Acyclic discrete phase type distributions: properties and a parameter estimation algorithm

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Abstract

This paper provides a detailed study on discrete phase type (DPH) distributions and its acyclic subclass referred to as acyclic-DPH (ADPH). Previously not considered similarities and differences between DPH and continuous phase type (CPH) distributions are investigated and minimal representations, called canonical forms, for the subclass of ADPH distributions are provided. We investigate the consequences of the recent result about the minimal coefficient of variation of the DPH class [The minimal coefficient of variation of discrete phase type distributions, in: Proceedings of the Third International Conference on Matrix-analytic Methods in Stochastic Models, July 2000] and show that below a given order (that is a function of the expected value) the minimal coefficient of variation of the DPH class is always less than the minimal coefficient of variation of the CPH class. Since all the previously introduced Phase Type fitting methods were designed for fitting over the CPH class we provide a DPH fitting method for the first time. The implementation of the DPH fitting algorithm is found to be simple and stable. The algorithm is tested over a benchmark consisting of 10 different continuous distributions. The error resulted when a continuous distribution sampled in discrete points is fitted by a DPH is also considered.

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1. Introduction

Discrete phase type (DPH) distributions have been introduced and formalized in [10], but they have received little attention in applied stochastic modeling since then, because the main research activity and application oriented work was addressed towards continuous phase type (CPH) distributions [11].
However, in recent years a new attention has been devoted to discrete models since it has been observed that they can be utilized in the numerical solution of non-Markovian processes, or they are more closely related to physical observations [15,16]. Moreover, new emphasis has been put on discrete stochastic Petri Nets [5,6,17]. Finally, DPHs may have a wide range of applicability in stochastic models in which random times must be combined with constant durations. In fact, one of the most interesting property of the DPH distributions is that they can represent in an exact way a number of distributions with finite support, like the deterministic and the (discrete) uniform, and hence one can mix inside the same formalism distributions with finite and infinite support.

In particular, while it is known that the minimal coefficient of variation for the CPH family depends only on the order $n$ and is attained by the Erlang distribution [1] ($cv = 1/n$), it is trivial to show, for the DPH family, that for any order $n$ the deterministic distribution with $cv = 0$ is a member of the family. Since, the range of applicability of the PH distributions may depend on the range of variability of the coefficient of variation given the order $n$, it is interesting to investigate, for the DPH family, how the coefficient of variation depends on the model parameters.

The convenience of using the DPH family in applied stochastic modeling has motivated the present paper whose aim is to investigate more closely the properties of the DPH family and to provide results that can be profitably exploited for the implementation of an algorithm to estimate the model parameters given an assigned distribution or a set of experimental points [4].

The DPH representation of a given distribution function is, in general, non-unique [13] and non-minimal. Hence, we first explore a subclass of the DPH class for which the representation is an acyclic graph (acyclic-DPH–ADPH) and we show that, similarly to the continuous case [8], the ADPH class admits a unique minimal representation, called canonical form.

We recall the theorem about the minimal coefficient of variation of the DPH class as a function of the order and of the mean [18]. This theorem shows that below a given order (that is a function of the mean) the minimal coefficient of variation of the DPH class is always less than the minimal coefficient of variation of the CPH class. This result, combined with the well known result of [1] (the minimal $cv$ for an $n$-phase CPH distribution is $1/n$ independent of its mean), offers the possibility of comparing the applicability of the CPH and DPH families to fit distributions with low $cv$.

An algorithm is presented for the estimation of the ADPH model parameters to fit distributions or a set of experimental data. The algorithm is based on the maximum likelihood (ML) principle. A $z$-transform version of the algorithm is derived from the continuous case [3], while a novel time domain version is provided. It is shown that the time domain algorithm is easier to implement and more stable. The algorithm is then tested on a benchmark of 10 different continuous distributions that have been already utilized for a similar study in the continuous case [4]. However, since a continuous distribution needs to be discretized in order to feed the fitting algorithm, the role of the discretization interval on the performance of the algorithm and on the goodness of the fit is extensively discussed.

The structure of the paper is as follows. Section 2 introduces the basic definitions and notation, and provides a simple example to emphasize some differences between the CPH and DPH class, differences that are not evident from a comparative analysis reported for instance in [9]. Section 3 derives the canonical form (and their main properties) for the class of acyclic-DPH (ADPH). Section 4 gives the theorem to describe the minimal coefficient of variation for the DPH class as a function of the order and of the mean and shows the shape of the structures that realize minimal coefficient of variation. Section 5 presents the ML estimation algorithm, both in $z$-transform domain and in time domain. Section 6 discusses the role of the discretization interval on the accuracy of the obtainable approximation, while
Section 7 is devoted to present the results of the benchmark analysis. Finally, Section 8 concludes the paper.

2. Definition and notation

A DPH distribution \([10,11]\) is the distribution of the time until absorption in a discrete-state discrete-time Markov chain (DTMC) with \(n\) transient states, and one absorbing state. (The case when \(n = \infty\) is not considered in this paper.) If the transient states are numbered \(1, 2, \ldots, n\) and the absorbing state is numbered \((n + 1)\), the one-step transition probability matrix of the corresponding DTMC can be partitioned as

\[
\hat{B} = \begin{bmatrix} B & b \\ 0 & 1 \end{bmatrix},
\]

where \(B = [b_{ij}]\) is the \((n \times n)\) matrix grouping the transition probabilities among the transient states, \(b = [b_{i,n+1}]^T\) is the \(n\)-dimensional column vector grouping the probabilities from any state to the absorbing one, and \(0 = [0]\) is the zero vector. Since \(\hat{B}\) is the transition probability matrix of a DTMC, the following relation holds:

\[
\sum_{j=1}^{n} b_{ij} = 1 - b_{i,n+1}.
\]

The initial probability vector of the DTMC is an \((n + 1)\)-dimensional vector \(\hat{\pi} = [\hat{\pi}, \alpha_{n+1}]\), with \(\sum_{j=1}^{n+1} \alpha_j = 1 - \alpha_{n+1}\). In the present paper, we only consider the class of DPH distributions for which \(\alpha_{n+1} = 0\), but the extension to the case when \(\alpha_{n+1} > 0\) is straightforward.

Let \(\tau\) be the time till absorption into state \((n + 1)\) in the DTMC. We say that \(\tau\) is a DPH r.v. of order \(n\) and representation \((\hat{\pi}, B)\) \([11]\). Let \(f(k), F(k)\) and \(F(z)\) be the probability mass, cumulative probability and probability generating function of \(\tau\), respectively. It follows:

\[
f(k) = \Pr\{\tau = k\} = \alpha b^{k-1}b \quad \text{for } k > 0,
\]

\[
F(k) = \Pr\{\tau \leq k\} = \alpha \sum_{i=0}^{k-1} b^i b = 1 - \alpha b^k e,
\]

\[
F(z) = E[z^\tau] = z\alpha(1 - zB)^{-1}b = \frac{U(z)}{V(z)} = \frac{z^n + u_{n-1} z^{n-1} + \cdots + u_0}{v_n z^n + v_{n-1} z^{n-1} + \cdots + v_0},
\]

where \(e\) is an \(n\)-dimensional column vector with all the entries equal to 1 and \(I\) is the \((n \times n)\) identity matrix. A DPH distribution is a non-negative, discrete distribution over \(\{1, 2, \ldots, n\}\).

2.1. Properties of DPHs different from CPHs

A number of properties of the DPH family have been derived in \([10]\). Moreover, the DPH family inherits many properties from the CPH family \([9]\), for which a more extensive literature exists \([2,7,12,14]\).
However, when DPHs and CPHs are used to approximate general distributions to transform a non-Markovian process into a DTMC or a CTMC over an expanded state space, a very crucial feature is to keep the order of the DPH or CPH distributions as low as possible, since the order affects multiplicatively the size of the expanded state space. Hence, it is very important to establish to what extent the properties of the family are dependent upon the order.

A well known and general result for CPH distributions [1] is that the squared coefficient of variation ($c^2v$) of a CPH of order $n$ is not less than $1/n$, and this limit is reached by the continuous Erlang, CE($\lambda$, $n$), (or Gamma($\lambda$, $n$)) distribution of order $n$ (independently of the parameter $\lambda$, and hence independently of the mean of the distribution).

The simple relation, established in [9], to compare the CPH and DPH classes, preserves the mean but not the coefficient of variation. Hence, in the case of the DPH family the consideration about the minimal coefficient of variation requires a more extensive analysis, and it is deferred to Section 4.

