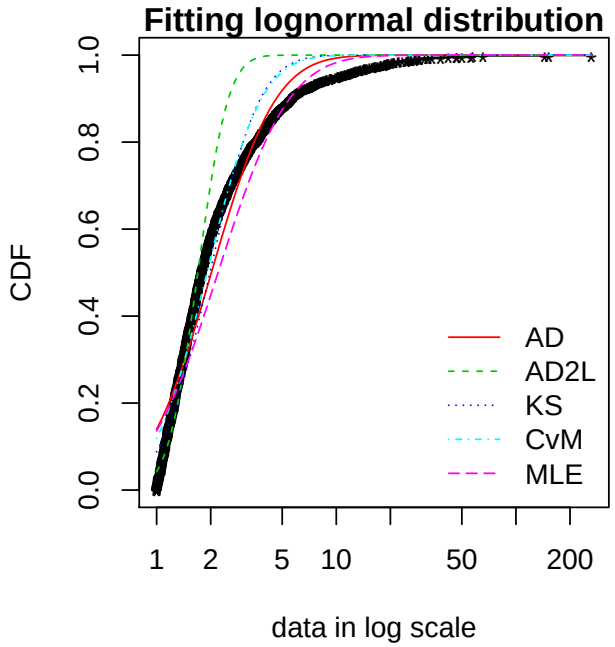


Figure 9: Comparison of statistical distance when fitting lognormal distribution on `danishuni`

Maximum goodness-of-fit estimation may also be useful to give more weight to data at one tail of the distribution. In ecotoxicology, species sensitivity distributions such as those presented in [22] are often fitted by a lognormal or a loglogistic distribution so as to estimate a low percentile, often 5% percentile, named the hazardous concentration 5% (HC5). This value is then interpreted as a value of the contaminant concentration protecting 95% of the species. In this context, one may consider to fit the parametric distribution by giving more weight to the left tail of the empirical distribution. In the following example of `endosulfan` data set, we use left tail Anderson-Darling distances of first or second order (see Figure 10).

```
> data(endosulfan)
> ATV <-subset(endosulfan,group == "NonArthroInvert")$ATV
> flnMGECvM <- fitdist(ATV,"lnorm",method="mge",gof="CvM")
> flnMGEAD <- fitdist(ATV,"lnorm",method="mge",gof="AD")
> flnMGEADL <- fitdist(ATV,"lnorm",method="mge",gof="ADL")
> flnMGEAD2L <- fitdist(ATV,"lnorm",method="mge",gof="AD2L")
> cdfcomp(list(flnMGECvM, flnMGEAD, flnMGEADL, flnMGEAD2L),
+ xlogscale = TRUE, main = "GOF estimation with different stat. distances",
+ legendtext = c("Cramer-von Mises (CvM)", "Anderson-Darling",
+ "Left-tail Anderson-Darling", "Left tailed Anderson-Darling of second order"),cex=0.7,
+ xlegend = 500, ylegend = 0.15)
```

4.1.2 Moment matching estimation

Another method commonly used to fit parametric distribution consists in estimating the parameters θ at the values that makes the first theoretical raw moments of the parametric distribution equal to the empirical moments (Equation 5).

$$E(X^k|\theta) = \frac{1}{n}\sum_{i=1}^{n} x_i^k \tag{5}$$

for $k = 1, \ldots, p$, 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 is also relevant to match centered moments as given by Equation (6).

$$E\left((X - E(X))^k|\theta\right) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x}_n)^k \tag{6}$$

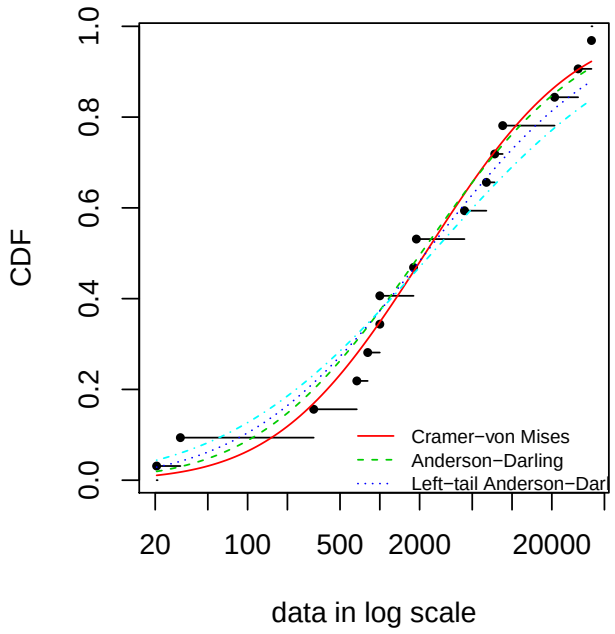


Figure 10: Comparison of one distribution fitted by maximum goodness-of-fit using various goodness-of-fit distances (a lognormal distribution fitted to acute toxicity values from the `endosulfan` data set)

This method called moment matching estimation can be performed fixing the argument `method` to `"mme"` in the call to fitdist. The estimate is computed by a closed formula for 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. [44]). 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 [14] for technical details).

