**MATRIXDIST: AN R PACKAGE FOR INHOMOGENEOUS PHASE–TYPE DISTRIBUTIONS**

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**Abstract.** Inhomogeneous phase-type distributions (IPH) are a broad class of laws which arise from the absorption times of Markov jump processes. In the time-homogeneous particular case, we recover phase-type (PH) distributions. In matrix notation, various functionals corresponding to their distributional properties are explicitly available and succinctly described. As the number of parameters increases, IPH distributions may converge weakly to any probability measure on the positive real line, making them particularly attractive candidates for statistical modelling purposes. Contrary to PH distributions, the IPH class allows for a wide range of tail behaviours, which often leads to adequate estimation with a moderate number of parameters. One of the main difficulties in estimating PH and IPH distributions is their large number of matrix parameters. This drawback is best handled through the expectation-maximisation (EM) algorithm, exploiting the underlying and unobserved Markov structure. The matrixdist package presents tools for IPH distributions to efficiently evaluate functionals, simulate, and carry out maximum likelihood estimation through a three-step EM algorithm. Aggregated and right-censored data are supported by the fitting routines, and in particular, one may estimate time-to-event data, histograms, or discretised theoretical distributions.

1. **Introduction**

Phase-type (PH) distributions ([7]) are a natural extension of the exponential distribution and are defined as the time to reach an absorbing state in an otherwise transient time-homogeneous pure-jump Markov process. The transient state space is of integer dimension \( p \geq 1 \). In the particular case \( p = 1 \) we recover the exponential distribution, and for general \( p \), the asymptotic tail behaviour remains exponential. Since we only observe the time to absorption but not the actual stochastic process trajectory, models based on phase-type distributions are hidden Markov models. They are typically estimated using the expectation-maximisation (EM) algorithm (see [6] for a MCMC approach). Closed-form formulae for functionals such as density, cumulative distribution function, Laplace transform, and moments are all explicitly available in terms of matrices and closely resemble their scalar counterparts.

Letting \( p \) grow indefinitely, one may choose the initial distribution of the Markov process, the sojourn (exponential) rates, and the transition rates between states in such a way that the resulting PH distributions converge weakly to any given and fixed distribution on the positive real line. Hence, we may regard PH distributions as a generalisation of the exponential distribution, which is as flexible as desired in the overall shape of its distribution function. However, the tail behaviour always remains exponential, and in many applications, a better description is required to estimate functionals based on quantiles correctly. This drawback naturally leads to considering classes which extend PH distributions and allow different tail behaviour while still enjoying closed-form formulae, the weak convergence property, and tractable estimation via the EM algorithm. One such class is comprised by inhomogeneous phase-type (IPH) distributions.

Inhomogeneous phase-type distributions ([1]) are equivalently defined as the law of a transformed PH distributed random variable or as the absorption time of a time-inhomogeneous pure-jump Markov process with \( p \) transient states and one additional absorbing state. Depending on the
chosen transformation, the tail behaviour of the resulting IPH distribution can be shown to be as heavy or light as desired. When considering parametric transformations, the estimation procedure was outlined in [2] for possibly aggregated data (see also [4] for extensions to right-censored data and survival regression models).

This paper presents the matrixdist package ([5]) to work with PH and IPH distributions, implemented in R ([13]). Various structures for the sub-intensity matrix of the underlying Markov process are considered, and several parametric transformations are provided, inspired by real-life applications. Most of the functions are coded in the language C++ for enhanced performance and made available in the language R through the package Rcpp. It is worth mentioning that the R package mapfit provides statistical routines for Markovian Arrival Processes (MAP), which can loosely speaking be seen as dependent concatenations of PH variables (arrivals), but only the time-homogeneous case is treated.

The remainder of the paper is organised as follows. Section 2 provides the mathematical formulation of PH and IPH distributions and their basic properties and inhomogeneity parametrisations. Estimation for aggregated and right-censored data via the EM algorithm is detailed in Section 3, for various sub-intensity matrix structures. In Section 4 the main methods of the matrixdist package for functional evaluation, simulation and estimation are presented. An illustration is provided in Section 5, and a condensed summary in Section 6.

2. Definitions and properties

2.1. Phase–type distributions. Let \((J_t)_{t \geq 0}\) be a time-homogeneous Markov jump process on a finite state space \(\{1, \ldots, p, p + 1\}\), where states \(1, \ldots, p\) are transient and state \(p + 1\) is absorbing. Then, the intensity matrix \(\Lambda\) of \((J_t)_{t \geq 0}\) is of the form

\[
\Lambda = \begin{pmatrix} S & s \\ 0 & 0 \end{pmatrix},
\]

