Moments characterization of order 3 matrix exponential distributions*

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Abstract. The class of order 3 phase type distributions (PH(3)) is known to be a proper subset of the class of order 3 matrix exponential distributions (ME(3)). In this paper we investigate the relation of these two sets for what concerns their moment bounds.

To this end we developed a procedure to check if a matrix exponential function of order 3 defines a ME(3) distribution or not. This procedure is based on the time domain analysis of the density function. The proposed procedure requires the numerical solution of a transcendent equation in some cases.

The presented moment bounds are based on some unproved conjectures which are verified only by numerical investigations.

Keywords: Matrix exponential distributions, Phase type distributions, moment bounds.

1 Introduction

The availability of efficient matrix analytic methods (see e.g., [7, 10]) reinforced the research of distributions with matrix exponential representation. The order of these distributions is defined as the (minimal) cardinality of the matrix that describes the distribution. The two main classes of these distributions are the class of phase type distributions [8, 9], which has a nice stochastic interpretation due to its underlying continuous time Markov chain, and the class of matrix exponential distributions [1], which does not allow for a simple stochastic interpretation.

It has been known for a long time that considering distributions of order 2 the two classes are identical, ME(2)≡PH(2), but for $n > 2$ PH(n) is a proper subset of ME(n) [12]. Unfortunately there are no tools to investigate the relation of the ME(n) and the PH(n) classes for $n > 2$. However, recent results on ME(3) [5] and PH(3) [6] distributions make it possible to investigate the relation of the ME(3) and the PH(3) classes.

The practical importance of low order PH and ME distributions comes from the fact that the complexity of the matrix analytic analysis increases rapidly

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with the order of the model components (e.g., PH distribution of the service time). Recent results suggest that matrix analytic methods are applicable for models with matrix exponential distributions as well as for models with phase type distributions [2]. Consequently, one can gain if the durations to be modelled can be described by a ME distribution with lower order than the application of a PH distributions would require.

We compare the flexibility of the ME(3) and the PH(3) classes through their moment bounds. It is not the only and not necessarily the easiest way to compare them, but this choice is motivated by the fact that moments and related measures (e.g., coefficient of variation) are the most frequently used parameters of distributions.

This paper is strongly related to the extensive work of Mark Fackrell in [5]. We reconsider some questions of [5] and complement those results with alternative ones. The main goal of this paper is to answer the following question ([5] p. 110) "The class of PH distributions is a proper subset of the class of ME distributions, but how much larger is the latter class than the former?". In [5] the question is answered for ME(n) and $\cup_{m \geq n}$ PH(m). We believe that this question has more practical importance for ME(n) and PH(n). In this work we try to answer this question for ME(3) and PH(3).

Related ME(3) results: [5] devotes its main attention to the matrix exponential distributions of order $n > 2$ and provides important necessary conditions for being a member of ME(n). Additionally, [5] provides necessary and sufficient conditions for being a member of ME(3). These conditions are given in the Laplace transform domain. Assuming that for a given triple $\{b_1, b_2, b_3\}$ the Laplace transform of a matrix exponential function takes the form

$$\frac{x_2 s^2 + x_1 s + b_1}{s^3 + b_3 s^2 + b_2 s + b_1}$$

(i.e., there is no probability mass at 0) the linear and parametric curves provided in [5] bound the region of $\{x_1, x_2\}$ where the matrix exponential function is a member of the ME(3) class.

Unfortunately, we did not find an easy implementation of these transform domain constraints, and this is why we developed a time domain counterpart for ME(3) characterization.

An important property of the ME(3) class, namely its minimal coefficient of variation, is studied in [4]. The results provided here verify the ones provided there.

Related PH(3) results: Another important preliminary work is [6] which provides a canonical representation of PH(3) distributions. More precisely, [6] presents an algorithm that transforms any order 3 matrix exponential function to PH(3) canonical form if it is possible. In this paper, this algorithm is used to characterize the borders of the PH(3) class.

The rest of the paper is organized as follows. Section 2 defines the class of matrix exponential distributions and the basic notations. Section 3 presents a procedure to check if a matrix exponential function of order 3 is a member of

the ME(3) class or not. Using this procedure and its counterpart for the PH(3) class from [6], Section 4 investigates the relation of the moment bounds of these two classes. The paper is concluded in Section 5.

2   Matrix exponential distributions

Definition 1. *The vector matrix pair $(\underline{v}, \boldsymbol{H})$ defines a matrix exponential distribution iff*

$$F(t) = Pr(X < t) = 1 - \underline{v}e^{\boldsymbol{H}t}\mathbb{1} , \qquad t \geq 0 \tag{1}$$

is a valid cumulative distribution function, i.e., $F(0) \geq 0$, $\lim_{t \to \infty} F(t) = 1$ and $F(t)$ is monotone increasing.

In (1), the row vector, $\underline{v}$, is referred to as the initial vector, the square matrix, $\boldsymbol{H}$, as the generator and $\mathbb{1}$ as the closing vector. Without loss of generality (see [8]), throughout this paper we assume that the closing vector is a column vector of ones, i.e., $\mathbb{1} = [1, 1, \ldots, 1]^T$.

The density, the Laplace transform and the moments of the matrix exponential distribution defined by $(\underline{v}, \boldsymbol{H})$ are

$$f(t) = \underline{v}e^{\boldsymbol{H}t}(-\boldsymbol{H})\mathbb{1} , \tag{2}$$

$$f^*(s) = E(e^{-sX}) = \underline{v}(s\boldsymbol{I} - \boldsymbol{H})^{-1}(-\boldsymbol{H})\mathbb{1} , \tag{3}$$

$$\mu_n = E(X^n) = n!\underline{v}(-\boldsymbol{H})^{-n}\mathbb{1} . \tag{4}$$

To ensure that $\lim_{t \to \infty} F(t) = 1$, $\boldsymbol{H}$ has to fulfill the necessary condition that the real parts of its eigenvalues are negative (consequently $\boldsymbol{H}$ is non-singular).