Our first example of fitting a lognormal distribution on `danish` data set uses a closed formula. Comparing the two fitted distributions functions, we observe on Figure 11 that the moment matching estimation is far more conservative than the maximum likelihood estimation, which is also more conservative than goodness-of-fit estimation.

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

Our second example is the fitting of a Pareto type II distribution. We use the implementation of **actuar** package providing moments and limited expected value for that distribution (in addition to `d`, `p`, `q` and `r` functions, see [20]). 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 a lower and an upper bounds for the optimization by `optim`. Our call below immadiately calls the L-BFGS-B optimization method, since this quasi-Newton allows box constraints[1]. We also observe that the fitting is relatively good when comparing empirical and fitted moments. Note that we have to pass a function for computing the empirical raw moment to `fitdist`.

```
> library(actuar)
> memp <- function(x, order) ifelse(order == 1, mean(x), sum(x^order)/length(x))
> fparedanishMME <- fitdist(danishuni$Loss, "pareto", method="mme", order=1:2,
+       memp="memp", start=c(shape=10, scale=10), lower=2+1e-6, upper=Inf)
> c(theo = mpareto(1, fparedanishMME$estimate[1], fparedanishMME$estimate[2]),
+ emp = memp(danishuni$Loss, 1))

 theo   emp
3.448 3.385

> c(theo = mpareto(2, fparedanishMME$estimate[1], fparedanishMME$estimate[2]),
+ emp = memp(danishuni$Loss, 2))
```

[1] That's what the B stands for.

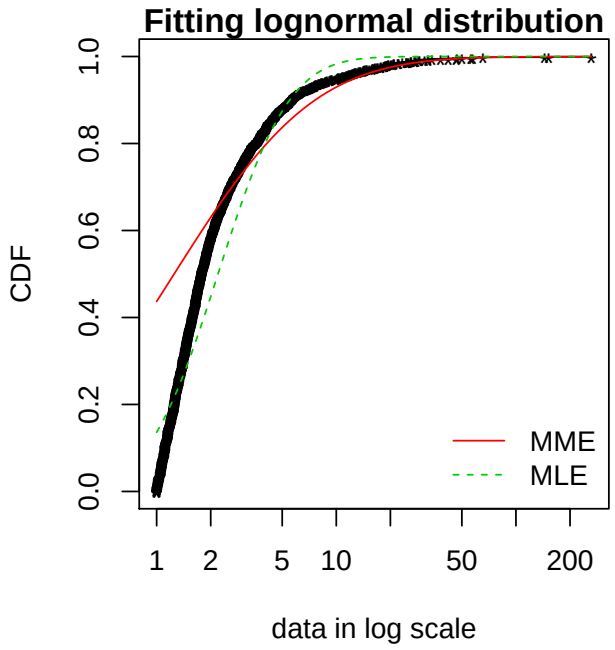


Figure 11: Comparison between MME and MLE when fitting lognormal distribution on `danishuni`

```
theo  emp
83.8 83.8
```

4.1.3 Quantile matching estimation

Fitting of a parametric distribution may also be done by matching theoretical quantiles of the parametric distributions (for specified probabilities) to the empirical quantiles. Equation (7) below is thus similar to Equations (5) and (6)