where \(S\) is a \(p \times p\) matrix and \(s\) is a \(p\)-dimensional column vector. Since every row of \(\Lambda\) sums to zero, it follows that \(s = -Se\), where \(e = (1, \ldots, 1)'\) is a \(p\)-dimensional column vector of ones. Assume that the process starts somewhere in the transient space with probability \(\alpha_k = P(J_0 = k), \quad k = 1, \ldots, p\), and let \(\alpha = (\alpha_1, \ldots, \alpha_p)\). Here it is assumed that the probability of starting in the absorbing state \(p + 1\) is zero, i.e., \(P(J_0 = p + 1) = 0\). Then, we say that the time until absorption \(Y\) has phase-type distribution with representation \((\alpha, S)\) and we write \(Y \sim \text{PH}(\alpha, S)\) or \(Y \sim \text{PH}_p(\alpha, S)\). The density \(f\) and distribution function \(F\) of \(Y \sim \text{PH}(\alpha, S)\) are given by

\[
\begin{align*}
    f(y) &= \alpha \exp (Sy)s, \quad y > 0, \\
    F(y) &= 1 - \alpha \exp (Sy)e, \quad y > 0,
\end{align*}
\]

where the exponential of a matrix \(A\) is defined by

\[
\exp (A) = \sum_{n=0}^{\infty} \frac{A^n}{n!}.
\]

The efficient computation of the exponential of a matrix is not a straightforward task in high dimensions (see [9]). The moments of \(Y \sim \text{PH}(\alpha, S)\) are given by

\[
\mathbb{E}(Y^{\theta}) = \Gamma(1 + \theta) \alpha (-S)^{-\theta} e, \quad \theta > 0.
\]

Let \(Y_1 \sim \text{PH}_{p_1}(\alpha_1, S_2)\) and \(Y_2 \sim \text{PH}_{p_2}(\alpha_2, S_2)\) be independent phase-type distributed random variables of dimensions \(p_1\) and \(p_2\) respectively. Then

\[
Y_1 + Y_2 \sim \text{PH}_{p_1+p_2}((\alpha_1, 0), \begin{pmatrix} S_1 & s_1 \alpha_2 \\ 0 & S_2 \end{pmatrix})
\]
\[ \min (Y_1, Y_2) \sim \text{PH} \left( \alpha_1 \otimes \alpha_2, S_1 \oplus S_2 \right), \tag{2.5} \]

and

\[ \max (Y_1, Y_2) \sim \text{PH} \left( \begin{pmatrix} \alpha_1 \otimes \alpha_2, 0, 0 \end{pmatrix}, \begin{pmatrix} S_1 \oplus S_2 & I \otimes S_2 & s_1 \otimes I \\ 0 & 0 & S_2 \end{pmatrix} \right), \tag{2.6} \]

where \( \otimes \) and \( \oplus \) denotes the Kronecker product and sum, respectively, and \( I \) is the identity matrix of appropriate dimension. In other words, the PH class is closed under addition, minima and maxima. In fact, it is also closed under any order statistic, and we confer to [7] for the exact and more involved expression.

By decomposing the matrix \( S \) into its Jordan normal form, it follows directly from the definition of survival function that the right tail of a PH distribution is asymptotically exponential. For a comprehensive reading on phase-type distributions we refer to [7].

2.2. Inhomogeneous phase–type distributions. In [1] the class of inhomogeneous phase-type distribution was introduced by allowing the Markov jump process to be time-inhomogeneous in the construction principle of phase-type distributions. In this way, \((J_t)_{t \geq 0}\) has an intensity matrix of the form

\[ \Lambda(t) = \begin{pmatrix} S(t) & s(t) \\ 0 & 0 \end{pmatrix}, \]

where \( s(t) = -S(t)e \). Here it is assumed the vector of initial probabilities is \( \alpha = (\alpha_1, \ldots, \alpha_p) \). Then, we say that the time until absorption \( X \) has inhomogeneous phase-type distribution with representation \((\alpha, S(t))\) and we write \( X \sim \text{IPH}(\alpha, S(t)) \). However, this setting is too general for applications, since its functionals are given in terms of product integrals. Thus, we consider the subclass of IPH distribution when the intensity matrix is of the form \( S(t) = \lambda(t)S \), where \( \lambda \) is some known non-negative real function and \( S \) is a sub-intensity matrix. In this case we write \( X \sim \text{IPH}(\alpha, S, \lambda) \). Note that with \( \lambda \equiv 1 \) one get the conventional phase-type distributions. This subclass is particularly suitable for applications due to the following property. If \( X \sim \text{IPH}(\alpha, S, \lambda) \), then there exists a function \( g \) such that

\[ X \sim g(Y), \]

where \( Y \sim \text{PH}(\alpha, S) \). The relationship between \( g \) and \( \lambda \) is given by the following expression

\[ g^{-1}(y) = \int_0^y \lambda(t)dt. \]

The density \( f \) and distribution function \( F \) of \( X \sim \text{IPH}(\alpha, S, \lambda) \) can again be expressed using the exponential of matrices, and are given by

\[ f(x) = \lambda(x) \alpha \exp \left( \int_0^x \lambda(t)dt \right) s, \quad x > 0, \tag{2.7} \]

\[ F(x) = 1 - \alpha \exp \left( \int_0^x \lambda(t)dt \right) e, \quad x > 0. \tag{2.8} \]

The class of IPH distributions is no longer confined to exponential tails, despite being defined in terms of matrix exponentials. Its exact asymptotic behaviour is determined by the function \( \lambda \) (see [4] for details).