The remaining constraint is the monotonicity of $F(t)$. It is the most difficult property to check. Instead of checking if $F(t)$ is monotone increasing, in the next section, we check if $f(t)$ is non-negative.

3   Matrix exponential distributions of order 3

We subdivide the class of ME(3) distributions according to the eigenvalue structure of $\boldsymbol{H}$. With $\lambda_1, \lambda_2, \lambda_3$ denoting the eigenvalues of the matrix $-\boldsymbol{H}$, we have the following possible cases:

- class A: $\lambda_1, \lambda_2, \lambda_3 \in \mathbb{R}^+$, $\lambda_1 < \lambda_2 < \lambda_3$
- class B: $\lambda_1, \lambda_2, \lambda_3 \in \mathbb{R}^+$, $\lambda_1 = \lambda_2 < \lambda_3$ or $\lambda_1 < \lambda_2 = \lambda_3$
- class C: $\lambda_1 = \lambda_2 = \lambda_3 \in \mathbb{R}^+$,
- class D: $\lambda_1 \in \mathbb{R}^+$, $\lambda_2 = \bar{\lambda}_3 \in \mathbb{C}^+$,

where $\mathbb{R}^+$ denotes the set of strictly positive real numbers and $\mathbb{C}^+$ the set of complex numbers with strictly positive real part. The following subsections consider these four cases.

3.1 Case A: 3 different real eigenvalues

In this case the general form of the density function and its derivative are

$$f(t) = a_1 e^{-\lambda_1 t} + a_2 e^{-\lambda_2 t} + a_3 e^{-\lambda_3 t} \tag{5}$$
$$f'(t) = -a_1 \lambda_1 e^{-\lambda_1 t} - a_2 \lambda_2 e^{-\lambda_2 t} - a_3 \lambda_3 e^{-\lambda_3 t} \tag{6}$$

Without loss of generality, we check the non-negativity of $f(t)$ assuming that $\lambda_1 < \lambda_2 < \lambda_3$.

Theorem 1. *$f(t)$ is non-negative for $t \geq 0$ iff*

- $a_1 + a_2 + a_3 \geq 0$ *and*
- $a_1 > 0$ *and*
- *if* $a_2 < -a_1 \dfrac{\lambda_3 - \lambda_1}{\lambda_3 - \lambda_2}$ *then* $a_3 \geq a_1 \dfrac{\lambda_2 - \lambda_1}{\lambda_3 - \lambda_2} \left(-\dfrac{a_2}{a_1} \dfrac{\lambda_3 - \lambda_2}{\lambda_3 - \lambda_1} \right)^{\frac{\lambda_3 - \lambda_1}{\lambda_2 - \lambda_1}}$.

Proof. First, we note that $f(t)$ is a monotone increasing function of a_1, a_2 and a_3 for $t \geq 0$ and both $f(t)$ and $f'(t)$ can have at most 2 roots in $(0, \infty)$ (excluding 0 and infinity).

The non-negativity of $f(t)$ at $t = 0$ results in the first condition and the non-negativity of $f(t)$ at $t \to \infty$ results in the second condition of the theorem.

In the rest we suppose that $a_1 > 0$ and $a_1 + a_2 + a_3 \geq 0$. We investigate the non-negativity of $f(t)$ by constructing $f^*(t) = a_1 e^{-\lambda_1 t} + a_2 e^{-\lambda_2 t} + a_3^* e^{-\lambda_3 t}$ such that a_3^* takes the minimal a_3 value with which $f(t)$ is still non-negative, i.e., we will have $f^*(c) = 0$ for some $c \geq 0$.

We have the following two cases:

a) $f^*(c)$ touches the x-axes at $c > 0$, that is, $f^*(c) = 0$ and $f'^*(c) = 0$,
b) $f^*(0) = 0$ and $f'^*(0) \geq 0$.

In case a) we have

$$f^*(c) = a_1 e^{-\lambda_1 c} + a_2 e^{-\lambda_2 c} + a_3^* e^{-\lambda_3 c} = 0, \tag{7}$$
$$f'^*(c) = -a_1 \lambda_1 e^{-\lambda_1 c} - a_2 \lambda_2 e^{-\lambda_2 c} - a_3^* \lambda_3 e^{-\lambda_3 c} = 0, \tag{8}$$

from which

$$\frac{a_2}{a_1} = -\frac{\lambda_3 - \lambda_1}{\lambda_3 - \lambda_2} \, e^{(\lambda_2 - \lambda_1)c}, \tag{9}$$

$$\frac{a_3^*}{a_1} = \frac{\lambda_2 - \lambda_1}{\lambda_3 - \lambda_2} \, e^{(\lambda_3 - \lambda_1)c}. \tag{10}$$

If $a_2 \geq -a_1 \dfrac{\lambda_3 - \lambda_1}{\lambda_3 - \lambda_2}$ then there is no $c > 0$ that satisfies (9), since the left hand side of (9) is negative and less than $-\dfrac{\lambda_3 - \lambda_1}{\lambda_3 - \lambda_2}$. Consequently, case a) is not possible when $a_2 \geq -a_1 \dfrac{\lambda_3 - \lambda_1}{\lambda_3 - \lambda_2}$.

If $a_2 < -a_1 \dfrac{\lambda_3 - \lambda_1}{\lambda_3 - \lambda_2}$ then c is obtained from (9) as

$$c = \frac{\log\left(-\dfrac{a_2}{a_1}\dfrac{\lambda_3 - \lambda_2}{\lambda_3 - \lambda_1}\right)}{\lambda_2 - \lambda_1},$$

and substituting it to (10) gives

$$a_3^* = a_1 \frac{\lambda_2 - \lambda_1}{\lambda_3 - \lambda_2}\left(-\frac{a_2}{a_1}\frac{\lambda_3 - \lambda_2}{\lambda_3 - \lambda_1}\right)^{\frac{\lambda_3 - \lambda_1}{\lambda_2 - \lambda_1}}.$$

In case b) we have

$$f^*(0) = a_1 + a_2 + a_3^* = 0, \tag{11}$$
$$f'^*(0) = -a_1\lambda_1 - a_2\lambda_2 - a_3^*\lambda_3 \geq 0. \tag{12}$$

Substituting $a_3^* = -a_1 - a_2$ from (11) into (12) we have that (12) holds when $a_2 \geq -a_1 \dfrac{\lambda_3 - \lambda_1}{\lambda_3 - \lambda_2}$. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

3.2 Case B: 2 different real eigenvalues

In this case we have two options.