$$F^{-1}(p^k|\theta) = Q_{n,p_k} \tag{7}$$

for $k = 1, \ldots, p$, 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 can be performed by fixing 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.

```
> flndanishQME1 <- fitdist(danishuni$Loss, "lnorm", method="qme", probs=c(1/3, 2/3))
> flndanishQME2 <- fitdist(danishuni$Loss, "lnorm", method="qme", probs=c(3/4, 4/5))
> cdfcomp(list(flndanishQME1, flndanishQME2, flndanishMLE),
+         legend=c("QME(1/3, 2/3)", "QME(3/4, 4/5)", "MLE"), main="Fitting 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 good precision around particular quantiles, e.g. $p = 99.5\%$ for Solvency II insurance context.

4.1.4 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 may then be 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` may be used in the call to `fitdist` or `fitdistcens`. It will internally be passed to `mledist` and to `optim`. This argument may be fixed to `"Nelder-Mead"` (the robust derivative-free Nelder and Mead method), `"BFGS"` (the BFGS quasi-Newton method), `"CG"` (the conjugate gradient hessian-free method), `"SANN"` (a

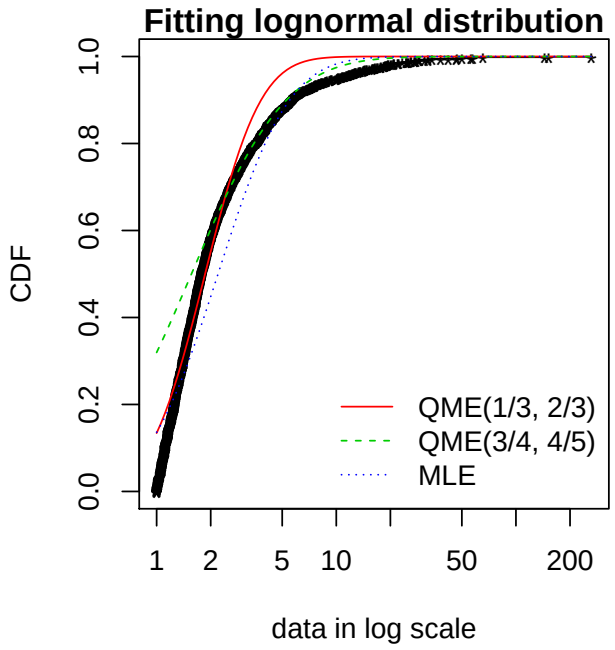


Figure 12: Comparison between QME and MLE when fitting lognormal distribution on `danishuni`

variant of (stochastic) simulated annealing) or `"L-BFGS-B"` (a modification of the BFGS quasi-Newton method which enables box constraints optimization and limited-memory usage). For the use of the last method the arguments `lower` and/or `upper` also have to be passed. More details on these optimization functions may be found in the help page of `optim` from the package **stats**.

Here are examples of fits of a gamma distribution to `groundbeef` data set with various options of `optim`. Note that the conjugate gradient algorithm 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)
```

You may also want to use another function than `optim` to maximize the likelihood. This optimization function has to be specified by the argument `custom.optim` in the call to `fitdist` or `fitdistcens`. But before that, it is necessary to customize this optimization function : `custom.optim` function must have (at least) the following arguments, `fn` for the function to be optimized, `par` for the initialized parameters. We assume that `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 `genoud` function from **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)
+ }
```

The customized optimization function may then be passed as the argument `custom.optim` in the call to `fitdist` or `fitdistcens`. The following code may 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 compare all the parameter estimates by the different algorithms: shape and rate parameters are relatively the same.

```
> 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 4.07079 4.12891 4.00834
rate  0.05442 0.05742 0.05507 0.05607 0.05443
```

4.2 Uncertainty in parameter estimates

4.2.1 Bootstrap procedures

The uncertainty in the parameters of the fitted distribution may be simulated by parametric or nonparametric bootstrap using the `boodist` function for non censored data and by nonparametric bootstrap using `boodistcens` function for censored data. These functions return 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` or `bootdistcens` 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 13).

Below is an example of the use of the `bootdist` function with the previous of the Weibull distribution to `groundbeef` data set.

```
> bw <- bootdist(fw, niter=1001)
> summary(bw)

Parametric bootstrap medians and 95% percentile CI
      Median   2.5%  97.5%
shape  2.198  2.003  2.438
scale 83.445 78.693 88.115

> plot(bw)
```

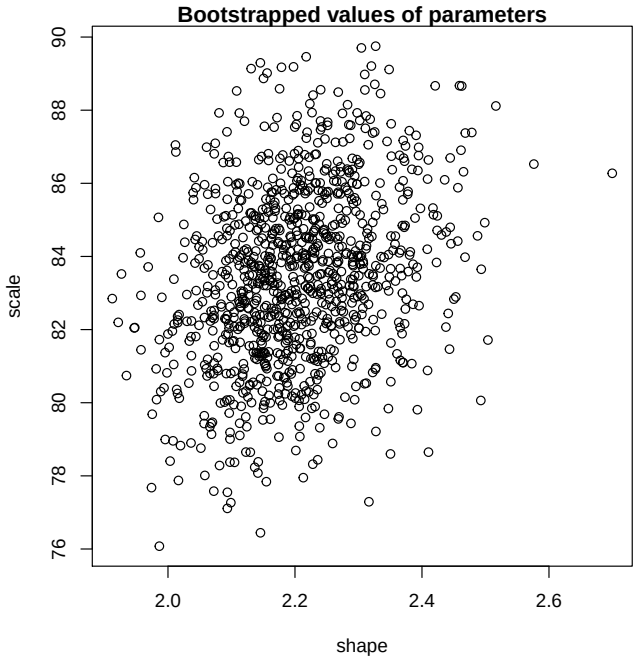
Then we fit the three-parameter distribution of Burr on `danishuni` data set. As when fitting the Pareto type II distribution, we have to use a lower bound when carrying out the optimization. Otherwise `optim` do not converge.