However, it is trivial to show that the mentioned property for CPHs does not hold for DPHs. In fact, for any order $n$, the DPH with representation $(\gamma, A)$ given by

\[ \gamma = [1, 0, \ldots, 0], \quad A = \begin{bmatrix} 0 & 1 & 0 & \ldots & 0 \\ 0 & 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & 0 \end{bmatrix}, \] (4)

represents a deterministic time to absorption $\tau = n$, with $c^2v = 0$. Hence for any order $n$ there exists at least one DPH with $c^2v = 0$. In order to emphasize other differences, we carry on a simple comparative example on a 2-CPH versus a 2-DPH.

**Example 1.** Let $\tau_C$ and $\tau_D$ be the CPH and DPH r.v. shown in Fig. 1, with representations $(\gamma, A)$ and $(\alpha, B)$, respectively

\[ \gamma = [1, 0], \quad A = \begin{bmatrix} -\lambda_1 & \lambda_1 \\ 0 & -\lambda_2 \end{bmatrix}, \quad \alpha = [1, 0], \quad B = \begin{bmatrix} 1 - \beta_1 & \beta_1 \\ 0 & 1 - \beta_2 \end{bmatrix}. \]

The mean $m$, the variance $\sigma^2$ and the squared coefficient of variation $c^2v$ of $\tau_C$ and $\tau_D$ are given below:

\[
\begin{align*}
  m_C &= \frac{1}{\lambda_1} + \frac{1}{\lambda_2}, \\
  m_D &= \frac{1}{\beta_1} + \frac{1}{\beta_2}, \\
  \sigma_C^2 &= \frac{1}{\lambda_1^2} + \frac{1}{\lambda_2^2}, \\
  \sigma_D^2 &= \frac{1}{\beta_1^2} + \frac{1}{\beta_2^2} - \frac{1}{\beta_1} - \frac{1}{\beta_2}, \\
  c^2v_C &= \frac{\sigma_C^2}{m_C^2} = \frac{\lambda_1^2 + \lambda_2^2}{(\lambda_1 + \lambda_2)^2}, \\
  c^2v_D &= \frac{\sigma_D^2}{m_D^2} = \frac{\beta_1^2 - \beta_1 \beta_2 + \beta_2^2 - \beta_1 \beta_2}{(\beta_1 + \beta_2)^2}.
\end{align*}
\]

(5)

Fig. 1. Two-state CPH and DPH structures.
Both distributions are characterized by two free parameters: the CPH by \((\lambda_1, \lambda_2)\), the DPH by \((\beta_1, \beta_2)\).

First, we suppose to fix the value of \(\lambda_1\) and \(\beta_1\), and to find the value \(\lambda_2^\text{min}\) and \(\beta_2^\text{min}\) that minimize the squared coefficient of variation in (5). The values \(\lambda_2^\text{min}\) and \(\beta_2^\text{min}\) are obtained by equating to 0 the derivative of \(cv^2\) with respect to \(\lambda_2\) and \(\beta_2\), and are given by

\[
\lambda_2^\text{min} = \lambda_1, \quad \beta_2^\text{min} = \frac{\beta_1(2 + \beta_1)}{2 - \beta_1},
\]

where \(0 \leq \beta_2, \beta_1 \leq 1\). The minimal coefficient of variation of the CPH structure is obtained when the parameters \(\lambda_1\) and \(\lambda_2\) are equal, while the DPH structure exhibits the minimal coefficient of variation when, in general, \(\beta_1\) differs from \(\beta_2\).

In order to investigate the dependence of the minimal coefficient of variation with respect to the mean, let us assume that the two free parameters of the considered structures are \((\lambda_2, m_C)\) and \((\beta_2, m_D)\).

Rearranging Eq. (5), we have

\[
\lambda_1 = \frac{\lambda_2}{m_C\lambda_2 - 1}, \quad \beta_1 = \frac{\beta_1}{m_D\beta_2 - 1}, \quad cv^2_C = \frac{2 - 2m_C\lambda_2 + m_C^2\lambda_2^2}{m_C^2},
\]

\[
\lambda_2 = \frac{2 - 2m_D\beta_2 - m_D\beta_2^2 + m_D^2\beta_2^2}{m_D^2}, \quad cv^2_D = \frac{1}{2} - \frac{1}{m_D}.
\]

For a given mean \((m_C, m_D)\), the minimal coefficient of variation is obtained by equating to 0 the derivative of \(cv^2\) with respect to \(\lambda_2\) and \(\beta_2\), respectively. It is obtained

\[
\lambda_2^\text{min} = \frac{2}{m_C}, \quad \beta_2^\text{min} = \frac{2}{m_D},
\]

where as a result of the given initial probability vector \([1, 0]\) the mean \(m_D \geq 2\) and \(\beta_2^\text{min} \leq 1\). Substituting this value into (6), we obtain

\[
\lambda_1 = \frac{2}{m_C}, \quad cv^2_C = \frac{1}{2}, \quad \beta_1 = \frac{2}{m_D}, \quad cv^2_D = \frac{1}{2} - \frac{1}{m_D}.
\]

In the CPH case, the minimal coefficient of variation is obtained (as in the previous case) when \(\lambda_1 = \lambda_2\) and it is independent of the mean \(m_C\). In the DPH case, differently from the previous case, the minimum is attained when \(\beta_1 = \beta_2\) (discrete Erlang distribution \(\text{DE}(2/m, 2)\)), but the value of the minimum depends on the mean \(m_D\).

3. Acyclic-DPHs

Definition 1. A DPH is called acyclic-DPH (ADPH) if its states can be ordered in such a way that matrix \(B\) is an upper triangular matrix.

By Definition 1, a generic ADPH of order \(n\) is characterized by \(N_f = (n^2 + 3n - 2)/2\) free parameters \((n(n + 1)/2\) in the upper triangular matrix \(B\) and \(n - 1\) in the initial probability vector \(\alpha\).

Definition 1 implies that a state \(i\) can be directly connected to a state \(j\) only if \(j \geq i\). In an ADPH, each state is visited only once before absorption. We define an absorbing path, or simply a path, the sequence
of states visited from an initial state to the absorbing one. In an ADPH of order \( n \), the number of paths is finite and is at most \( 2^n - 1 \). The length of a path is the (integer) number of states visited via the path before absorption.

The \( k \)th path, \( r_k \), of length \( \ell \leq n \), is characterized by a set of indices, representing the states visited before absorption

\[
r_k = (x_1, x_2, \ldots, x_\ell)
\]

such that

\[
\begin{align*}
1 \leq x_j & \leq n & \forall j : 1 \leq j \leq \ell, \\
x_j < x_{j+1} & \forall j : 1 \leq j < \ell, \\
b_{x_j, x_{j+1}} > 0 & \forall j : 1 \leq j < \ell, \\
b_{x_\ell, n+1} > 0 &
\end{align*}
\]

(7)

where the last two conditions mean that in a path any two subsequent indices represent states that are connected by a direct arc (non-zero entry in the \( B \) matrix), and the last index represents a state that is connected by a direct arc to the absorbing state \((n+1)\). Note that the path description, \( r_k \), defines explicitly the initial state of the underlying DTMC. The below defined quantities \((P(r_k), F(z, r_k))\) are all conditional to the initial state \((x_1)\).

Assuming that the underlying DTMC starts in state with index \( x_1 \), the path \( r_k \) in (7), occurs with probability

\[
P(r_k) = \prod_{j=1}^{\ell} \frac{b_{x_j, x_{j+1}}}{1 - b_{x_j, x_{j+1}}},
\]

(8)

and the generating function of the time to arrive to the absorbing state through path \( r_k \) is

\[
F(z, r_k) = \prod_{j=1}^{\ell} \frac{(1 - b_{x_j, x_{j+1}})z}{1 - b_{x_j, x_{j+1}}},
\]

(9)

\( P(r_k) \) is the product of the probabilities of choosing the consecutive states of the path and \( F(z, r_k) \) is the product of the generating functions of the sojourn times spent in the consecutive states of the path.

Let \( L_i \) be the set of all the paths starting from state \( i \) (i.e., for which \( x_1 = i \)). The generating function of the time to absorption assuming the DTMC starts from state \( i \) is

\[
F_i(z) = \sum_{r \in L_i} P(r) F(z, r),
\]

where it is clear from (8) that \( \sum_{r \in L_i} P(r) = 1 \).