– The multiplicity of the dominant eigenvalue, λ_1, $(\lambda_1 < \lambda_2)$ is one and hence the general form of the density function is

$$f_1(t) = a_1\,e^{-\lambda_1 t} + (a_2 + a_{21}t)\,e^{-\lambda_2 t}. \tag{13}$$

– The multiplicity of the dominant eigenvalue , λ_1, $(\lambda_1 < \lambda_2)$ is two and hence the general form of the density function is

$$f_2(t) = (a_1 + a_{11}t)\,e^{-\lambda_1 t} + a_2\,e^{-\lambda_2 t}. \tag{14}$$

Theorem 2. *$f_1(t)$ is non-negative for $t \geq 0$ iff*

– *$a_1 + a_2 > 0$ and*
– *$a_1 \geq 0$ and*
– *$a_{21} \geq a_{21}^*$*

where a_{21}^* is that solution of

$$a_{21}\,e^{a_2\lambda_2/a_{21}} + a_1(\lambda_2 - \lambda_1)\,e^{1+a_2\lambda_1/a_{21}} = 0 \tag{15}$$

which satisfies $a_{21}(1 - (\lambda_2 - \lambda_1)) > a_2(\lambda_2 - \lambda_1)$.

Proof. $f_1(t)$ is a monotone increasing function of a_1, a_2 and a_{21} for $t \geq 0$ and both $f_1(t)$ and $f_1'(t)$ can have at most 2 roots in $(0, \infty)$ (excluding 0 and infinity).

The non-negativity of $f_1(t)$ at $t = 0$ results in the first condition and the non-negativity of $f_1(t)$ at $t \to \infty$ results in the second condition. The minimal a_{21} value for which $f_1(t)$ is non-negative is obtained assuming that $f_1(t)$ touches the x axes at $t = c > 0$, i.e., $f_1(c) = 0$ and $f_1'(c) = 0$. Solving this set of equations for a_{21} and c, we have

$$c = \frac{a_{21} - a_2(\lambda_2 - \lambda_1)}{a_{21}(\lambda_2 - \lambda_1)},$$

and (15) and the $a_{21}(1 - (\lambda_2 - \lambda_1)) > a_2(\lambda_2 - \lambda_1)$ condition is equivalent with $c > 0$. $\qquad\square$

Theorem 3. *$f_2(t)$ is non-negative for $t \geq 0$ iff*

- $a_1 + a_2 > 0$ *and*
- $a_{11} \geq 0$ *and*
- $a_{11} \geq a_{11}^*$

where a_{11}^* is that solution of

$$a_2\, e^{\lambda_2\left(\frac{a_1}{a_{11}} - \frac{1}{\lambda_2 - \lambda_1}\right)} - a_{11}(\lambda_2 - \lambda_1)\, e^{\lambda_1\left(\frac{a_1}{a_{11}} - \frac{1}{\lambda_2 - \lambda_1}\right)} = 0 \qquad (16)$$

which satisfies $-a_1(\lambda_2 - \lambda_1) > a_{11}(1 + \lambda_2 - \lambda_1)$.

Proof. The proof follows the same pattern as the one for $f_1(t)$. $\qquad\square$

It has to be noted that the third condition of Theorem 2 and 3 are transcendent, and consequently, numerical methods are required to compute them.

3.3 Case C: 1 real eigenvalue

In this case the general form of the density function is

$$f(t) = (a_0 + a_1 t + a_2 t^2)\, e^{-\lambda t} \qquad (17)$$

$$(18)$$

Theorem 4. *$f(t)$ is non-negative for $t \geq 0$ iff*

- $a_0 > 0$ *and*
- $a_2 > 0$ *and*
- $a_1 \geq -2\sqrt{a_0 a_2}$.

Proof. $f(t)$ is a monotone increasing function of a_0, a_1 and a_2 for $t \geq 0$ and both $f(t)$ and $f'(t)$ can have at most 2 roots in $(0, \infty)$ (excluding 0 and infinity).

The non-negativity of $f(t)$ at $t = 0$ results in the first condition and the non-negativity of $f(t)$ at $t \to \infty$ results in the second condition.

Supposing that $a_0 > 0$ and $a_2 > 0$ we have the following two cases:

- if $a_1 \geq 0$ then $a_0 + a_1 t + a_2 t^2$ is monotone increasing on $(0, \infty)$,
- if $a_1 < 0$ then $a_0 + a_1 t + a_2 t^2$ has a minimum at $t = -\frac{a_1}{2a_2}$ which is $a_0 - \frac{a_1^2}{4a_2}$.

From which the third condition comes. $\qquad\square$

3.4 Case D: one real and a pair of complex eigenvalues

In this case the general form of the density function is

$$f(t) = a_1\, e^{-\lambda_1 t} + a_2 \cos(\omega t + \phi)\, e^{-\lambda_c t} \tag{19}$$

where, for uniqueness, a_2 and ϕ are defined such that $a_2 > 0$ and $-\pi < \phi \le \pi$.