It turns out that a number of IPH distributions can be expressed as classical distributions with matrix-valued parameters, properly defined using functional calculus. Tables 2.1, 2.2 and 2.3 contain the IPH transformations, densities and cumulative distribution functions in closed-form.
matrix notation as implemented in the \texttt{matrixdist} package (cf. [1, 2, 4] for details and motivation on the various parametrisations).

\begin{table}[h]
\centering
\begin{tabular}{|l|l|l|}
\hline
\textbf{Matrix-Pareto} & $\lambda(t) = (t + \beta)^{-1}$ & $g(y) = \beta (\exp(y) - 1)$ \\
\hline
\textbf{Matrix-Weibull} & $\lambda(t) = \beta t^{\beta - 1}$ & $g(y) = y^{1/\beta}$ \\
\hline
\textbf{Matrix-Lognormal} & $\lambda(t) = \frac{\gamma (\log(s+1))^{\gamma - 1}}{s+1}$ & $g(y) = \exp(y^{1/\gamma}) - 1$ \\
\hline
\textbf{Matrix-Loglogistic} & $\lambda(t) = \theta t^{\theta - 1} / (t^\theta + \gamma^\theta)$ & $g(y) = \gamma (\exp(y) - 1)^{1/\theta}$ \\
\hline
\textbf{Matrix-Gompertz} & $\lambda(t) = \exp(\beta t) \log(\beta y + 1) / \beta$ & $g(y) = \beta > 0$ \\
\hline
\textbf{Matrix-GEV} & $\lambda(t) = \exp(\beta t)$ & $g(y) = \log(\beta y + 1) / \beta$ \\
\hline
\end{tabular}
\caption{Transformations}
\end{table}

\begin{table}[h]
\centering
\begin{tabular}{|l|l|}
\hline
\textbf{Matrix-Pareto} & $f(x) = \alpha \left(\frac{x}{\beta} + 1\right)^{S-1} s^{-1/s}$ \\
\hline
\textbf{Matrix-Weibull} & $f(x) = \alpha \exp(Sx^\beta) s x^{\beta-1}$ \\
\hline
\textbf{Matrix-Lognormal} & $f(x) = \alpha \exp(S (\log(x+1))^\gamma) s^{\gamma / x+1}$ \\
\hline
\textbf{Matrix-Loglogistic} & $f(x) = \alpha \exp(S \log((x/\gamma)^\theta + 1)) \theta x^{\theta-1} / (x^\theta + \gamma^\theta)$ \\
\hline
\textbf{Matrix-Gompertz} & $f(x) = \alpha \exp(S (\exp(βx) - 1) / β) s \exp(βx)$ \\
\hline
\textbf{Matrix-GEV (ξ ≠ 0)} & $f(x) = \frac{1}{\sigma} \alpha \exp \left( S \left( 1 + \frac{x - μ}{σ} \right)^{-1/ξ} \right) s \left( 1 + \frac{x - μ}{σ} \right)^{-1/ξ}$ \\
\hline
\textbf{Matrix-GEV (ξ = 0)} & $f(x) = \frac{1}{\sigma} \alpha \exp \left( S \exp \left( -\frac{x - μ}{σ} \right) \right) s \exp \left( -\frac{x - μ}{σ} \right)$ \\
\hline
\end{tabular}
\caption{Densities}
\end{table}

\begin{table}[h]
\centering
\begin{tabular}{|l|l|}
\hline
\textbf{Matrix-Pareto} & $F(x) = 1 - \alpha \left(\frac{x}{\beta} + 1\right)^{S}$ \\
\hline
\textbf{Matrix-Weibull} & $F(x) = 1 - \alpha \exp(Sx^\beta)$ \\
\hline
\textbf{Matrix-Lognormal} & $F(x) = 1 - \alpha \exp(S (\log(x+1))^\gamma)$ \\
\hline
\textbf{Matrix-Loglogistic} & $F(x) = 1 - \alpha \exp(S \log((x/\gamma)^\theta + 1))$ \\
\hline
\textbf{Matrix-Gompertz} & $F(x) = 1 - \alpha \exp(S (\exp(βx) - 1) / β)$ \\
\hline
\textbf{Matrix-GEV (ξ ≠ 0)} & $F(x) = \alpha \exp \left( S \left( 1 + \frac{x - μ}{σ} \right)^{-1/ξ} \right)$ \\
\hline
\textbf{Matrix-GEV (ξ = 0)} & $F(x) = \alpha \exp \left( S \exp \left( -\frac{x - μ}{σ} \right) \right)$ \\
\hline
\end{tabular}
\caption{Cumulative distribution functions}
\end{table}

For a randomly generated 5-dimensional general phase-type distribution, Figure 2.1 depicts the density, distribution function, hazard rate and quantile function of the following \texttt{ph} and \texttt{iph} objects:
set.seed(1)
x <- ph(structure = "general", dimension = 5)
x1 <- iph(x, gfun = "pareto", gfun_pars = 0.5)
x2 <- iph(x, gfun = "weibull", gfun_pars = 1.5)
x3 <- iph(x, gfun = "lognormal", gfun_pars = 2)
x4 <- iph(x, gfun = "gompertz", gfun_pars = 1)