Corollary 1. The generating function of an ADPH is the mixture of the generating functions of its paths (see also [8]):

\[
F_{ADPH}(z) = \sum_{i=1}^{n} a_i \sum_{r \in L_i} P(r) F(z, r),
\]

(10)
Example 2. Let us consider the ADPH in Fig. 2, with representation
\[ \alpha = [ \alpha_1 \ \alpha_2 ], \quad B = \begin{bmatrix} 0.3 & 0.5 \\ 0 & 0.6 \end{bmatrix}. \]  
(11)

Three different paths can be identified to reach the absorbing state. The paths are depicted in Fig. 3 and have the following structure:

- \( r_1 \) is a path of length 1 starting from state 1. Eqs. (8) and (9) applied to \( r_1 \) provide
  \[ P(r_1) = \frac{b_{13}}{1 - b_{11}} = 2, \quad F(z, r_1) = \frac{(1 - b_{11})z}{1 - b_{11}z} = \frac{0.7z}{1 - 0.3z}. \]

- \( r_2 \) is a path of length 2 starting from state 1. Eqs. (8) and (9) provide
  \[ P(r_2) = \frac{b_{12}b_{23}}{1 - b_{11}1 - b_{22}} = 5, \quad F(z, r_2) = \frac{(1 - b_{11})z(1 - b_{22})z}{1 - b_{11}z1 - b_{22}z} = \frac{0.7z \cdot 0.4z}{1 - 0.3z1 - 0.6z}. \]

- \( r_3 \) is a path of length 1 starting from state 2. Eqs. (8) and (9) provide
  \[ P(r_3) = \frac{b_{23}}{1 - b_{22}} = 1, \quad F(z, r_3) = \frac{(1 - b_{22})z}{1 - b_{22}z} = \frac{0.4z}{1 - 0.6z}. \]

From (9) and from Corollary 1, it follows that the generating function of the time to absorption does not depend on the particular order of the geometrically distributed sojourn times. Hence, we can reorder the eigenvalues (diagonal elements) of the matrix \( B \) into a decreasing sequence \( q_1 \geq q_2 \geq \cdots \geq q_n \). For the sake of convenience, we define the symbols \( p_i = (1 - q_i) \) which represent the exit rate from state \( i \).

Since the sequence of the \( q_i \)'s is in a decreasing order, the sequence of the \( p_i \)'s is in an increasing order: \( p_1 \leq p_2 \leq \cdots \leq p_n \).
Any path \( r_k \) can be described as a binary vector \( u_k = [u_i] \) of length \( n \) defined over the ordered sequence of the \( q_i \)'s. Each entry of the vector is equal to 1 if the corresponding eigenvalue \( q_i \) is present in the path, otherwise the entry is equal to 0. Hence, any path \( r_k \) of length \( \ell \) has \( \ell \) ones in the vector \( u_k \). With this representation any path is characterized by a unique binary number \( 1 \leq \#u_k \leq 2^n - 1 \).

**Definition 2.** A path \( r_k \) of length \( \ell \) of an ADPH is called a basic path (basic series [8]) if it contains the \( \ell \) fastest phases \( q_{n-\ell+1}, \ldots , q_n \). The binary vector associated to a basic path is called a basic vector and it contains \((n-\ell)\) initial 0's and \( \ell \) terminal 1's, so that the unique binary number of a basic vector is \( \#u_k = 2^\ell - 1 \).

**Theorem 1.** The generating function of a path of an ADPH is a mixture of the generating functions of its basic paths.

**Proof.** The following lemma gives the basic relationship to prove the theorem.

**Lemma 1.** The generating function of a phase with parameter \( q_i \) can be represented as the mixture of the generating functions of a phase with parameter \( q_{i+1} \) and a sequence of two phases with parameter \( q_i \) and \( q_{i+1} \).

The above lemma is a consequence of the relationship

\[
\frac{(1-q_i)z}{1-q_{i+1}z} = w_i \frac{(1-q_{i+1})z}{1-q_{i+1}z} + (1-w_i) \frac{(1-q_i)z}{1-q_{i+1}z},
\]

(12)

where \( w_i = (1-q_i)/(1-q_{i+1}) \), hence \( 0 \leq w_i \leq 1 \).

A path \( r_k \) is composed by geometric phases according to its associated binary vector \( u_k \). Starting from the rightmost component of \( u_k \) which is not ordered as a basic path (Definition 2), the application of (12) splits the path into two paths which are enriched in components with higher indices. Repeated application of (12) can transform any path into a mixture of basic paths. Cumani [8] has provided an algorithm which performs the transformation of any path into a mixture of basic paths in a finite number of steps.

**Example 3.** Let \( n = 5 \) and let \( r_k \) be a path of length \( \ell = 2 \) characterized by the binary vector \( u_k = [0, 1, 0, 1, 0] \) (corresponding to the phases with parameters \( q_2 \) and \( q_4 \)). By applying Lemma 1 to the rightmost phase of \( r_k \) (phase 4), the associated binary vector \( u_k \) can be decomposed in a mixture of two binary vectors one containing phase 5 and the second one containing the sequence of phases (4,5). Thus the original path is split into the mixture of the following two paths:

\[
\begin{align*}
u_k &= [0, 1, 0, 1, 0] \\
&\Rightarrow [0, 1, 0, 0, 1],
\end{align*}
\]

\[
\begin{align*}
u_k &= [0, 1, 0, 1, 0] \\
&\Rightarrow [0, 1, 0, 1, 1].
\end{align*}
\]

Now for each obtained binary vector, we take the rightmost phase which is not already ordered in a basic path, and we decompose the corresponding path into two paths according to Eq. (12). The complete decomposition tree is shown next, where all the final binary vectors are basic vectors according
to Definition 2:

\[ u_k = [0, 1, 0, 1, 0] \Rightarrow \begin{cases} [0, 1, 0, 0, 1] & \{ [0, 0, 0, 1, 1] \\ [0, 0, 1, 0, 1] \\ [0, 1, 0, 1, 1] \\ [0, 0, 1, 1, 1] \\ [0, 1, 1, 1, 1] \} \\ [0, 1, 0, 1, 1] \{ [0, 0, 1, 1, 1] \\ [0, 1, 1, 1, 1] \} \end{cases} \]

Corollary 2 (Canonical form CF1). Any ADPH has a unique representation as a mixture of basic paths called canonical form 1 (CF1). The DTMC associated to the CF1 is given in Fig. 4, and its matrix representation \((a, P)\) takes the form:

\[
a = [a_1, a_2, \ldots, a_n], \quad P = \begin{bmatrix} q_1 & p_1 & 0 & 0 & \cdots & 0 \\ 0 & q_2 & p_2 & 0 & \cdots & 0 \\ & \vdots & \vdots & \vdots & \ddots & \vdots \\ & 0 & 0 & 0 & \cdots & q_n \end{bmatrix}
\]

with \(\sum a_i = 1\) and \(p_1 \leq p_2 \leq \cdots \leq p_n\).

**Proof.** The corollary is a direct consequence of Theorem 1.

Due to the particular structure of the matrix in (13), the relevant elements can be stored into an \(n\)-dimensional vector \(p\) containing the \(p_i\)'s, so that we will use the notation \((a, p)\) as the representation of a CF1, where \(a\) and \(p\) are \(n\)-dimensional vectors (where \(0 \leq a_i \leq 1, 0 < p_i \leq 1\)).

**Example 4.** The transformation of the ADPH of Fig. 2 into the canonical form CF1 proceeds along the following steps. We first order the eigenvalues of the matrix \(B\) into a decreasing sequence to obtain: \(q_1 = b_{22} = 0.6\) and \(q_2 = b_{11} = 0.3\) with \(q_1 \geq q_2\). Then, any path is assigned its characteristic binary vector. If the binary vector is not in basic form, each path is transformed into a mixture of basic paths by repeated application of (12), along the line shown in Example 3. Since the ADPH of Fig. 2 is of order \(n = 2\), we have two basic paths \(b_1 = [0, 1]\) and \(b_2 = [1, 1]\).

Path \(r_1\). The associated binary vector is \(u_1 = [0, 1]\) and is coincident with the basic path \(b_1\). Hence \(F(z, r_1) = F(z, b_1)\).
Path $r_2$. The associated binary vector is $u_2 = [1, 1]$ and is coincident with the basic path $b_2$. Hence
\[ F(z, r_2) = F(z, b_2). \]

Path $r_3$. The associated binary vector is $u_3 = [1, 0]$ and is not a basic path. Hence, $r_3$ must be transformed in a mixture of basic paths as shown in Fig. 5. Application of (12) provides
\[ F(z, r_3) = w_1 F(z, b_1) + (1 - w_1) F(z, b_2) \]
with $w_1 = p_1 / p_2 = 4/7$.

The generating function of the ADPH can be finally written as
\[ F(z) = a_1 F(z, b_1) + a_2 F(z, b_2). \] (15)

The DTMC associated to the obtained CF1 is depicted in Fig. 6, and its representation is
\[ a = [a_1, a_2], \quad p = [0.4, 0.7]. \] (16)

3.1. Properties of canonical forms

Property 1. The CF1 is a minimal representation of an ADPH.