Theorem 5. *$f(t)$ is non-negative for $t \ge 0$ iff*

- $a_1 + a_2 \cos(\phi) > 0$ *and*
- $a_1 > 0$ *and*
- $\lambda_1 \le \lambda_c$ *and*
- $a_2 < a_1 e^{(\lambda_c - \lambda_1)\frac{2\pi}{\omega}}$ *and*
- *if $a_1 < a_2$ ($< a_1 e^{(\lambda_c - \lambda_1)\frac{2\pi}{\omega}}$) then $f(\check{t}) \ge 0$ and $f(\hat{t}) \ge 0$ and*
- *if $a_1 < a_2$ ($< a_1 e^{(\lambda_c - \lambda_1)\frac{2\pi}{\omega}}$) and $f'(t)$ has roots in $[\check{t}, \hat{t}]$ then $f(t) \ge 0$ at those roots,*

where $\check{t} = \max\left(0, \frac{\pi - 2\phi}{2\omega}\right)$ and $\hat{t} = \min\left(\frac{1}{\lambda_c - \lambda_1} \log\left(\frac{a_2}{a_1}\right), \frac{\pi - \phi}{\omega}\right)$.

Proof. The non-negativity of $f(t)$ at $t = 0$ results in the first condition and the non-negativity of $f(t)$ at $t \to \infty$ results in the second and the third conditions. The sign of $f(t)$ is determined by two main factors:

- the relation of the two exponential functions $a_1\, e^{-\lambda_1 t}$ and $a_2\, e^{-\lambda_c t}$,
- the value of the cyclic term $\cos(\omega t + \phi)$.

Supposing that the first 3 conditions hold, $f(t)$ has the following properties:

- $f(t)$ is a monotone increasing function of a_1 for $t \ge 0$.
- Both $f(t)$ and $f'(t)$ might have infinitely many roots in $(0, \infty)$ (excluding 0 and infinity).
- If $a_1 > a_2$ then $a_1\, e^{-\lambda_1 t} > a_2\, e^{-\lambda_c t}$ for $\forall t > 0$, and consequently $f(t) > 0$ for $\forall t > 0$. If $a_1 < a_2$ and $\lambda_1 < \lambda_c$ then $a_1\, e^{-\lambda_1 t} > a_2\, e^{-\lambda_c t}$ for $\forall t > t_r = \frac{1}{\lambda_c - \lambda_1} \log(\frac{a_2}{a_1})$, and consequently $f(t) > 0$ for $\forall t > t_r$, since t_r is the solution of $a_1\, e^{-\lambda_1 t_r} > a_2\, e^{-\lambda_c t_r}$ and the quicker decay of $e^{-\lambda_c t}$ ensures the last statement.
- If at the end of the first period of $\cos(\omega t + \phi)$, i.e., at $t_p = \frac{2\pi}{\omega}$ we have $a_1\, e^{-\lambda_1 t_p} < a_2\, e^{-\lambda_c t_p}$, then for $t = \frac{\pi - \phi}{\omega} < t_p$ we have

$$f(\tfrac{\pi - \phi}{\omega}) = a_1\, e^{-\lambda_1 \frac{\pi - \phi}{\omega}} + a_2 \cos(\omega \tfrac{\pi - \phi}{\omega} + \phi)\, e^{-\lambda_c \frac{\pi - \phi}{\omega}}$$

$$= a_1\, e^{-\lambda_1 \frac{\pi - \phi}{\omega}} - a_2\, e^{-\lambda_c \frac{\pi - \phi}{\omega}} < a_1\, e^{-\lambda_1 t_p} - a_2\, e^{-\lambda_c t_p} < 0 \ .$$

- If $f(t) > 0$ for $\forall t > 0$ for a given a_2 then $\tilde{f}(t) = a_1\, e^{-\lambda_1 t} + \tilde{a}_2 \cos(\omega t + \phi)\, e^{-\lambda_c t} > 0$ for $\forall t > 0$ and $\forall \tilde{a}_2 \in [0, a_2]$.
- If $f(t) \ge 0$ for $\forall t \in [0, t_p]$ then $f(t) \ge 0$ for $\forall t > 0$, because the non-negativity of $f(t)$ for $[t_p, \infty)$ is equivalent with the non-negativity of $a_1\, e^{-\lambda_1 t} + \tilde{a}_2\, \cos(\omega t + \phi)\, e^{-\lambda_c t}$, where $\tilde{a}_2 = a_2\, e^{-(\lambda_c - \lambda_1)t_p} \le a_2$.

According to these properties, if $\lambda_1 < \lambda_c$,

- $a_2 \leq a_1$ implies that $f(t)$ is non-negative.
- $a_2 > a_1 e^{(\lambda_c - \lambda_1)\frac{2\pi}{\omega}}$ or equivalently $t_r > t_p$ implies that $f(t)$ is not non-negative,
- if $a_1 < a_2 \leq a_1 e^{(\lambda_c - \lambda_1)\frac{2\pi}{\omega}}$ then $f(t)$ can become negative depending on the initial phase of the cosine term. $f(t)$ can become negative only when the cosine term is negative, e.g., $t \in (\frac{\pi - 2\phi}{2\omega}, \frac{3\pi - 2\phi}{2\omega})$, but due to the faster decay of the $e^{-\lambda_c t}$ term it is enough to study the first interval, where the cosine term takes the values from 0 to -1, i.e., $(\frac{\pi - 2\phi}{2\omega}, \frac{\pi - \phi}{\omega})$. Depending on the initial phase, ϕ, $\frac{\pi - 2\phi}{2\omega}$ can be less than 0 and $\frac{\pi - \phi}{\omega}$ can be greater than t_r. Considering these additional constraints $\check{t}$ and $\hat{t}$ defines the borders of the decisive interval. If $f(t)$ is non-negative on $[\check{t}, \hat{t}]$ it is non-negative for $\forall t > 0$. $f'(\check{t}) < 0$ because both $e^{-\lambda_1 t}$ and $\cos(\omega t + \phi)\,e^{-\lambda_c t}$ decay at $t = \check{t}$.
  If $f'(\hat{t})$ is non-positive, $f'(t)$ has 0, 1, or 2 roots in $[\check{t}, \hat{t}]$, and the sign of $f(t)$ at these roots decides the non-negativity of $f(t)$.
  If $f'(\hat{t})$ is positive, $f(t)$ has a single minimum in $[\check{t}, \hat{t}]$, and the sign of this minimum decides the non-negativity of $f(t)$. $\qquad\square$

4 Moments bounds of the ME(3) class

The previous section provides results to check the ME(3) membership of order 3 matrix exponential functions. We implemented those checks in a Mathematica function. Using this implementation, in this section, we numerically investigate the flexibility of the ME(3) class compared to the limits of the PH(3) class, for which similar results are provided in [6] to check PH(3) membership.