Figure 2.1. Functionals of 5-dimensional inhomogeneous phase-type distributions with the same underlying structure.
3. **Inference algorithms**

3.1. **Estimation of PH distributions.** The expectation-maximisation (EM) algorithm is an iterative method for maximum likelihood (ML) estimation. This algorithm is particularly suitable for situations best described as *incomplete-data* problems, where ML estimation is difficult due to the absence of some part of data in a more familiar and simpler data structure. Examples of incomplete data settings include: missing data, truncated distributions, and censored or grouped observations. Consider \( y_1, \ldots, y_M \) an i.i.d. sample from a phase-type distributed random variable. Since each \( y_i, i = 1, \ldots, M \), is a replication of the absorption time of a Markov-jump process whose trajectory is unobserved, we are clearly in an incomplete data set-up. This was first exploited in [3] where the authors proposed the use of an EM algorithm for ML estimation for PH distributions and derived explicit formulae for the E- and M- steps. We now briefly describe such method.

Let \( B_k \) be the number of times the Markov process underlying the phase-type distribution initiates in state \( k \), \( N_{kl} \) the total number of transitions from state \( k \) to \( l \), \( N_k \) the number of times an exit to the absorbing state was caused by a jump from state \( k \), and \( Z_k \) the total time the Markov process has spent in state \( k \). The complete data likelihood \( L_c \) is then given by

\[
L_c(\alpha, S, \beta; y) = \prod_{k=1}^{p} \alpha_k e_k \prod_{k=1}^{p} \prod_{l \neq k} s_{kl}^{-N_{kl}} e^{-s_{kl}Z_k} \prod_{k=1}^{p} s_k^{-N_k} e^{-s_kZ_k},
\]

leading to the EM algorithm 3.1, where \( e_k \) denotes a \( p \)-dimensional column vector with all entries equal to zero except from the \( k \)-th entry which is equal to one.

**Algorithm 3.1** (EM algorithm for PH distributions).

**Input:** observations \( y_1, \ldots, y_M \), number of iterations to perform \( N \), initial parameters \((\alpha, S)\).

**Loop** over \( 1 \leq n \leq N \):

1. **(E-step) Calculate**

\[
\mathbb{E}(B_k | Y = y) = \sum_{i=1}^{M} \alpha_k e_k \frac{\exp(Sy_i)s}{\alpha \exp(Sy_i)s}.
\]

\[
\mathbb{E}(Z_k | Y = y) = \sum_{i=1}^{M} \int_{0}^{y_i} e_k \frac{\exp(S(y_i - u))sa \exp(Su)e_k du}{\alpha \exp(Sy_i)s}.
\]

\[
\mathbb{E}(N_{kl} | Y = y) = \sum_{i=1}^{M} s_{kl} \int_{0}^{y_i} e_k \frac{\exp(S(y_i - u))sa \exp(Su)e_k du}{\alpha \exp(Sy_i)s}.
\]

\[
\mathbb{E}(N_k | Y = y) = \sum_{i=1}^{M} s_k \frac{sa \exp(Sy_i)e_k}{\alpha \exp(Sy_i)s}.
\]

2. **(M-step) Let**

\[
\hat{\alpha}_k = \frac{\mathbb{E}(B_k | Y = y)}{M}, \quad \hat{s}_{kl} = \frac{\mathbb{E}(N_{kl} | Y = y)}{\mathbb{E}(Z_k | Y = y)},
\]

\[
\hat{s}_k = \frac{\mathbb{E}(N_k | Y = y)}{\mathbb{E}(Z_k | Y = y)}, \quad \hat{s}_{kk} = -\sum_{l \neq k} \hat{t}_{kl} - \hat{t}_k.
\]

Let \( \hat{\alpha} = (\hat{\alpha}_1, \ldots, \hat{\alpha}_p) \), \( \hat{S} = \{\hat{s}_{kl}\}_{k,l=1,\ldots,p} \) and \( \hat{s} = (\hat{s}_1, \ldots, \hat{s}_p)' \).
(3) Assign \( \alpha := \hat{\alpha}, \ S := \hat{S}, \ s := \hat{s} \) and GOTO 1.

**Output:** fitted parameters \((\alpha, S)\).

Let \((\alpha_n, S_n)\) be the parameter values after the \(n\)-th iteration. The EM algorithm ensures that each new estimate is better than the previous one in the sense that

\[
L(\alpha_n, S_n; y) \leq L(\alpha_{n+1}, S_{n+1}; y),
\]

where \(L(\alpha, S; y) = \prod_{i=1}^{M} \alpha \exp (S y_i) s\) is the likelihood function. In other words, the likelihood function increases for each iteration, and hence converges to some maximum. In general, there is no way of guaranteeing that such maximum is global. In practice, a commonly used criterion for determining the number of iterations is consider a large enough number such that subsequent changes in the log-likelihood are negligible.