```
> fdan <- fitdist(danishuni$Loss, "burr", method="mle",
+   start=c(shape1=5, shape2=5, rate=10), lower=1e-1)
> bdan <- bootdist(fdan,  bootmethod="param", niter=101)
> summary(bdan)

Parametric bootstrap medians and 95% percentile CI
        Median    2.5%   97.5%
shape1  0.1000  0.1000  0.1146
shape2 14.4049 12.7866 14.8343
rate    0.9198  0.9041  0.9320

The estimation method converged only for  99  among  101  iterations

> plot(bdan)
```

4.2.2 Use of bootstrap samples

Bootstrap samples of parameter estimates may be used to calculate confidence intervals on each parameter of the fitted distribution, but it is also interesting to look at the marginal distribution of the bootstrap values in a scatterplot (or a matrix of scatterplots if the number of parameters exceeds two), and especially to look at the potential structural correlation between parameters.

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 **mc2d** ([33]). One could refer to Pouillot *et al.* ([32]) for an introduction to the use of **mc2d** and **fitdistrplus** packages in the context of quantitative risk assessment.



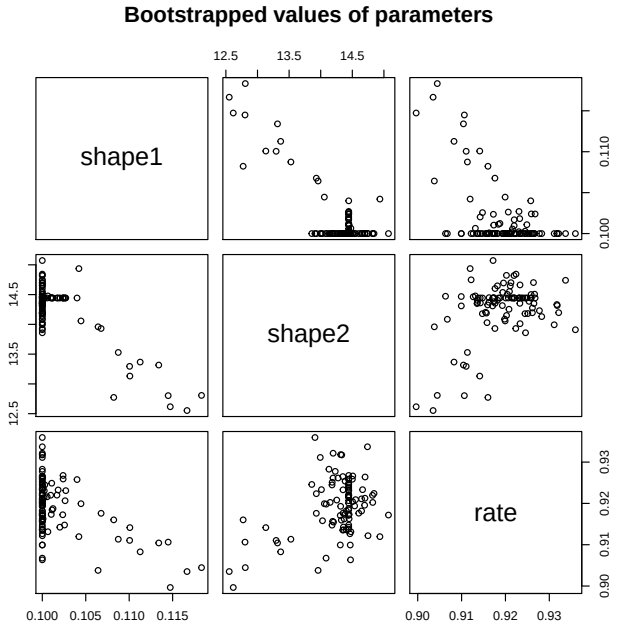


Figure 13: Bootstrappped values of parameters for a fit of a distribution characterized by two parameters (example on the fit of a Weibull distribution to serving sizes from the `groundbeef` data set)

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 `fitdist` for non censored data and `fitdistcens` for censored data. They must be called with a first argument corresponding to an object of class `fitdist` or `fitdistcens`, and as a second argument the vector of probabilities at which the quantiles of the fitted distribution must be estimated. By default quantiles calculated at the estimated parameters are provided, followed by 95% bootstrap confidence intervals for each quantile. These two functions are internally calling to `bootdist` or `bootdistcens` and give the complete results of these calls as a part of their output, in `resbootdist` and `resbootdistcens`. The `quantile` function is of great interest in the ecotoxicology field, while a hazardous concentration at x% (HCx) is computed from species sensitivity distributions, that is interpreted as the contaminant concentration protecting $(100 - x)$% of the species. Below is an example of use of `quantile` to estimate HCx values for different x-values, with 95% bootstrap confidence intervals, using the maximum likelihood fit of a lognormal distribution on the `endosulfan` data set.

```
> flnMLE <- fitdist(ATV,"lnorm")
> quantile(flnMLE, probs = c(0.05, 0.10, 0.20, 0.50))

Estimated quantiles for each specified probability
  prob=0.05 prob=0.1 prob=0.2 prob=0.5
1     55.49    120.3    306.8     1840

two-sided 95% CI of each quantile
      prob=0.05 prob=0.1 prob=0.2 prob=0.5
2.5%      13.61    34.69    100.2    644.6
97.5%    300.01   549.85   1104.6   5263.3
```

5 Conclusion

Papers citing **fitdistrplus** are [27, 8, 38, 28, 23, 45, 6, 1, 40, 39, 34, 30, 25, 21, 24, 19, 17, 10, 9, 4, 3, 16, 37]

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