In fact, the number of free parameters of a CF1-ADPH of order $n$ is $N_F = 2n - 1$ and is equal to the number of degrees of freedom $N_G$ computed from (3).
Given a canonical form CF1 of order \( n \) and representation \((a, p)\) (Fig. 4), the mean, the second moment and the probability generating function are expressed as

\[
m = \sum_{i=1}^{n} a_i \sum_{j=i}^{n} \frac{1}{p_j},
\]

\[
d = \sum_{i=1}^{n} a_i \left[ \sum_{j=i}^{n} \left( \frac{1}{p_j} - \frac{1}{p_i} \right) + \left( \sum_{j=i}^{n} \frac{1}{p_j} \right)^2 \right],
\]

\[
F(z) = \sum_{i=1}^{n} a_i \prod_{j=i}^{n} \frac{p_j z}{1 - (1 - p_j) z}.
\]

Even if the canonical form CF1 is the simplest minimal form to use in computations, sometimes it can be more convenient to have a minimal representation in which the initial probability is concentrated in the first state. Borrowing terminology from the continuous case\[8\], we define the following.

**Definition 3** (Canonical form CF2). An ADPH is in canonical form CF2 (Fig. 7) if transitions are possible from phase 1 to all the other phases (including the absorbing one), and from phase \( i \) (\( 2 \leq i \leq n \)) to phase \( i \) itself and \( i + 1 \). The initial probability is 1 for phase \( i = 1 \) and 0 for any phase \( i \neq 1 \).

The matrix representation of the canonical form CF2 is

\[
\alpha = \begin{bmatrix} 1 & 0 & \cdots & 0 \end{bmatrix}, \quad B = \begin{bmatrix} q_0 & c_1 & c_2 & \cdots & c_{n-1} \\
0 & q_1 & p_1 & 0 & \cdots & 0 \\
0 & 0 & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & \cdots & 0 & q_{n-1} \\
0 & 0 & \cdots & 0 & q_n & \cdots & q_{n-1} \\
0 & 0 & \cdots & 0 & \cdots & 0 & q_n \end{bmatrix}.
\]

It is trivial to verify that CF2 is a minimal form and that the equivalence of distributions of the time to absorption between CF1 and CF2 is established by the following relationship:

\[
c_k = a_k p_{n-k}.
\]

**Definition 4** (Canonical form CF3). An ADPH is in canonical form CF3 (Fig. 8) if from any phase \( i \) (\( 1 \leq i \leq n \)) transitions are possible to phase \( i \) itself, \( i + 1 \) and \( n + 1 \). The initial probability is 1 for phase \( i = 1 \) and 0 for any phase \( i \neq 1 \).
The matrix representation of CF3 is

\[ \alpha = [1 \ 0 \ \cdots \ 0], \quad B = \begin{bmatrix} q_0 & e'_0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & q_{n-1} & e'_{n-1} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & q_2 & e'_2 \\ 0 & 0 & 0 & 0 & \cdots & 0 & q_1 \end{bmatrix} \] (22)

It is also easy to verify that CF3 is a minimal form and that the equivalence of the distribution of the time to absorption between CF1 and CF3 is established by

\[ s_i = \sum_{j=1}^{i} a_{j}, \quad e'_i = \frac{a_i}{p_i}, \quad e_j = \frac{x_{j-1}}{x_j} \]

In CF3 the phases are ordered according to decreasing sojourn time. A path through the last \( i \) phases of a CF1 is represented by a path through the first \( i \) phases and a jump to the absorbing state in CF3.

4. Comparing the minimal coefficient of variation for CPH and DPH

It has been shown in Section 2.1, that a deterministic distribution with \( cv = 0 \) is a member of the DPH as well as the ADPH class (4), and moreover that the minimal \( cv \) depends on the mean. Since the flexibility in approximating a given distribution function may depend on the range of variability of the coefficient of variation, in this section we compare the CPH and DPH families from the point of minimal coefficient of variation. For this purpose we recall the theorem that describes the minimal coefficient of variation for the DPH class [18].

To state the theorem, the following notation is introduced. \( \tau_n(m) \) is a DPH of order \( n \) with mean \( m \). Given a real number \( x \), define \( f(x) = \lfloor x \rfloor \) the integer part of \( x \) and \( R(x) \) the fractional part of \( x \), respectively, i.e., \( x = f(x) + R(x), 0 \leq R(x) < 1 \).

**Theorem 2.** The minimal squared coefficient of variation, \( cv^2_{\text{min}} \), of a DPH \( \tau_n(m) \) of order \( n \) with mean \( m \) is

\[
cv^2_{\text{min}}(\tau_n(m)) = \begin{cases} 
\frac{R(m)(1 - R(m))}{n} & \text{if } m \leq n, \\
1 - \frac{1}{m} & \text{if } m > n.
\end{cases}
\] (23)
The DPH which exhibits this minimal $c_v^2$ is referred to as MDPH, and has the following structure (in CF1 form):

- if $m \leq n$: $p_i = 1$, $\forall i$ and the non-zero initial probabilities are $a_{n-I(m)} = R(m)$ and $a_{n-I(m)+1} = 1 - R(m)$ (Fig. 9);
- if $m > n$: $p_i = n/m$, $\forall i$ and the only non-zero initial probability is $a_1 = 1$ (discrete Erlang distribution DE($n/m, n$)) (Fig. 10).

Comment. The MDPH structure is uniquely specified given the order $n$ and the mean $m$. The MDPH structure with $m \leq n$ is the mixture of two deterministic CF1-ADPHs with length $I(m) + 1$ and initial probability $R(m)$ and with length $I(m)$ and initial probability $1 - R(m)$. This structure derives from the following identity: if $x$ is real, $x = R(x)(I(x) + 1) + (1 - R(x))I(x)$. Hence, for $m \leq n$, the corresponding MDPH structure has an effective order $I(m) + 1$, being the initial probabilities from state 1 to $n - I(m)$ equal to 0. Hence, in contrast with the continuous case, increasing the order beyond $n > m$ does not have any effect on the minimal $c_v$. The case $m > n$ is more similar to the CPH case, and tends to be equal to the CPH case as $n \rightarrow \infty$.

Theorem 2, combined with the well known result of [1] (the minimal $c_v^2$ for a CPH of order $n$ is equal to $1/n$ independent of its mean), offers the possibility of comparing the variability of the CPH and DPH families.

For fixed $m$, as the order $n$ increases beyond $n > m$ the minimal $c_v^2$ of the DPH remains unchanged, while the minimal $c_v^2$ of the CPH decreases as $1/n$. Hence, given $m$ a value $n = n_C$ can be found, such that the minimal $c_v^2$ of the CPH of order $n_C$ is less or equal then the minimal $c_v^2$ of the DPH of the same order. Recalling Eq. (23), the value of $n_C$ is the smallest positive integer which satisfies

$$\frac{1}{n_C} < \frac{R(m)(1 - R(m))}{m^2}. \quad (24)$$

It is clear from (24) that if $m$ is integer, $R(m) = 0$ and $n_C \rightarrow \infty$. Using the relation $m = I(m) + R(m)$, in Eq. (24), we can find the value of $R(m)$ that minimizes (24), for any positive integer $I(m)$, and the corresponding minimal value of $n_C$. 

Fig. 9. MDPH with $m \leq n$.

Fig. 10. MDPH with $m > n$. 
Setting the derivative of \( C \) with respect to \( R(m) \) to zero with \( I(m) = \) constant, we get

\[
\frac{dC}{dR(m)} = 0 \quad \text{iff} \quad R(m) = \frac{I(m)}{1 + 2I(m)}.
\]

From which the minimal value of \( C \), corresponding to any mean with integer part equal to \( I(m) \), is given by

\[
C_{\text{min}} = 4I(m)(1 + I(m))
\] (25)

From Eq. (25) we can get Table 1 which gives us the minimal order \( nC_{\text{min}} \) as a function of the integer part of the mean \( I(m) \) for which the CPH class provides a minimal \( cV^2 \) less than the DPH of the same order.

**Example 5.** Fig. 11 shows the minimal \( cV^2 \) as a function of the number of phases for the DPH family versus the CPH family, when the mean is \( m = 4.5 \). (Note that in Fig. 11, \( m < n \) when \( n \geq 5 \).) According to Theorem 2 the minimal \( cV^2 \) for the DPH class remains unchanged (\( cV^2_{\text{min}} = 1/81 \)) for \( n \geq 5 \), while the the minimal \( cV^2 \) for the CPH class (\( C_{\text{min}} = 1/n \)) decreases to 0 as \( n \to \infty \).

Application of Eq. (25) tells us that if \( I(m) = 4 \) (i.e., the mean is any value \( 4 \leq m < 5 \)), the minimal number of phases for which the CPH has a \( cV^2 \) less than the DPH is \( nC_{\text{min}} = 80 \), corresponding to a mean \( m = 4.444 \cdots \).
Fig. 12. Minimal squared coefficient of variation for $n = 5$.