Note that the EM algorithm 3.1 preserves zeros in \(\alpha\) and \(S\). This means, that when an element has been estimated to zero, it will remain zero in subsequent iterations. Thus, one can initiate the algorithm with a specific initial structure and it will be preserved. The matrixdist package includes the following preset structures:

- **General PH.** No restrictions, all elements are allowed to be non-zero.
- **Hyperexponential.** Also known as mixture of exponentials. Here, the Markov process is allowed to start in any of the transient states but gets absorbed without visiting any other state. This means that the matrix \(S\) is non-zero only in the diagonal.
- **Generalised Erlang.** Also known as sum of exponentials. Here, the Markov process starts in state 1 with probability one, i.e., \(\alpha = (1, 0, \ldots, 0)\) and then visits each subsequent state \(2, \ldots, p\), in that order, and finally reaches the absorbing state.
- **Coxian.** Same structure as the generalised Erlang, but the Markov process is allowed to reach absorption from any of the transient states.
- **Generalised Coxian.** Same structure as the Coxian, but the Markov process is allowed to start in any state.

The main computational burden lies in the E-steps where the computation of matrix exponentials is required. While this can be done in multiple ways (see [9]), the matrixdist package employs the approach described in [3] that consists of converting the problem into a system of ODE’s. More specifically, we consider the \(p\)-dimensional vector functions

\[
a(y | \alpha, S) = \alpha \exp (S y), \quad b(y | \alpha, S) = \exp (S y) s,
\]

\[
c(y, k | \alpha, S) = \int_{0}^{y} \alpha \exp (Su) e_k \exp (S(y - u)) \ dt \ , \quad k = 1, \ldots, p,
\]

Note that the E-step can be computed from the knowledge of the above functions. Thus, for fixed \(\alpha\) and \(S\), we get the following system of ODE’s

\[
a^{(1)}(y | \alpha, S) = a(y | \alpha, S) S, \quad b^{(1)}(y | \alpha, S) = S b(y | \alpha, S),
\]

\[
c^{(1)}(y, k | \alpha, S) = S c(y, k | \alpha, S) + a_i(y | \alpha, S) s, \quad k = 1, \ldots, p,
\]

where \(a_i(y | \alpha, S)\) is the \(i\)-th component of the vector \(a(y | \alpha, S)\). Here, the superscript \((k)\) denotes the \(k\)-th order derivative. The initial conditions of the system are

\[
a(0 | \alpha, S) = \alpha, \quad b(0 | \alpha, S) = s.
\]
The system is then solved numerically via a Runge-Kutta method of fourth order. This is also the method employed in the EMpht programme ([12]). We made use of the same default step-length of $0.1 / \max_{i=1, \ldots, p} |s_{ii}|$ as in the EMpht programme, but the user may input a custom step-length if desired. An important consideration in the implementation of this method is that the sample must be ordered, which is done automatically by the \texttt{matrixdist} package. See [2, 10] for other methods based on uniformisation.

3.2. Censored data. In [11] an EM algorithm for ML estimation of PH distributions in the presence of censored data was derived. The only difference with respect to the algorithm in [3] is in the E-step. The authors derived explicit formulae for left-censoring, right-censoring and, more generally, interval censoring. The \texttt{matrixdist} package includes the right-censoring case, which is arguably the most commonly encountered setting in application areas such as survival analysis. Next we present the missing formulae which are needed for this specific case.

\[
\mathbb{E}(B_k \mid Y > v) = \frac{\alpha_k e_k' \exp(Sv)e}{\alpha \exp(Sv)e},
\]

\[
\mathbb{E}(Z_k \mid Y > v) = \int_0^v e_k' \exp(\{S\{v - u\}\})e\alpha \exp(\{Su\})e_k du,
\]

\[
\mathbb{E}(N_{kl} \mid Y > v) = s_{kl} \int_0^v e_l' \exp(\{S\{v - u\}\})e\alpha \exp(\{Su\})e_k du.
\]

Note that the contribution from $N_k$, given that $Y > v$, must be zero since absorption has not yet taken place. The computation of this expression is performed via a Runge-Kutta method of fourth order as well (we refer to [11] for further details).

3.3. Weighted data. Suppose that for a given sample set there are $y_1, \ldots, y_D$ distinct values and that $y_i$ appears $M_i \geq 1$ times in the original sample, $i = 1, \ldots, D$. In this way, $M_1 + \cdots + M_D = M$ and the sums over all sample points in the E-step may be reduced to weighted sums of fewer terms. For instance,

\[
\mathbb{E}(B_k \mid Y = y) = \sum_{i=1}^D M_i \frac{\alpha_k e_k' \exp(Sy_i)e}{\alpha \exp(Sy_i)e}.
\]

This is particularly useful when data are represented by a histogram rather than raw data. The \texttt{matrixdist} package allows weighted data sets as input to estimation routines. In absence of weight input, an equal weight is assigned to each observation by default.

