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A NOTE ON UNICYCLIC REPRESENTATIONS OF PHASE TYPE DISTRIBUTIONS

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□ *In this note, we study the unicyclic representation introduced in O'Cinneide[21]. First, we present a counterexample to the conjecture that every PH-representation has an equivalent unicyclic representation of the same order. Then we show that the conjecture holds if the order of the PH-representation is 3. We also introduce an algorithm for computing a unicyclic generator of order 3, which PH-majorizes the original PH-generator, for any PH-generator of order 3. For the general case, we develop a nonlinear program for computing unicyclic representations for PH-distributions.*

Keywords Matrix analytic methods; Phase type distribution; Probability distribution.

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1. INTRODUCTION

It is well known that the *PH*-representation of a phase type (*PH*) distribution is not unique (Neuts[15,16]). Because of that, finding smaller and simpler matrix representations for *PH*-distributions has become an important theoretical and practical issue. On one hand, it is interesting to find a *PH*-representation with the smallest number of phases for a *PH*-representation (Asmussen and Bladt[1]; Commault[2]; Commault and Mocanu[4,5]; Neuts[15]; O'Cinneide[17–21], etc.) This problem is known as the minimal representation problem of *PH*-distributions. On the other hand, it is useful to construct *PH*-representations with a simple structure for

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PH-distributions (Commault and Chemla[3]; Commault and Mocanu[4,5]; Cumani[7]; Dehon and Latouche[8]; He and Zhang[9–11]; Mocanu and Commault[14]; O'Cinneide[17,20,21]). The focus of this note is on a simple *PH*-representation known as the unicyclic representation.

In Cumani[7], it was shown that every triangular *PH*-representation has an ordered Coxian representation of the same order (or a bi-diagonal *PH*-representation) (also see Dehon and Latouche[8]). In O'Cinneide[20], it was shown that any *PH*-distribution whose Laplace Stieltjes transform has only real poles has a triangular *PH*-representation. He and Zhang[9–11] introduced spectral polynomial algorithms for computing ordered Coxian representations (Cox[6]) for *PH*-distributions with only real poles. It was shown that any symmetric *PH*-generator is *PH*-majorized by a Coxian generator (He and Zhang[9]). Those works apply to *PH*-distributions whose Laplace Stieltjes transforms have only real poles. For *PH*-distributions whose Laplace Stieltjes transforms have complex poles, Mocanu and Commault[14] (see also Commault and Mocanu[5]) introduced and studied sparse representations. Similar to the sparse structure introduced in Mocanu and Commault[14], the unicyclic representation was introduced in O'Cinneide[21] as an extension of the Coxian representation. Unlike the Coxian representations, which are for *PH*-distributions with only real poles, the unicyclic representations were proposed for all *PH*-distributions. Numerical examples show that many *PH*-distributions do have a unicyclic representation. Since the simple structure of the unicyclic *PH*-generator may bring in computational advantages in applications, it is worth to investigate such a class of *PH*-representations in more detail. We start our exploration on the unicyclic representation with this note.

It is well known that any *PH*-representation of order 2 has an equivalent Coxian representation of order 1 or 2. It is also known that any *PH*-representation with a triangular or symmetric *PH*-generator has an equivalent Coxian representation of the same or a smaller order. Since Coxian representation is a special type of unicyclic representation, a unicyclic representation of the same or a smaller order exists for these special *PH*-representations. However, little is known on cases other than these special ones. For instance, we do not know whether or not a *PH*-representation has an equivalent unicyclic representation of the same order. More generally, we do not know whether or not a *PH*-distribution has a unicyclic representation of some order. In this note, we shall provide answers to some of those questions.

More specifically, section 2 presents a *PH*-representation of order 6 that has no equivalent unicyclic representation of the same order. In section 3, we show that there exists a unicyclic generator of order 3, which *PH*-majorizes the original *PH*-generator, for any *PH*-generator of order 3. We introduce an algorithm for computing such a unicyclic generator for any PH-generator of order 3. Section 4 presents a nonlinear program for computing equivalent unicyclic representations for PH-distributions. Section 5 concludes this note.