Let us now consider the dual case, in which we fix the order $n$. We already know from Table 1 that if $n < n_{c_{\min}}$ no CPH can have a minimal $c v^2$ less than the DPH. However, if $m$ increases with fixed $n$, we arrive in a situation in which $m > n$, and applying the second part of (23) we see that $c v^2_{\min} \to 1/n$ as $m \to \infty$. Hence, as $m$ increases, the behavior of the DPH class tends to be similar to the one of the CPH class.

Example 6. Fig. 12 shows the minimal $c v^2$ as a function of the mean for a DPH of order $n = 5$. Note that for $m \leq n (= 5)$, $c v^2_{\min}$ equals zero for any $m$ integer, and $c v^2_{\min}$ tends to the value of the CPH class $(1/n)$ as $m \to \infty$.

5. A fitting algorithm for parameter estimation

We describe a fitting algorithm for estimating the parameters of an ADPH in CF1 form, based on the ML principle [3,4]. We first derive the closed form expression for the pmf both in the z-transform domain and in the time domain, and for its derivatives with respect to the model parameters, then the implemented ML estimation algorithm is briefly sketched. The range of applicability of both techniques is finally discussed.

5.1. The probability mass function

The generating function of a CF1-ADPH with $n$ phases and representation $(a, p)$ is provided in (19) and may be written as

$$F(z) = \sum_{j \in S} a_j F(z)^{p_j},$$  \hspace{1cm} (26)
where $F(i)$ is the generating function of a path of length $(n - i + 1)$ from phase $i$ to $(n+1)$, and is given by

$$F(i)(z) = \prod_{k=i}^{n} \frac{1-q_{k}}{1-q_{k}}.$$  \hspace{1cm} (27)

Let $\sigma_i (\sigma_i \leq n - i + 1)$ denote the number of distinct eigenvalues out of the set $\{q_i, q_{i+1}, \ldots, q_n\}$ and let us further denote by $(\hat{q}_i^{(1)}, \hat{q}_i^{(2)}, \ldots, \hat{q}_i^{(\sigma_i)})$ the $\sigma_i$-dimensional vector of the distinct eigenvalues and by $(\hat{m}_1^{(i)}, \hat{m}_2^{(i)}, \ldots, \hat{m}_{\sigma_i}^{(i)})$ the vector of their multiplicities. With this notations, $\hat{m}_j^{(i)}$ is the multiplicity of $\hat{q}_j^{(i)}$ and $\sum_{j=1}^{\sigma_i} \hat{m}_j^{(i)} = n - 1 + i$. Eq. (27) can be rewritten as

$$F(i)(z) = \prod_{j=1}^{\sigma_i} \frac{(1-\hat{q}_j^{(i)})^{\hat{m}_j^{(i)}}}{(z-1-\hat{q}_j^{(i)})^{\hat{m}_j^{(i)}}}.$$ \hspace{1cm} (28)

After a partial fraction decomposition, we have

$$F(i)(z) = \sum_{j=1}^{\sigma_i} \frac{\hat{m}_j^{(i)}}{\sum_{l=2}^{\hat{m}_j^{(i)}} c(i)_j l} \left( \frac{1-\hat{q}_j^{(i)}}{z-1-\hat{q}_j^{(i)}} \right)^{\hat{m}_j^{(i)}}, \hspace{1cm} (29)$$

where $c(i)_j (j \in \{1, 2, \ldots, \sigma_i\}$ and $l \in \{1, 2, \ldots, \hat{m}_j^{(i)}\}$) are coefficients determined by the partial fraction decomposition. In [3], a recursive algorithm is proposed for the computation of the coefficients $c(i)_j$.

Using the fact that the $z$-transform of a series like

$$h(k) = \begin{cases} 0 & \text{if } 0 \leq k < l, \\ \frac{(k-1)(k-2)\cdots(k-(l-1))}{(l-1)!} q^{k-l} & \text{if } k \geq l \geq 2, \end{cases}$$

is

$$H(z) = \frac{c(i)_j}{(1-qz)^l}$$

($h(k)$ is the geometric series for $l = 1$), the inverse of (28) is

$$f^{(i)}(k) = \sum_{j=1}^{\sigma_i} \frac{\hat{m}_j^{(i)}}{\sum_{l=2}^{\hat{m}_j^{(i)}} c(i)_j l} \left( \frac{1-\hat{q}_j^{(i)}}{z-1-\hat{q}_j^{(i)}} \right)^{\hat{m}_j^{(i)}}, \hspace{1cm} k \geq 1, \hspace{1cm} (29)$$

which is the conditional pmf of absorption in $k$ steps in state $(n+1)$ assuming that the chain started from phase $i$. Applying (26), the unconditional pmf of absorption in $k$ steps becomes

$$f(k) = \sum_{i=1}^{n} a_i f^{(i)}(k). \hspace{1cm} (30)$$

In the time domain, the pmf of the time to absorption is obtained from (1)

$$f(k) = aP^{k-1}p_n,$$ \hspace{1cm} (31)

where $a$ and $P$ are given in (13), and $p_n$ is a $n$-dimensional column vector whose first $n-1$ elements are equal to 0, and the nth element is equal to $p_n$. 


5.2. The derivatives of the probability mass function

In order to solve the non-linear constrained optimization problem that arises from the application of the ML principle (see Section 5.3), the derivatives of the pmf with respect to the parameters \((a, p)\) are needed. Because the pmf depends linearly on the entries of \(a\), the derivatives with respect to these parameters are immediate. In order to express the derivative of the pmf with respect to \(p_j\), we rearrange (19):

\[
F(z) = \frac{p_j}{z - 1} - \frac{1}{q_j} - \frac{1}{q_j} + \sum_{i=1}^{n} a_i \prod_{k=i}^{n} \frac{p_k}{z - 1 - q_k} + \sum_{i=j+1}^{n} a_i \prod_{k=i}^{n} p_k,
\]

where the second term of the r.h.s. does not depend on \(p_j\). The derivative of (32) with respect to \(p_j\) is

\[
\frac{\partial F(z)}{\partial p_j} = \left[ \frac{1}{z - 1 - q_j} \right] \sum_{i=1}^{n} a_i \prod_{k=i}^{n} \frac{p_k}{z - 1 - q_k} = \frac{1}{p_j} \left[ \sum_{i=1}^{j} a_i F^{(i)}(z) - \frac{p_j}{z - 1 - q_j} \sum_{i=1}^{j} a_i F^{(i)}(z) \right],
\]

where \(F^{(i)}(z)\) is given in (27). The second term in the r.h.s. may be interpreted as the generating function of a CF1-like model that is obtained by adding one further phase, with exit probability \(p_j\), and null initial probability (Fig. 13) to the original CF1 model. Hence, any algorithm that can be used to evaluate the CF1 structure of Fig. 4, can be utilized to evaluate the derivatives with respect to the \(p\) factors as in Fig. 13.

Using the partial fraction decomposition method, the coefficients of the augmented model of Fig. 13, may be calculated by iterating the same recursive algorithm described earlier [3], just one step more. Using the matrix formulation (31), the time domain equivalent of (33) becomes

\[
\frac{\partial f(k)}{\partial p_j} = \frac{1}{p_j} \left[ \hat{a} \hat{P}^{k-1} \hat{p}_n - \hat{a} (\hat{P})^{k-1} [\hat{p}_{n+1}] \right],
\]

where \(\hat{a} (\hat{P})\) is a row vector of length \(n+1\) with elements \(\hat{a}_i = \hat{a}_j = a_i\) if \(1 \leq i \leq j\), and \(\hat{a}_i = \hat{a}_j = 0\) otherwise, \(\hat{p}_{n+1}\) is a column vector of length \(n+1\) with elements \(\hat{p}_i = 0\) if \(1 \leq i \leq n\), \(\hat{p}_{n+1} = p_j\), and

\[
\hat{P} = \begin{bmatrix}
1 - p_1 & p_1 & \cdots & 0 \\
0 & 1 - p_2 & p_2 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & \cdots & \cdots & 1 - p_n & p_n \\
0 & \cdots & \cdots & 0 & 1 - p_j
\end{bmatrix}
\]

Fig. 13. Structure used to determine the derivative with respect to \(p_j\).
is the transition probability matrix that is obtained by adding one more transient phase to the original CF1 structure as in Fig. 13.

Since $P$ and $P^j$ ($j = 1, \ldots, n$) are upper triangular matrices whose only non-zero elements are located in the main diagonal or in the first (upper) subdiagonal the numerical solution of Eqs. (31) and (34) does not require the complexity of a general vector matrix multiplication algorithm.