Another situation where weighted samples are useful is to fit PH distributions to a theoretical given distribution. In [3] it was shown that the EM algorithm can be modified to this case and expressions in terms of integrals are given. However, in general none of the integrals have explicit solutions, and approximations have to be employed. These integrals can be approximated by a weighted sum over a finite grid, i.e., if $h$ is the theoretical given density then the integrals are approximated as $\int_{-\infty}^{\infty} \cdots h(y)dy = \sum_{i=1}^D M_i y_i$. Thus, the problem is reduced to having a weighted sample as input.

3.4. Estimation of IPH distributions. An EM algorithm for ML estimation of IPH distribution was recently introduced in [2]. The main idea is to allow the inhomogeneity function $\lambda(\cdot; \beta)$ to depend on a parameter $\beta$ in the representation $X \sim \text{IPH}(\alpha, S, \lambda(\cdot; \beta))$. In particular, $g^{-1}(X : \beta) \sim \text{PH}(\alpha, S)$, where $g^{-1}(x : \beta) = \int_0^x \lambda(t; \beta)dt$. 

Notice that the parameter $\beta$ must also be estimated, such that the approach of transforming into the PH domain taken in [1] is not applicable in this parametric setting. Instead, [2, 4] considered estimating $\beta$ separately from the other parameters and performing a new transformation to the PH domain after each set of E- and M- steps. In this way, one obtains the EM algorithm 3.2, which is also guaranteed to increase the likelihood at each iteration, thus converging to a (possibly local) maximum.

It is worth noting that algorithm 3.2 will increase the likelihood at each iteration even if the maximum in Step 2 is not fully reached, as long as there is no decrease of likelihood in the numerical optimisation routine involved in that step. Hence, to speed-up convergence, a pre-set number of iterations, or depth, may be specified for Step 2.

Extensions to censored and weighted data can be handled in an analogous way as the PH case and are also implemented in the matrixdist package, but are presently omitted for conciseness. We refer to [4] for further details on these algorithms, as well as other covariate-dependent extensions.

Algorithm 3.2 (EM algorithm for IPH distributions).

**Input:** observations $x_1, \ldots, x_M$, number of iterations to perform $N$, initial parameters $(\alpha, S, \beta)$.

**Loop** over $1 \leq n \leq N$:

1. Transform the data into $y_i = g^{-1}(x_i; \beta)$, $i = 1, \ldots, M$, and apply the E- and M-steps EM algorithm 3.1 by which we obtain the estimators $(\hat{\alpha}, \hat{S})$.

2. Compute

$$\hat{\beta} = \arg \max_\beta \sum_{i=1}^{M} \log \left( f_X \left( x_i; \hat{\alpha}, \hat{S}, \beta \right) \right)$$

$$= \arg \max_\beta \sum_{i=1}^{M} \log \left( \lambda(x_i; \beta) \hat{\alpha} \exp \left( \int_0^{x_i} \lambda(t; \beta)dt \hat{S} \right) \right) .$$

3. Assign $(\alpha, S, \beta) = (\hat{\alpha}, \hat{S}, \hat{\beta})$ and GOTO 1.

**Output:** fitted parameters $(\alpha, S, \beta)$.

4. Methods for PH and IPH distributions

The matrixdist provides an object-oriented interface for PH and IPH distributions. The constructor function $\text{ph}$ will admit structural parameters $\alpha$ and $S$ and create an object of class $\text{ph}$. Alternatively, one may input a structure (“general”, “coxian”, “gcxian”, “hyperexponential”, or “gerlang”) and a randomly generated valid structure of the provided dimension will be generated. The constructor function $\text{iph}$ will admit a $\text{ph}$ object together with the inhomogeneity function $g$ (“pareto”, “weibull”, “lognormal”, “loglogistic”, “gompertz”, or “gev”), or alternatively will admit the same input as the $\text{ph}$ constructor function and the inhomogeneity specifications. Once a $\text{ph}$ or $\text{iph}$ object has been created, a suite of methods are available for the efficient evaluation of functionals, simulation, and estimation. We describe in this section the implementation of these methods.

**Density function** The $\text{dens}$ method calculates the density function of a $\text{ph}$ or $\text{iph}$ object. For $\text{ph}$ objects, an internal function $\text{phdensity}$ is called from c++, which implements formula (2.1), and in particular calculates the matrix exponential using a similar implementation to MATLAB’s built-in algorithm, the Pade approximation ([9]).
For *iph* objects, the expressions in Table 2.2 are implemented individually and called through their *g* function name. For instance, the *c++* function `mweibullden` is called for Matrix-Weibull objects. This implementation is faster than inputting an inhomogeneity function into a generic function of the type (2.7).

**Cumulative distribution function** The *cdf* method calculates the cumulative distribution function of a *ph* or *iph* object. For *ph* objects, an internal function `phcdf` is called from *c++*, which implements formula (2.2), and once again calculates the matrix exponential using the Pade approximation.

For *iph* objects, the expressions in Table 2.3 are implemented individually and called through their *g* function name. For instance, the *c++* function `mparetocdf` is called for Matrix-Pareto objects. As for densities, the implementation is faster than inputting an inhomogeneity function into formula (2.8).