2. A COUNTEREXAMPLE

Define a continuous time Markov chain with $m+1$ states and an infinitesimal generator

$$\begin{pmatrix} T & -T\mathbf{e} \\ 0 & 0 \end{pmatrix}, \tag{2.1}$$

where the $(m+1)$st state is an absorption state, T is a *PH-generator* of order m, and $\mathbf{e}$ is the column vector with all elements being one. We assume that states $\{1, 2, \ldots, m\}$ are transient. Let $\boldsymbol{\alpha}$ be a nonnegative vector of size m for which the sum of its elements is less than or equal to one. We call the distribution of the absorption time of the Markov chain to state $m+1$, with initial distribution $(\boldsymbol{\alpha}, 1-\boldsymbol{\alpha}\mathbf{e})$, a *phase type distribution* (PH-distribution). We call the 2-tuple $(\boldsymbol{\alpha}, T)$ a *PH-representation* of that PH-distribution. Without loss of generality, we shall assume that $\boldsymbol{\alpha}\mathbf{e} = 1$ throughout this paper. That is, we assume that all PH-distributions considered in this note have a zero mass at zero. We refer to Chapter 2 in Neuts[16] for basic properties of PH-distributions.

According to O'Cinneide[21], *a unicyclic representation* $(\boldsymbol{\beta}, U(\mathbf{x}))$ of a PH-distribution is a PH-representation for which the PH-generator $U(\mathbf{x})$ is given as

$$U(\mathbf{x}) = \begin{pmatrix} -x_1 & x_{1,2} & x_{1,3} & \cdots & x_{1,m} \\ x_2 & -x_2 & 0 & \cdots & 0 \\ 0 & x_3 & -x_3 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & x_m & -x_m \end{pmatrix}, \tag{2.2}$$

where $\mathbf{x} = (x_1, x_2, \ldots, x_m,\ x_{1,2}, \ldots, x_{1,m})$ with positive elements $\{x_1, x_2, \ldots, x_m\}$, non-negative elements $\{x_{1,2}, \ldots, x_{1,m}\}$, and $x_1 > x_{1,2} + \cdots + x_{1,m}$. If $x_{1,2} = \cdots = x_{1,m} = 0$, $U(\mathbf{x})$ is called a *Coxian generator* and $(\boldsymbol{\beta}, U(\mathbf{x}))$ is a *Coxian representation* that represents a *Coxian distribution.* Furthermore, if $x_1 \geq x_2 \geq \cdots \geq x_m > 0$ and $x_{1,2} = \cdots = x_{1,m} = 0$, $U(\mathbf{x})$ is called an *ordered Coxian generator.*

Conjecture 4 in O'Cinneide[21] states "Every phase-type distribution of order m has a unicyclic representation of order m." Next, we present a counterexample to that conjecture. In fact, we shall prove the following stronger statement.

Statement 1. Not every *PH*-representation has a *generalized unicyclic representation* $(\boldsymbol{\beta}, U(\mathbf{x},\mathbf{y}))$ of the same order, where

$$U(\mathbf{x},\mathbf{y}) = \begin{pmatrix} -x_1 & x_{1,2} & x_{1,3} & \cdots & x_{1,m} \\ y_2 & -x_2 & 0 & \cdots & 0 \\ 0 & y_3 & -x_3 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & y_m & -x_m \end{pmatrix}, \tag{2.3}$$

$\mathbf{x} = (x_1, x_2, \ldots, x_m,\ x_{1,2}, \ldots, x_{1,m})$ with positive elements $\{x_1, x_2, \ldots, x_m\}$ and non-negative elements $\{x_{1,2}, \ldots, x_{1,m}\}$, $x_1 \geq x_{1,2} + \cdots + x_{1,m}$, $\mathbf{y} = (y_2, \ldots, y_m)$, $x_i \geq y_i \geq 0$, $2 \leq i \leq m$, and $U(\mathbf{x},\mathbf{y})$ is a *PH*-generator.