5.3. ML estimation

Let $\phi = \phi_1, \ldots, \phi_\nu$ be a set of $\nu$ integer data samples. Values in $\phi$ may derive from experimental observations or from the discretization of a continuous cdf. Let us denote $\hat{a}$ and $\hat{p}$ the ML estimators of $a$ and $p$, respectively. The likelihood function has the form

$$L(\phi, a, p) = \prod_{i=1}^\nu f(\phi_i, a, p).$$

The estimation problem consists of finding the parameters $(\hat{a}, \hat{p})$ such that the likelihood function $L(\phi, \hat{a}, \hat{p})$ is maximal, under the constraints of the CF1 form

- $0 \leq p_1 \leq p_2 \leq \cdots \leq p_n \leq 1$,
- $a_i \geq 0$, $\sum_{i=1}^n a_i = 1$.

The estimation problem is then formulated in terms of a non-linear constrained optimization problem, that is solved by resorting to an iterative application of a linear programming algorithm. The logarithm of the likelihood function is linearized around the current point by means of a first order series expansion:

$$\log L(\phi, a + \Delta a, p + \Delta p) = \log L(\phi, a, p) + \frac{\partial \log L(\phi, a, p)}{\partial a} \Delta a + \frac{\partial \log L(\phi, a, p)}{\partial p} \Delta p^T. \quad (35)$$

Given an initial guess $a_0, p_0$, $L(\phi, a, p)$ is linearized according to (35) and linear programming is used to find the maximum of the linearized function inside a small box around $a_0, p_0$ according to the constraints. The solution of this step is used as the initial guess in the subsequent step of the iterative procedure, and the procedure is iterated until a preassigned tolerance level is reached or the maximum number of iterations is exceeded.

5.4. Comparison of the algorithms

The $z$-transform algorithm is based on a partial fraction decomposition method applied to Eqs. (27) and (28) for the computation of the pmf, and to Eq. (33) for the computation of the derivatives. The most time consuming and unstable part of the algorithm is the evaluation of the coefficients $c_{jl}$ in (28). The instability comes from the fact that when two eigenvalues tend to be equal, the associated coefficients grow unboundedly, and when the eigenvalues are coincident the expression of the partial fraction expansion changes.

During the iterative estimation procedure the $p$ parameters may become closer, and a criterion should be set to decide whether two close eigenvalues are “coincident” and to modify the partial fraction expansion accordingly. Practically, a small quantity $\epsilon$ is assigned, and when the difference between two eigenvalues becomes less than $\epsilon$, they are considered to be coincident. However, this procedure introduces numerical instabilities and inaccuracies.
Once the coefficients $c_{jl}^{(i)}$ are determined, the evaluation of the pmf and of its derivatives even for a large $k$ can be done recursively at a very low computational cost.

On the other hand, using the time domain analysis, the pmf is evaluated through Eq. (31) while the derivatives are evaluated through Eq. (34). The solution of both equations requires a vector matrix multiplication that must be replicated $k$ times. Due, however, to the very special and sparse structure of the involved matrices and vectors a very specialized algorithm can be used. Moreover, since all the entries in the vectors and matrices are non-negative numbers less than 1, the vector matrix multiplication remains very stable for any value of $k$. Of course, in this case, the complexity of the algorithm increases with $k$. Hence, the time domain algorithm is much simpler to be implemented, more stable and faster. Only when the time span over which the solution is required becomes very high, the use of the z-transform algorithm may be justified.

We have implemented and experimented both algorithms, but, since the time domain computation proved to be more applicable for high number of phases, the results we show in the next section are all obtained by means of the time domain algorithm.

6. Approximating continuous distributions

When using ADPH distributions to approximate random variables arising in practical problems, there are cases in which a discrete sample of data points is directly derived from the application. But there are also cases in which the distributions to be approximated are not discrete. For example, ADPH distributions can be utilized to approximate continuous distributions.

The ADPH approximation of a continuous distribution requires two steps:

1. The distribution is discretized according to a given discretization step. Indeed, discrete samples and associated mass probability values are generated.
2. The ADPH estimation algorithm is run over the discrete sample provided in the previous step.

The discretization of a continuous distribution is a delicate step that introduces errors, and the amplitude of the introduced errors is mainly related to the size of the discretization interval. Therefore, the role of the discretization interval and its impact on the goodness of fit of DPH estimation algorithms is investigated in the following sections.

6.1. The role of the discretization interval

There are several ways to “discretize” a general distribution, i.e., to assign a probability mass to the elements of a discrete, finite (ordered) set $S = \{x_1, x_2, x_3, \ldots\}$ (where $x_1 < x_2 < x_3 < \cdots$). The most common case of discretization is when the elements of the discrete set are integer multiples of a discretization interval ($\delta$), i.e., $x_i = i\delta$.

Given a r.v. $X$ whose cdf is $F_X(x)$, a simple rule for discretizing $F_X(x)$ over the discrete set $S = \{x_1, x_2, x_3, \ldots\}$ is to use the following:

$$p_i = F_X\left(\frac{x_i + x_{i+1}}{2}\right) - F_X\left(\frac{x_{i-1} + x_i}{2}\right), \quad i > 1, \quad \text{and} \quad p_1 = F_X\left(\frac{x_1 + x_2}{2}\right).$$

(36)

where $p_i$ is the probability associated with $x_i$. This discretization does not preserve the moments of the distribution.
Since there are various potential ways to discretize a given distribution function, here we try to provide some general guidelines.

In general, the smaller is the discretization interval the closer is the discretized distribution to the original one. Hence, on the one hand, the discretization error decreases by decreasing the discretization interval: this remark suggests the use of a small $\delta$. On the other hand, the discretization interval changes the scale of the representation. Indeed, let $X$ be the original (non-negative) random variable expressed in a natural time unit (e.g., seconds); its discretized counterpart $X_d$ is expressed in $\delta$ unit. For any reasonable discretization procedure, we must have

$$E(X_i) \sim \delta E(X_i^d), \quad i \geq 1,$$

being $E(X_i)$ and $E(X_i^d)$ the $i$th moment of $X$ and $X_d^i$, respectively. Eq. (37) shows that a discretization procedure modifies the mean of the distribution ($E(X) \sim \delta E(X_d)$) (since the mean of the discretized distribution is $\delta$ times lower than the mean of the original distribution), but leaves (almost) unchanged its coefficient of variation ($cv(X) \sim cv(X_d)$). Since the minimal $cv$ of a DPH distribution is a function of its mean the chosen discretization interval may play a significant role in the variability of the DPH and, hence, in the goodness of the fit.

6.1.1. Bounds of the discretization interval

The following considerations provide practical upper and lower bounds to guide in the choice of a suitable discretization interval $\delta$, and are mainly based on the dependence of the minimal coefficient of variation of an ADPH on the order $n$ and on the mean $m$.

Since we only consider DPH distributions with no mass at zero, the mean of any DPH distribution is greater than 1, which means that, $\delta$ should be less than $E(X)$. However, given the number of phases $n$, in order to completely exploit the flexibility associated with the $n$ phases, a better upper bound is

$$\delta \leq \frac{E(X)}{n-1},$$

(38)

If the squared coefficient of variation of the distribution to be approximated ($cv^2(X_d)$) is greater than $1/n$ (i.e., $cv^2(X) \sim cv^2(X_d) > 1/n$), any small value of $\delta$ provides a suitable discretization interval. Instead, if $cv^2(X) \sim cv^2(X_d) \leq 1/n$, in order to allow the ADPH to reach this low coefficient of variation (lower than the bound of any CPH as established in [1]), $\delta$ should satisfy the following relation:

$$\delta > \left( \frac{1}{n} - cv^2(X) \right) E(X),$$

(39)

based on the theorem about the minimal $cv$ of ADPH distributions (Section 4).

The effect on the goodness of the attainable approximation of different discretization intervals ($\delta$) is illustrated utilizing a Lognormal distribution with parameters (1, 0.2), whose mean is 1 and $cv^2$ is 0.0408 (this Lognormal distribution is the test case L3 of the benchmark considered in Section 7).

Fig. 14 reports the discretized Lognormal distribution together with the best fit ADPHs of order $n = 2, 4, 8, 12$ and 16 (only for $\delta = 0.025$) obtained applying the ML algorithm, for two different values of the discretization interval $\delta = 0.05$ and $\delta = 0.025$. The discretized mass of the continuous Lognormal distribution at $\delta k$ is $(F(k\delta) - F((k-1)\delta))/\delta$, where $F(t)$ is the cdf of the Lognormal distribution. Note that the discretized distribution is a function of the discretization interval. The lower and upper bounds of $\delta$, computed from Eqs. (38) and (39), are reported in Table 2 as a function of the order of the ADPH (the same orders $n = 2, 4, 8, 12$ as in Fig. 14 are used).
Table 2
Upper and lower bound for $\delta$ as a function of the order

<table>
<thead>
<tr>
<th>$n$</th>
<th>Lower bound of $\delta$ Eq. (39)</th>
<th>Upper bound of $\delta$ Eq. (38)</th>
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</thead>
<tbody>
<tr>
<td>4</td>
<td>0.2092</td>
<td>0.333</td>
</tr>
<tr>
<td>8</td>
<td>0.0842</td>
<td>0.1429</td>
</tr>
<tr>
<td>12</td>
<td>0.0425</td>
<td>0.0909</td>
</tr>
<tr>
<td>16</td>
<td>0.0217</td>
<td>0.0667</td>
</tr>
</tbody>
</table>

Fig. 14. Effect of changing the discretization step.
In Fig. 14, it can be seen that when $\delta$ is less than its lower bound the required low $cv$ cannot be attained; while when $\delta$ is in the proper range (e.g., $n = 12; \delta = 0.05$ and $n = 16; \delta = 0.025$) a reasonably good fit is obtained.