**Quantile function** The *quan* method calculates the quantile function of a *ph* or *iph* object, defined as

\[ Q(p) = \inf\{x \in \mathbb{R} : p \leq F(x)\}, \quad 0 < p < 1. \]

No general closed-form formula exists for PH and IPH distributions, so the R function `stats::uniroot` function is called to numerically find such infimum. For very few special cases, such as a one-dimensional *ph* object, i.e. an exponential distribution, explicit formulae for quantiles are mathematically available and thus their direct implementation will be faster.

**Hazard rate function** The *haz* method calculates the hazard rate of a *ph* or *iph* object, defined as

\[ h(x) = \frac{f(x)}{1 - F(x)}, \quad x > 0, \]

and is implemented precisely as such ratio, using the methods `dens` and `cdf`.

**Moments** The *moment* method calculates the fractional moments of a *ph* object, or of the underlying *ph* object of an *iph* object, as given by formula (2.3). The method is implemented for diagonalisable matrices $S$, and uses the built-in R functions `eigen` and `solve` to compute the matrix function involved in (2.3).

**Random sampling** The *sim* method performs random sampling from a *ph* or *iph* object. For *ph* objects, an internal function `rphasetype` is called from *c++*, which simulates a path of a time-homogeneous Markov jump process and outputs the absorption time as the corresponding PH variate.

For *iph* objects, the *c++* function `riph` uses the transforms of Table 2.1 to simulate from a path of a time-inhomogeneous Markov jump process, and output the absorption time as the corresponding IPH variate. A special implementation for the Matrix-GEV distribution is provided using the *c++* function `rmatrixgev`, since this case is not obtainable through straightforward time transformation for any $\xi$.

**Sum, minimum and maximum** The "+", *minimum* and *maximum* methods admit two *ph* objects and construct another *ph* object according to formulae (2.4), (2.5) and (2.6), respectively. Their implementation is straightforward using the *ph* constructor function, the built-in R function `kronecker` for computing Kronecker product of matrices, and the function `kronecker_sum` from the `matrixdist` package for computing the Kronecker sum of matrices.

For the special case when two *iph* objects have the same *g* function and parameter, the minimum and maximum is again an IPH distribution with the same *g* function and parameter, and underlying
structures (2.5) and (2.6), respectively. Thus, the minimum and maximum methods also work for this particular case of IPH distributions.

**Estimation via the EM algorithm** The fit method estimates a ph or iph object based on given data and an initial ph or iph object, respectively. The data should be positive (except when considering the Matrix-GEV distribution, which is allowed to take negative values as well) and may be aggregated or right-censored. Algorithms 3.1 and 3.2 and their censored and aggregated data versions are implemented.

For ph objects, the c++ function EMstep_RK is called at each iteration to perform an E- and M-step. The c++ function default_step_length re-calculates the default step-size of the Runge-Kutta method at each iteration, unless it is user specified. The function logLikelihoodPH_RK calculates and prints the log-likelihood every pre-set number of steps, is implemented in c++, and re-uses some of the by-products of the EM step via the Runge-Kutta method to improve evaluation speed.

For iph objects, the c++ function EMstep_RK is called at each iteration to perform an E- and M-step, and then the optimisation in Step 2 of algorithm 3.2 is performed using the R built-in optimiser optim. The objective function in the latter optimisation depends on the g inhomogeneity function. For instance, logLikelihoodMlognormal_RK is a c++ function which is called to perform log-likelihood evaluations for the Matrix-Lognormal distribution using the by-products of the EM step via the Runge-Kutta method. As before, the step size is re-calculated at every iteration, and the log-likelihood is printed at every pre-set number of steps, this time using the output of the optim function.

The object-oriented interface of the matrixdist package is particularly convenient for estimation using the fit method, since one may re-start the EM algorithm to perform more iterations by simply using a fitted object as the initial object of a new fit to the same data. Furthermore, for large datasets, one may fit on a histogram to get a near-optimal fit, and then finish off the estimation using the entire dataset. All previous methods for ph and iph objects are again available for fitted objects, since they are once again of the same class.

**Other methods** The show, logLik and coef methods admit ph objects and work in the same manner as the usual R methods with the same names.

5. **Illustrations**

In this section we provide two detailed illustrations of the estimation of PH and IPH distributions using the matrixdist package. These examples also provide some guidance on how to employ the fitting functionalities of the package. In what follows, the number of iterations was chosen in such a way that the changes in the successive log-likelihood values became negligible.

5.1. **Truncated normal distribution.** Let Z be a normally distributed random variable with mean $\mu$ and standard deviation $\sigma$. Then, we say that the conditional distribution of Z given $a < Z < b$, $-\infty \leq a < b \leq \infty$, is a truncated normal distribution with density function $h$ given by

$$h(x) = \frac{\phi \left( \frac{(x - \mu)}{\sigma} \right)}{\sigma \left( \Phi \left( \frac{(b - \mu)}{\sigma} \right) - \Phi \left( \frac{(a - \mu)}{\sigma} \right) \right)}, \quad a < x < b,$$

where $\phi$ and $\Phi$ are the density and distribution functions of a standard normal distribution, respectively.