A continuous ME(3) or PH(3) distribution is uniquely characterized by its first 5 moments. For a given set of $\{\mu_1, \ldots, \mu_5\}$ moments we check the ME(3) and PH(3) membership with a two step procedure.

- The first step is to compute a vector and matrix pair of order 3, $(\underline{v}, \boldsymbol{H})$, for which $i!\underline{v}(-\boldsymbol{H})^{-i}\mathbb{I} = \mu_i, i = 1, \ldots, 5$. The procedure of Appie van de Liefvoort in [12] provides such $(\underline{v}, \boldsymbol{H})$ pair with a proper transformation of the closing vector[3].
- Starting from $(\underline{v}, \boldsymbol{H})$, if the PH(3) transformation procedure in [6] generates a valid canonical representation then $\{\mu_1, \ldots \mu_5\}$ represents a member of the PH(3) set. Similarly, if the matrix exponential function, $\underline{v}e^{\boldsymbol{H}t}(-\boldsymbol{H})\mathbb{I}$, is non-negative according to the checks of the previous section then $\{\mu_1, \ldots \mu_5\}$ represents a member of the ME(3) set.

As in previous works, to reduce the number of parameters we introduce the normalized moments, $n_i = \frac{\mu_i}{\mu_{i-1}\mu_1}$, which eliminate a scaling factor and represent the shape of ME(3) and PH(3) distributions with 4 parameters, $\{n_2, n_3, n_4, n_5\}$.

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[3] In [12] the initial and the closing vectors are $\{1, 0, 0, \ldots, 0\}$. In our case the closing vector is $\{1, 1, \ldots, 1\}$, hence a similarity transformation is required as described in [11].

The subsequent numerical results are divided into investigations of the n_2, n_3 domain with arbitrary n_4, n_5 and investigations of the n_4, n_5 domain with given n_2, n_3.

4.1 The second and third normalized moments

The n_2, n_3 normalized moment bounds of the PH(3) class are not completely known yet. There is a proved result for the valid range of the APH(3) class [3], and there is a numerically checked conjecture that the related borders of the PH(3) class coincide with the ones of the APH(3) class [6]. Here we compare the borders of the ME(3) class with these borders of the PH(3) class.

To check if an n_2, n_3 pair is inside the range of the ME(3) class is rather difficult. We have tools to check if $\{n_2, n_3, n_4, n_5\}$ defines an ME(3) distribution. Based on this tool, for a given n_2, n_3 pair a natural procedure would be to check the ME(3) membership of $\{n_2, n_3, x, y\}$, where x and y run through the positive quarter plain. Unfortunately, this procedure is infeasible, because it is practically impossible to find valid n_4, n_5 pairs with exhaustive search.

To get around this problem we applied special ME(3) subclasses whose structure is defined by 2 shape parameters and a scaling factor. Having these subclasses we set the 2 shape parameters to match n_2, n_3 and checked if we obtained a valid distribution.

The Exp-Erlang and the Erlang-Exp distributions in [3] form such subsets, which we used for n_2, n_3 pairs inside the range of the PH(3) class.

For n_2, n_3 pairs outside the range of the PH(3) class we used the following function with complex roots ($a_1 = a_2 = a$, $\lambda_1 = \lambda_2 = \lambda$ in (19))

$$f(t) = a \ e^{-\lambda t}(1 + \cos(\omega t + \phi)) \tag{20}$$

where a is a normalizing constant ($\int_t e^{-\lambda t}(1 + \cos(\omega t + \phi))dt = 1/a$), λ is the scaling factor and ω and ϕ are the two shape parameters. When $\lambda = 1$

$$n_2 = \frac{2\left(\sqrt{1+\omega^2} + \cos(\phi + \arctan(\omega))\right)\left(\left(1+\omega^2\right)^{\frac{3}{2}} + \cos(\phi + 3\ \arctan(\omega))\right)}{\left(1+\omega^2 + \cos(\phi + 2\ \arctan(\omega))\right)^2},$$

$$n_3 = \frac{3\left(\sqrt{1+\omega^2} + \cos(\phi + \arctan(\omega))\right)\left(\left(1+\omega^2\right)^2 + \cos(\phi + 4\ \arctan(\omega))\right)}{\left(1+\omega^2 + \cos(\phi + 2\ \arctan(\omega))\right)\left(\left(1+\omega^2\right)^{\frac{3}{2}} + \cos(\phi + 3\ \arctan(\omega))\right)}.$$

For a given n_2, n_3 pair solving this equation for the ϕ, ω pair gives a matrix exponential function whose second and third normalized moments are n_2 and n_3. The non-negativity of this function can be checked by Theorem 5.

Figure 1 depicts the borders of the ME(3) class (obtained for subclass (20)) and the borders of the PH(3) class (inner borders of the figure) on the n_2, n_3 plain. Our numerical investigations suggest that the outer borders in Figure 1 are the borders of the whole ME(3) class, but we cannot prove it. The left most point of these borders, $n_2 = 1.200902$ gives the ME(3) distribution with

minimal n_2 or, equivalently, with minimal coefficient of variation, and this point corresponds to the minimal coefficient of variation of the ME(3) class reported in [4]. The PH(3) class, and consequently the ME(3) class, are known to be only lower bounded when $n_2 > 1.5$. That is why the upper bound curves end at $n_2 = 1.5$.