Fig. 15 depicts the cdf and the pmf of three PH distributions approximating distribution L3 using different discretization steps (0.1, 0.05, 0.025). The figure shows the cdf and the pdf of the original distribution and the approximating CPH as well. (When plotting the pmf the probabilities of the approximating PH distributions are multiplied by $1/\delta$ in order to have the values in the same range. This is done to illustrate in a single figure how the mass functions with different discretization steps follow the shape of the original continuous curve and where the CPH approximation is located compared to them.) All the PH distributions have eight phases. Having 0.1 as discretization step eight phases are enough to capture the
low $c_v$ of the distribution $L_3$ (Table 3), this DPH approximation follows the steep changes of the pdf and the cdf as well. As the discretization step is decreased the discrete approximation is getting worse and is approaching the continuous approximation.

### 6.1.2. The required number of phases with a given discretization step

In Fig. 14, it is also visible that the lower $\delta$ we use (the higher the mean of the discretized distribution with respect to the discretization interval) the more phases are needed in order to achieve the same goodness of fit. In fact, according to the theorem given in Section 4 about the minimal $c_v$ of the ADPH family, more phases are needed to attain a given coefficient of variation. The minimal number of phases ($n$) that are needed to reach a given $c_v^2$ when the mean is $E(X_d)$ is given by the next expression

$$n \geq \frac{E(X_d)}{c_v^2(X_d)E(X_d)} + 1$$

if $c_v^2 > \frac{R(E(X_d))(1 - R(E(X_d)))}{E(X_d)^2}$.

Table 3 reports, for the Lognormal distribution of Fig. 14, the mean $E(X_d)$ and the coefficient of variation $c_v^2(X_d)$ of the discretized distribution together with the minimal number of phases needed to reach the coefficient of variation of the original distribution ($c_v^2 = 0.0408$), as a function of different discretization steps.

Table 3 also shows how the discretization modifies the mean and the $c_v$ as a function of the discretization step.

### 7. Examples for the estimation process

This section reports the results of the numerical experiments that have been carried out to test the goodness of fit of the proposed ML fitting algorithm. The experiments are based on a benchmark (composed of continuous distributions only) already proposed in [4] to test the goodness of fit of algorithms for CPH distributions (the origin and the motivations behind the proposed benchmark are discussed in [4]). Hence, the present results allows us to compare the features of the discrete and the CPH fitting.

Table 4 summarizes the distributions that compose the benchmark. In Table 4, the continuous exponential distribution has been added, which was not present in the original benchmark in [4], since the continuous exponential is not a DPH distribution.

Since in our experiments we have to approximate continuous distributions, we have to discretize them before approximation. In the present experiments, we have used the following discretization method. We conventionally assume that the largest sample in the discretized distribution corresponds to the discrete
Table 4
Test cases of the benchmark

<table>
<thead>
<tr>
<th>Density</th>
<th>Symbol</th>
<th>Numerical cases</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weibull</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$f(t) = \frac{\beta}{\eta} \left( \frac{t}{\eta} \right)^{\beta-1} e^{-\left( \frac{t}{\eta} \right)^\beta}$</td>
<td>W1</td>
<td>$\eta = 1, \beta = 1.5$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\eta = 1, \beta = 0.5$</td>
</tr>
<tr>
<td>Lognormal</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$f(t) = \frac{1}{\sigma \sqrt{2\pi}} \exp \left[ -\frac{\left( \log(t/\phi) + \sigma^2/2 \right)^2}{2\sigma^2} \right]$</td>
<td>L1</td>
<td>$\phi = 1, \sigma = 1.8$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\phi = 1, \sigma = 0.8$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\phi = 1, \sigma = 0.2$</td>
</tr>
<tr>
<td>Uniform on (a, b)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$f(t) = \frac{1}{b-a}$</td>
<td>U1</td>
<td>$a = 0, b = 1$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$a = 1, b = 2$</td>
</tr>
<tr>
<td>Shifted exponential</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$f(t) = \frac{1}{2} e^{-t} + \frac{1}{2} e^{-\left( t-1 \right)} 1(t \geq 1)$</td>
<td>SE</td>
<td></td>
</tr>
<tr>
<td>Exponential</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$f(t) = \lambda e^{-\lambda t}$</td>
<td>EX</td>
<td>$\lambda = 1$</td>
</tr>
</tbody>
</table>

point closest to $\hat{x}$ where $F(\hat{x}) = 0.995$, and we assign a probability mass to all points from 1 to $\hat{x}$ based on the rule in (36). As mentioned in the previous section, this discretization rule does not preserve the moments, so that the moments of the discretized distribution (including the expected value) are not coincident with the ones of the original continuous distribution.

For further reference let us denote $F(\cdot)$, $f(\cdot)$, $\bar{F}(\cdot)$, $\bar{f}(\cdot)$ the cdf and pmf of the original distribution, the discretized distribution, and the one resulting from the ML estimation algorithm, respectively.

According to [4], five different measures have been chosen to evaluate the goodness of the fit. The five measures are defined in Table 5, where $c_1(F)$, $c_2(F)$ and $c_3(F)$ represent the first three centered moments of $F(\cdot)$.

While in [4], measures 4 and 5 were defined over continuous functions (as integrals over the support of the distribution), in Table 5 the discretized version has been reported. Hence, the first three measures in

Table 5
Measures for evaluating the goodness of fit

<table>
<thead>
<tr>
<th>Measure</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Relative error in the first moment</td>
<td>$\bar{e}_1 = \frac{</td>
</tr>
<tr>
<td>2. Relative error in the second moment</td>
<td>$\bar{e}_2 = \frac{</td>
</tr>
<tr>
<td>3. Relative error in the third moment</td>
<td>$\bar{e}_3 = \frac{</td>
</tr>
<tr>
<td>4. pmf absolute area difference</td>
<td>$\bar{H} = \sum_{i=1}^{\infty}</td>
</tr>
<tr>
<td>5. Minus cross entropy</td>
<td>$\bar{H} = \sum_{i=1}^{\infty} f(i) \log(\bar{f}(i))$</td>
</tr>
</tbody>
</table>
Table 5 are computed between the original and the ML estimation, the last two measures are computed between the discretized and the ML estimation.

7.1. Results

Fig. 16 plots the results obtained for the 10 distributions of the benchmark in term of their pmf’s. For each distribution of Table 4, Fig. 16 reports the discretized distribution \( f_d(\cdot) \) (in solid line) and the ML estimations \( \bar{f}(\cdot) \), computed for CF1 with two, four and eight phases, respectively. The discretization step is assumed \( \delta = 0.1 \) in all the plots.

A detailed description of the measures obtained for all the distributions in the benchmark is reported in Tables 6–10. In each table, the measures are reported for CF1 of order 2, 4 and 8, respectively, and for two discretization intervals, namely: \( \delta = 0.1 \) (as in Fig. 16 and \( \delta = 0.05 \)).