Presently, we consider a truncated normal distribution with support in the interval $(0, \infty)$ and $\mu = \sigma = 1$. Then, we employ algorithms 3.1 and 3.2 to estimate PH and IPH models to this theoretical given distribution. To this end, we first discretise the theoretical model’s density.
this can be done in several ways, such as using Simpson’s rule, we proceeded with a simplified
approximation which yielded the following data set

\[
y <- \text{seq}(0.01, 5, \text{by} = 0.05)\\
weights <- 0.05 * \text{dnorm}(y, \text{mean} = 1)/\text{pnorm}(0, \text{mean} = 1, \text{lower.tail} = \text{FALSE})
\]

Then, we fitted a PH model with 10 phases and Coxian structure

```r
set.seed(1)
x1 <- ph(structure = "coxian", dimension = 10)
x_fit1 <- fit(x1, y, weight = weights, stepsEM = 20000)
```

The run time was of 131.28 seconds in a usual PC with a 2.4 GHz 8-Core Intel Core i9 processor. As a second model, we considered a Matrix-Gompertz model with Coxian structure of dimension 2.

```r
set.seed(1)
x2 <- iph(ph(structure = "coxian", dimension = 2), gfun = "gompertz")
x_fit2 <- fit(x2, y, weight = weights, stepsEM = 600)
```

Here the run time was 1.33 seconds. Figure 5.1 shows that the matrix-Gompertz model provides a better fit with substantially less phases. Note that the AIC displayed is for comparison purposes only. In general, one should proceed with great caution when employing information criteria (especially in high dimensions) due to the well-known identifiability issues for PH and IPH distributions.

5.2. **Loss insurance data.** The data consist of 1500 insurance claims from a real-life insurance company. Each claim consists of an indemnity payment (loss) and an allocated loss adjustment expense (ALAE). This data set is available in the `copula` package and has been previously studied in the literature (e.g. [8]). We presently consider only the loss component, for which 34 observations are right-censored, and proceed to fit Pareto and Matrix-Pareto models. As a first step, we split the data into censored and non-censored observations

```r
data(loss, package="copula")
y <- loss$loss[loss$censored == 0]
rcens <- loss$loss[loss$censored == 1]
```

Subsequently, we fitted the Pareto model, which is a special case of the matrix-Pareto with \( p = 1 \). Thus we may employ algorithm 3.2 for its estimation as well.

```r
set.seed(1)
x1 <- iph(ph(structure = "general", dimension = 1), gfun = "pareto")
x_fit1 <- fit(x1, y, rcen = rcens, stepsEM = 1000)
```

The running time was of 5.34 seconds with a log-likelihood of \(-16537.36\). Moreover, the tail index, which determines the heaviness of the tail is of 0.88, very close to the one of 0.89 from the Pareto model in [8].

Next we fitted a Matrix-Pareto distribution win Coxian structure of dimension 4

```r
set.seed(1)
x2 <- iph(ph(structure = "coxian", dimension = 4), gfun = "pareto")
x_fit2 <- fit(x2, y, rcen = rcens, stepsEM = 2000)
```

In this case, the running time was 13.66 seconds. Note that the log-likelihood here is of \(-16528.92\), significantly higher than the Pareto model, indicating that the matrix-Pareto model provides a better fit. This is further supported by figure 5.1, where we see that the cumulative hazard of the
matrix-Pareto model is closer to the non-parametric Nelson-Aalen estimator, the later computed using the \texttt{survival} package. Note that the tail index in the Matrix-Pareto fit is of 0.67, suggesting that a model with a lighter tail behaviour is more adequate. This can also be seen directly from the cumulative hazard plot. The tail indexes were computed as follows (see [4] for the mathematics behind these formulae, and in general for the asymptotic behaviour of IPH distributions)

\begin{verbatim}
x1 <- 1/-max(eigen(coef(x_fit1)$S)$values)
x2 <- 1/-max(eigen(coef(x_fit2)$S)$values)
\end{verbatim}

![Fits to truncated N(1,1)](image1)

**Figure 5.1.** Left panel: two approximations of a truncated normal distribution; right panel: fitted cumulative hazards to the loss data compared to the Nelson-Aalen implied hazard.

6. **Summary**

We surveyed the basic properties of phase-type and inhomogeneous phase-type distributions and introduced the \texttt{matrixdist} package, which provides tools for their statistical analysis. The package includes methods for computing various functionals, creating more complicated objects based on simpler building blocks, simulation, and estimation via the EM algorithm. Particular emphasis was given to the estimation routines, where we reviewed the most useful existing algorithms and touched upon some computational aspects.

The package’s major novelty is the implementation of all methods concerning IPH distributions. However, functional evaluation (and some new techniques) together with manipulating conventional PH distributions comprehensively in an object-oriented manner are useful tools that fill a gap in their own right.

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