The results of Section 3 indicate already that the borders of the ME(3) class do not exhibit nice closed form expressions, but numerical methods are required for their evaluation. We used the standard floating point precision of Mathematica to compute the presented results, but these computations are numerically sensitive.
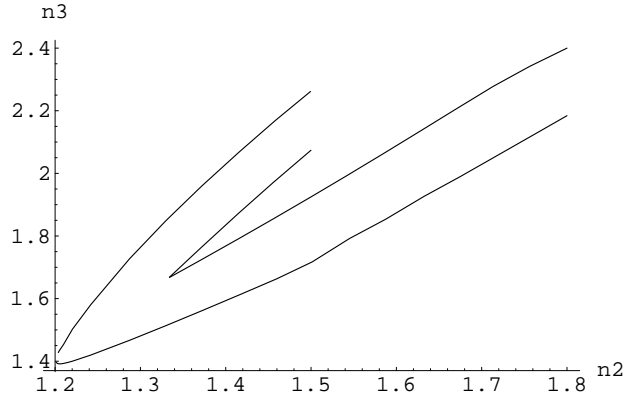
Fig. 1. The range of second and third normalized moments of the PH(3) and ME(3) classes

4.2 The fourth and fifth normalized moments

In this section we study the region of realizable fourth and fifth normalized moments (n_4 and n_5) for a given pair of second and third normalized moments (n_2 and n_3). In order to find this region we make use of the subclasses presented in Section 4.1. We use Erlang-Exp distributions [3] inside the PH(3) borders of Figure 1 and the subclass defined by (20) between the PH(3) and the ME(3) borders. First we generate a matrix exponential function from the given ME(3) subclass that realizes the pair (n_2, n_3). Then we calculate n_4 and n_5 for this matrix exponential function and use them as starting point in exploring the realizable region of n_4 and n_5. Since the realizable region of the PH(3) class is a subregion of the realizable region of the ME(3) class, it is easier to start from a PH(3) point if possible.

We start by considering cases for which $n_2 = 1.45$. Based on the results presented in Section 4.1, with this value of n_2 the interval of realizable third normalized moments is $(1.6517, 2.1498)$ with ME(3) while it is $(1.8457, 1.9573)$

with PH(3). First we look at the middle point of the n_3 interval that can be realized with a PH(3), i.e., $n_3 = 1.9015$. Figure 2 depicts the realizable region of n_4 and n_5 for both PH(3) and ME(3). In all the figures we have n_4 on the x-axes and n_5 on the y-axes. Further, the lighter gray region contains the points that are realized with a ME(3) or PH(3) with one real and a pair of complex eigenvalues (class D) while the darker gray area contains points where the ME(3) or PH(3) is realized with three real eigenvalues. It is clear from Figure 2 that the ME(3) gives much higher flexibility than the PH(3) does. In Figure 3 we concentrate on the lower peak of the regions depicted in Figure 2. ME(3) is somewhat more flexible in this subregion as well and one can observe that the flexibility is increased both for what concerns the distribution with one real and two complex eigenvalues and for what concerns the distributions with three real eigenvalues.
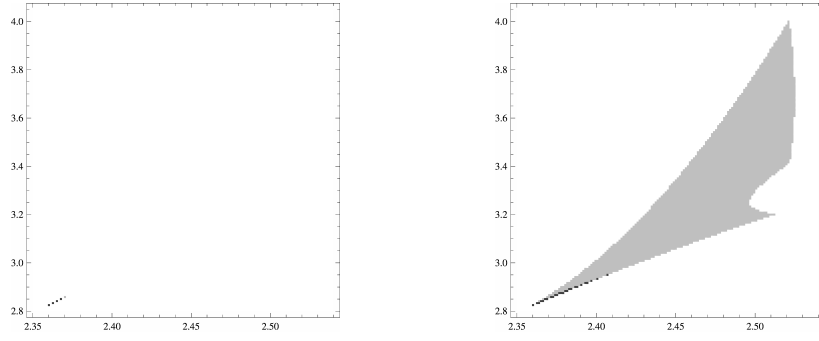
Fig. 2. Realizable n_4, n_5 normalized moments with PH(3) (on the left) and ME(3) (on the right) in case of $n_2 = 1.45$ and $n_3 = 1.9015$
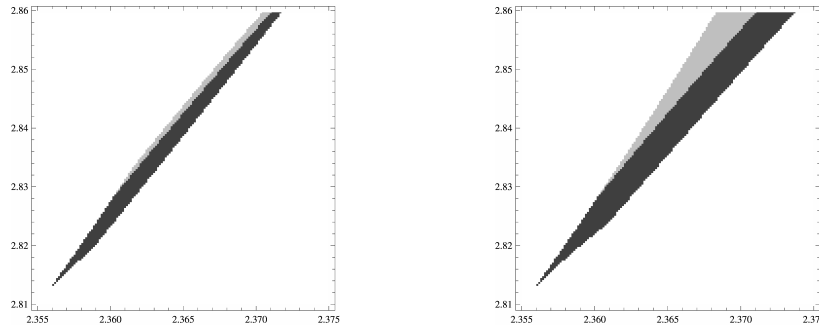
Fig. 3. Lower peak of the realizable n_4, n_5 region with PH(3) (on the left) and ME(3) (on the right) in case of $n_2 = 1.45$ and $n_3 = 1.9015$