<table>
<thead>
<tr>
<th>Distribution</th>
<th>( e_1(F) )</th>
<th>Relative error ( \hat{e}_1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Two phases</td>
<td>( \delta = 0.1 )</td>
</tr>
<tr>
<td>W1</td>
<td>0.9027</td>
<td>0.0144</td>
</tr>
<tr>
<td>W2</td>
<td>2.0000</td>
<td>0.5148</td>
</tr>
<tr>
<td>L1</td>
<td>1.0000</td>
<td>0.2195</td>
</tr>
<tr>
<td>L2</td>
<td>1.0000</td>
<td>0.0918</td>
</tr>
<tr>
<td>L3</td>
<td>1.0000</td>
<td>0.01194</td>
</tr>
<tr>
<td>U1</td>
<td>0.5000</td>
<td>0.0904</td>
</tr>
<tr>
<td>U2</td>
<td>1.5000</td>
<td>0.01038</td>
</tr>
<tr>
<td>SE</td>
<td>1.5000</td>
<td>0.0114</td>
</tr>
<tr>
<td>ME</td>
<td>1.4945</td>
<td>0.0706</td>
</tr>
<tr>
<td>EX</td>
<td>1.0000</td>
<td>0.01181</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Distribution</th>
<th>( e_2(F) )</th>
<th>(( cv ))^2</th>
<th>Relative error ( \hat{e}_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Original distribution</td>
<td>Two phases</td>
<td>( \delta = 0.1 )</td>
</tr>
<tr>
<td>W1</td>
<td>0.3776</td>
<td>0.4610</td>
<td>0.1704</td>
</tr>
<tr>
<td>W2</td>
<td>20.000</td>
<td>5.0000</td>
<td>0.9161</td>
</tr>
<tr>
<td>L1</td>
<td>24.534</td>
<td>24.534</td>
<td>0.9282</td>
</tr>
<tr>
<td>L2</td>
<td>0.8964</td>
<td>0.8964</td>
<td>0.4661</td>
</tr>
<tr>
<td>L3</td>
<td>0.4048</td>
<td>0.4048</td>
<td>0.9922</td>
</tr>
<tr>
<td>U1</td>
<td>0.0833</td>
<td>0.3333</td>
<td>0.6109</td>
</tr>
<tr>
<td>U2</td>
<td>0.0833</td>
<td>0.0370</td>
<td>1.479</td>
</tr>
<tr>
<td>SE</td>
<td>1.2500</td>
<td>0.5555</td>
<td>0.0890</td>
</tr>
<tr>
<td>ME</td>
<td>0.9530</td>
<td>0.8653</td>
<td>0.3267</td>
</tr>
<tr>
<td>EX</td>
<td>1.0000</td>
<td>1.0000</td>
<td>0.0396</td>
</tr>
</tbody>
</table>
Fig. 16. Probability mass functions of the discretized and the approximating ADPH distributions.
### Table 8
Relative error in the third moment

<table>
<thead>
<tr>
<th>Distribution</th>
<th>$c_3(F)$</th>
<th>Relative error $\hat{c}_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Two phases</td>
<td>Four phases</td>
</tr>
<tr>
<td></td>
<td>$\delta = 0.1$</td>
<td>$\delta = 0.05$</td>
</tr>
<tr>
<td>W1</td>
<td>0.2468</td>
<td>0.7011</td>
</tr>
<tr>
<td>W2</td>
<td>592.00</td>
<td>0.9917</td>
</tr>
<tr>
<td>L1</td>
<td>16573</td>
<td>0.9995</td>
</tr>
<tr>
<td>L2</td>
<td>3.1315</td>
<td>0.0961</td>
</tr>
<tr>
<td>L3</td>
<td>0.0050</td>
<td>74.82</td>
</tr>
<tr>
<td>U1</td>
<td>0.0000</td>
<td>0.3949</td>
</tr>
<tr>
<td>U2</td>
<td>0.0000</td>
<td>8.5742</td>
</tr>
<tr>
<td>SE</td>
<td>2.0000</td>
<td>0.1740</td>
</tr>
<tr>
<td>ME</td>
<td>1.9929</td>
<td>0.4958</td>
</tr>
<tr>
<td>EX</td>
<td>2.0000</td>
<td>0.0490</td>
</tr>
</tbody>
</table>
For most of the cases the results of the discrete approximation are comparable with the results obtained from the continuous approximation [4]. However, for the cases where the distribution has a low coefficient of variation the DPH approximation shows a better fit, which is in line with the result on the minimal \(cv\) of the ADPH class, discussed in Section 4. As the relation between the order \(n\) and the discretization interval \(\delta\) fits the bounds established in Section 6, the ADPH approximation can attain lower coefficients of variations with respect to the CPHs of the same order. This can be seen for the test case L3, when \(n = 8\) and \(\delta = 0.1\).

In the benchmark, there are test cases whose discretized version is a DPH distribution. For example, the two uniform distributions (U1 and U2), using a discretization interval \(\delta = 0.1\), can be represented...
as, respectively
\[
\begin{align*}
    a_1 &= [0.1, 0.1, 0.1, 0.1, 0.1, 0.1, 0.1, 0.1], \\
    p_1 &= [1, 1, 1, 1, 1, 1, 1, 1],
\end{align*}
\]
and
\[
\begin{align*}
    a_2 &= [0.1, 0.1, 0.1, 0.1, 0.1, 0.1, 0.1, 0.1, 0.1, 0.0, 0.0, 0.0, 0.0, 0.0], \\
    p_2 &= [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1].
\end{align*}
\]
The proposed estimation algorithm is able to find exactly these forms. For example, with \( \delta = 0.1 \), \( n = 10 \) phases are needed to represent exactly the discretized version of U1; however, it is interesting to observe by a visual inspection of Fig. 16 how the approximating ADPH improves the fit passing from \( n = 2 \) to \( n = 8 \).

7.2. Empirical guidelines of ADPH fitting

In this section, we try to draw a general conclusion about the applicability of ADPH distribution fitting based on our fitting experience.

The following specific properties of the class of ADPH distributions limit their applicability in distribution fitting:

- bounded moments;
- limited number of waves of the pmf;
- sharp changes of the pmf is not possible at high (\( \gg n \)) time instances (where \( n \) is the order of the ADPH distribution);
- exponentially decaying tail distribution.

The bounds of the first two moments of ADPH distributions are already mentioned above (\( m \geq 1 \), and Theorem 2). These bounds already indicate that the ADPH class cannot exhibit all the possible sets of moments that can be obtained by positive distributions. Similar bounds hold for higher moments as well. This means that the moments of the distribution to be fitted should be realizable by ADPH distributions of the given order.

The number of waves exhibited by the pmf of an ADPH distribution of order \( n \) is not greater than \( n/2 \). The sharpest possible change of the pmf of an ADPH of order \( n \) at time \( k (k \gg n) \) is obtained by the discrete Erlang(\( n \)) distribution. Hence distributions with sharp changes at time \( k \gg n \) is not possible to approximate closely. For example, the jumps of the discrete uniform distribution between \( a \) and \( b \), with \( a < n \) and \( b \gg n \), cannot be equally well captured. It is possible to capture the sharp jump at time \( a \), but the best ADPH fitting of the jump at \( b \) is distributed in a wide range.

With respect to the tail behavior, it is possible to approximate both heavier or lighter tail behavior than exponential decay to some upper limit, but after a limit all ADPH distributions have an exponentially decaying tail behavior.

As a conclusion, based on our experiences and the above considerations, we would predict a “close” ADPH fit when the distribution to be fitted has moments achievable with ADPH of order \( n \), has less than \( n/2 \) waves, has a smoothly changing pmf especially after time \( n \), and has an approximately exponentially decaying tail behavior.
8. Conclusion

Some previously not considered properties of the DPH distributions, which are essential for DPH fitting, are investigated and compared with the known properties of the CPH distributions. Similarly to the continuous family, acyclic-DPH distributions admit a minimal representation called canonical form. resorting to the canonical form, we have investigated the dependence of the minimal squared coefficient of variation on the mean and on the order, and we have established the conditions for which the minimal coefficient of variation for the DPH family is less than the one for the CPH family of the same order.

The results about the wider variability of the DPH class can be very relevant in stochastic modeling. When PH distributions are used in modeling, the number of states in the model depends multiplicatively on the number of phases. Keeping the order as low as possible increases the capability of the approach.

Furthermore, since the deterministic distribution is a member of the ADPH class, the use of DPH distributions offers a viable technique to handle random execution times and constant durations inside the same formalism.

A DPH fitting method is presented for the first time. Similar to the continuous case we used an ML estimation procedure for the evaluation of the parameters of an ADPH distribution in canonical form CF1. While previous estimation algorithms for the CPH family were based on a transform domain analysis, we have shown that the time domain analysis is also possible, and the estimation algorithm based on time domain expressions is easier to implement, numerically simpler and more stable.

The goodness of fit of this new algorithm has been tested with respect to a benchmark composed of 10 different continuous distributions. However, in order to apply the proposed procedure to a continuous distribution, the continuous function must be discretized according to a given discretization interval. The role of the discretization interval has been discussed, and the way to chose a suitable discretization interval as a function of the mean and of the coefficient of variation has been indicated.

As it could have been expected from the properties of the ADPH family, the fitting algorithm performs better than the CPH one in the cases in which the coefficient of variation is low, and in the cases of distributions with finite support (like the uniform).

Acknowledgements

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References

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M. Telek received the M.Sc. degree in electrical engineering from the Technical University of Budapest in 1987. After graduation he joined the Hungarian Post Research Institute where he studied the modelling, analysis and planning aspects of communication networks. Since 1990 he has been with the Department of Telecommunications of the Technical University of Budapest, where he is an Associate Professor now. He received the candidate of science degree from the Hungarian Academy of Science in 1995. His current research interest includes stochastic performance modeling and analysis of computer and communication systems.