Now we turn our attention to such n_3 values that cannot be realized by a PH(3) with $n_2 = 1.45$. In particular, Figure 4 depicts the realizable n_4, n_5 regions for $n_2 = 1.45, n_3 = 1.725$ and $n_2 = 1.45, n_3 = 2.1$ which lie respectively beneath and above the n_3 interval that can be realized with PH(3). By comparison with Figure 2 it is clear that approaching the possible minimum and maximum values of n_3 the realizable n_4, n_5 region not only changes its shape but it is shrinking as well. To illustrate further this shrinking, Figure 5 depicts the realizable n_4, n_5 region for $n_2 = 1.45, n_3 = 2.1249$ and $n_2 = 1.45, n_3 = 2.1373$ where the realizable region gets narrower and shorter.
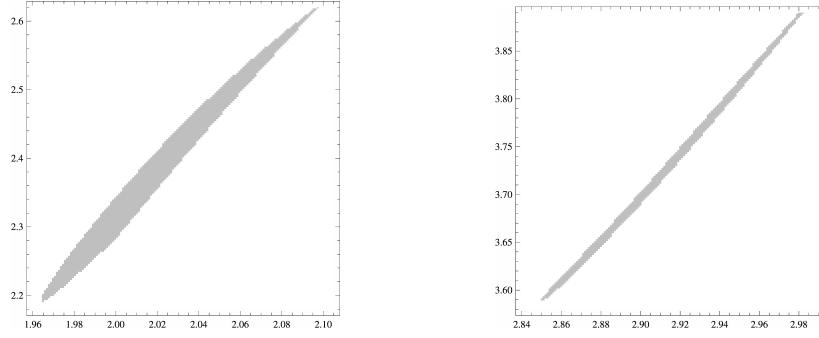
Fig. 4. Realizable n_4, n_5 normalized moments with ME(3) for $n_2 = 1.45$ and $n_3 = 1.725$ (on the left) and $n_2 = 1.45$ and $n_3 = 2.1$ (on the right)
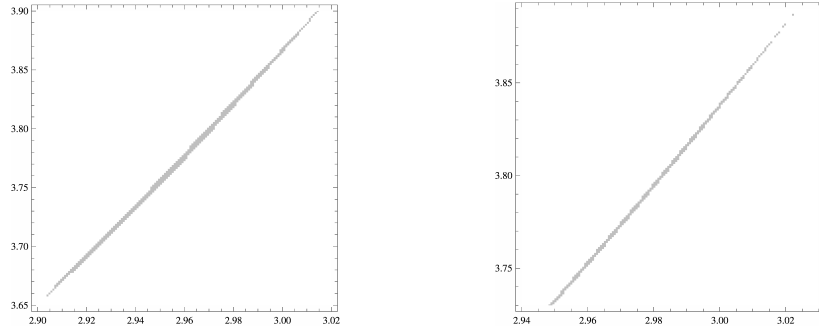
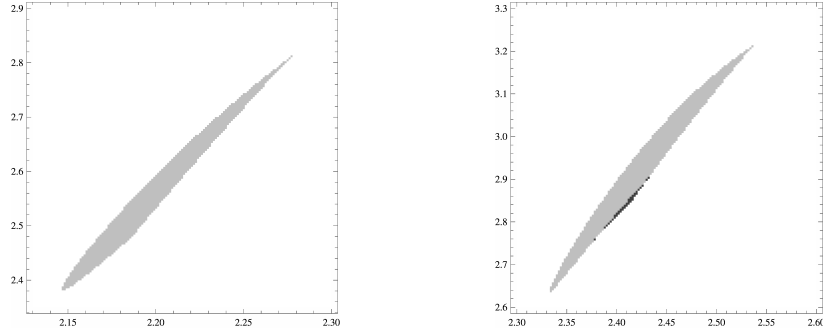**Fig. 5.** Realizable n_4, n_5 normalized moments with ME(3) for $n_2 = 1.45$ and $n_3 = 2.1249$ (on the left) and $n_2 = 1.45$ and $n_3 = 2.1373$ (on the right)

Next we investigate a few cases with $n_2 = 1.6$. We start with two such values of n_3, namely 1.9 and 2.0, that cannot be realized with a PH(3). The realizable n_4, n_5 pairs are depicted in Figure 6. Diverging from the minimal n_3 value, i.e. by

increasing the actual value of n_3 the realizable region becomes larger. Diverging further from the minimal n_3 value, we choose $n_3 = 2.2$ which can be realized by PH(3). Figure 7 depicts the lower peak of the realizable n_4, n_5 region for PH(3) and ME(3). This figure reports new qualitative properties. It indicates that the realizable n_4, n_5 region can be composed by more than two areas and the arias are not concave. The $n_2 = 1.6$, $n_3 = 2.2$ case is further illustrated by Figure 8, there is no upper bound for n_4 and n_5. Figure 9 illustrates instead how the realizable n_4, n_5 is changed and moved by increasing n_3 to 2.3.

Fig. 6. Realizable n_4, n_5 normalized moments with ME(3) for $n_2 = 1.6$ and $n_3 = 1.9$ (on the left) and $n_2 = 1.6$ and $n_3 = 2.0$ (on the right)
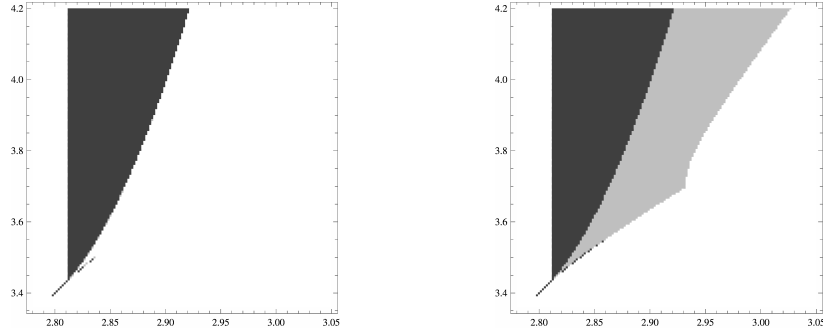

Fig. 7. Lower peak of the realizable n_4, n_5 region with PH(3) (on the left) and ME(3) (on the right) in case of $n_2 = 1.6$ and $n_3 = 2.2$

In the following we investigate cases with $n_2 = 2.2$. Figure 10 depicts the realizable region for $n_3 = 2.7333$ which cannot be realized by PH(3) and $n_3 = 2.9333$ which is the lower limit for PH(3), i.e., in this point a single (n_4, n_5) point can be realized with PH(3). For $n_3 = 3.1333$ the regions are shown in Figure 11
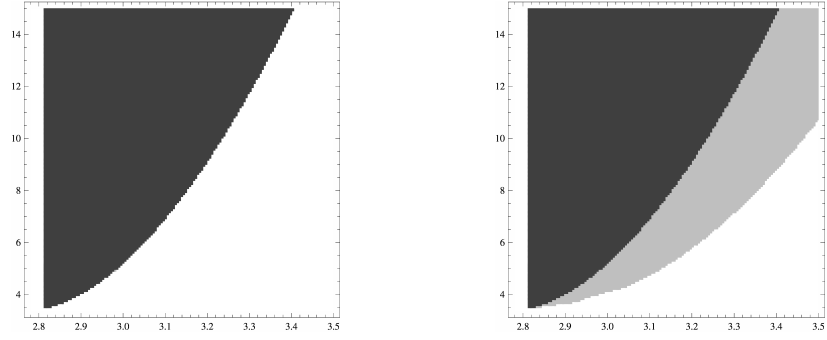
Fig. 8. Realizable n_4, n_5 region with PH(3) (on the left) and ME(3) (on the right) in case of $n_2 = 1.6$ and $n_3 = 2.2$
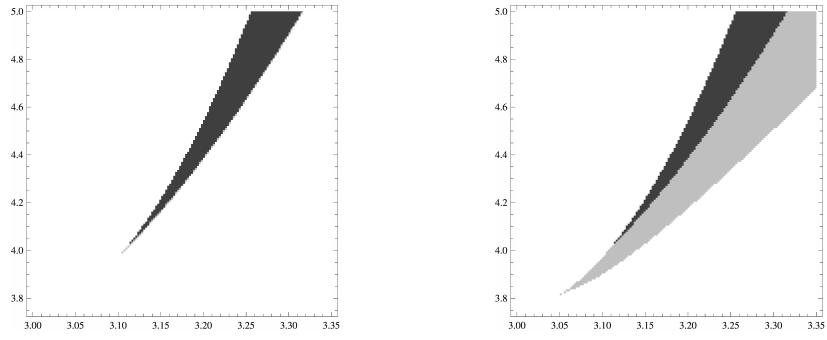

Fig. 9. Realizable n_4, n_5 region with PH(3) (on the left) and ME(3) (on the right) in case of $n_2 = 1.6$ and $n_3 = 2.3$

and for $n_3 = 3.3333$ in Figure 12. With $n_3 = 3.1333$ there are upper bounds for n_4 and n_5 which are not present with $n_3 = 3.3333$.
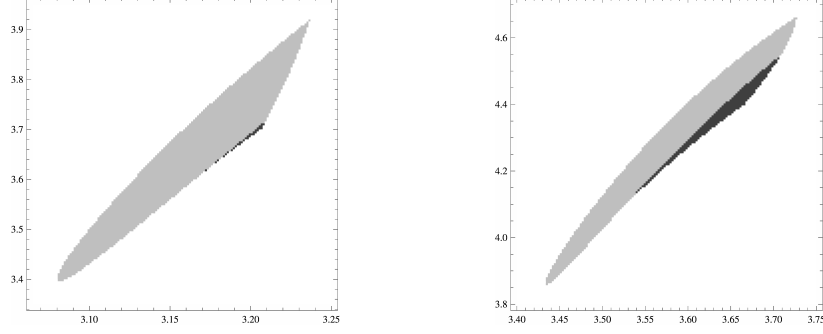

Fig. 10. Realizable n_4, n_5 region with ME(3) for $n_3 = 2.7333$ (on the left) and $n_3 = 2.9333$ (on the right) in case of $n_2 = 2.6$
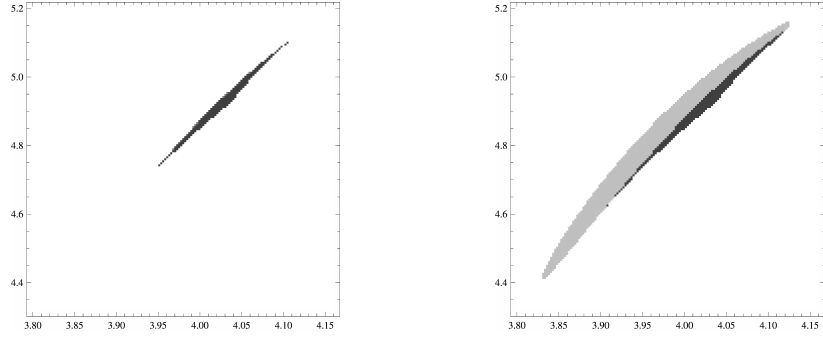

Fig. 11. Realizable n_4, n_5 region with PH(3) (on the left) and ME(3) (on the right) in case of $n_2 = 2.2$ and $n_3 = 3.1333$

5   Conclusions

This paper is devoted to the investigation of the border of ME(3) distributions. To this end we collected necessary and sufficient conditions for different kinds of order 3 matrix exponential functions to be non-negative. It turned out that these conditions are explicit in some cases, but they require the solution of a transcendent equation in other cases. Due to this fact, only numerical methods are available for the investigation of ME(3) borders.
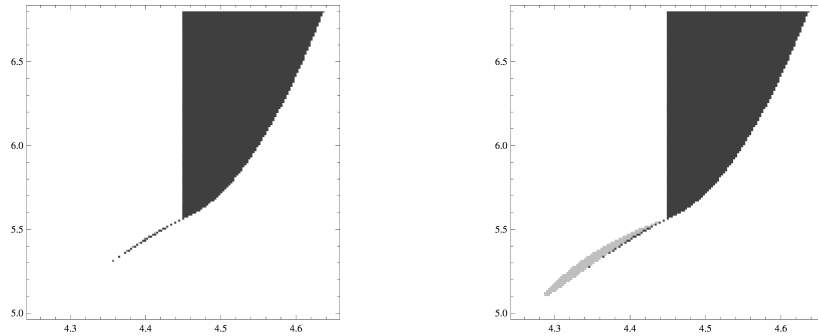
Fig. 12. Realizable n_4, n_5 region with PH(3) (on the left) and ME(3) (on the right) in case of $n_2 = 2.2$ and $n_3 = 3.3333$

Using those necessary and sufficient conditions we completed a set of numerical evaluations. The results show, in accordance with the common expectations, that the ME(3) set has very complex moments borders and it is significantly larger than the PH(3) set.

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