Consider a *PH*-generator T of order 6 defined as

$$T = \begin{pmatrix} T_1 & 0 \\ 0 & T_2 \end{pmatrix}, \quad \text{where} \quad T_1 = \begin{pmatrix} -1 & 0 & 0.5 \\ 1 & -1 & 0 \\ 0 & 1 & -1 \end{pmatrix} \quad \text{and}$$

$$T_2 = \begin{pmatrix} -1 & 0 & 0.9 \\ 1 & -1 & 0 \\ 0 & 1 & -1 \end{pmatrix}. \tag{2.4}$$

Apparently, for *PH*-generator T given in equation (2.4), any *PH*-distribution $(\boldsymbol{\alpha}, T)$ is the mixture of two *PH*-distributions with *PH*-generators T_1 and T_2, respectively. The matrix T has six distinct eigenvalues $\{-1.3969 + 0.6874i, -1.3969 - 0.6874i, -0.2063, -1.4827 + 0.8361i, -1.4827 - 0.8361i, -0.0345\}$, where $i = \sqrt{-1}$. We consider a *PH*-distribution $(\boldsymbol{\alpha}, T)$ with $\boldsymbol{\alpha} = (0, 0, 0.6, 0, 0, 0.4)$. It can be shown that the distribution function of $(\boldsymbol{\alpha}, T)$ is given by

$$\begin{aligned} F(t) \quad &= 1 - [(-0.0847 + 0.0567i)\exp\{(-1.3969 + 0.6874i)t\} \\ &\qquad + (-0.0847 - 0.0567i)\exp\{(-1.3969 - 0.6874i)t\} \\ &\qquad + 0.7695\exp\{-0.2063t\}] \\ &\quad - [(-0.0072 + 0.0043i)\exp\{(-1.4827 + 0.8361i)t\} \\ &\qquad + (-0.0072 - 0.0043i)\exp\{(-1.4827 - 0.8361i)t\} \\ &\qquad + 0.4145\exp\{-0.0345t\}]. \end{aligned} \tag{2.5}$$

According to equation (2.5), the Laplace Stieltjes transform of the distribution $(\boldsymbol{\alpha}, T)$ has six distinct poles, which are the eigenvalues of T.

Suppose that ($\boldsymbol{\beta}$, $U(\mathbf{x},\mathbf{y})$) is a generalized unicyclic representation of order 6 that is equivalent to $(\boldsymbol{\alpha}, T)$, i.e., ($\boldsymbol{\beta}$, $U(\mathbf{x},\mathbf{y})$) and $(\boldsymbol{\alpha}, T)$ represent the same probability distribution. Then the Laplace Stieltjes transform of ($\boldsymbol{\beta}$, $U(\mathbf{x},\mathbf{y})$) must have the same six poles. Since the order of $U(\mathbf{x},\mathbf{y})$ is 6, the six distinct poles of the Laplace Stieltjes transform of $(\boldsymbol{\alpha}, T)$ must be the eigenvalues of $U(\mathbf{x},\mathbf{y})$. Therefore, $U(\mathbf{x},\mathbf{y})$ and T have the same eigenvalues. Consequently, the matrices $U(\mathbf{x},\mathbf{y})$ and T have the same characteristic polynomial, i.e., $\det(\lambda I - T) = \det(\lambda I - U(\mathbf{x},\mathbf{y}))$ (Lancaster and Tismenetsky[12]). By routine calculations, we obtain

$$\begin{aligned}\det(\lambda I - T) &= \left[(\lambda+1)^3 - 0.5\right]\left[(\lambda+1)^3 - 0.9\right]\\ &= \lambda^6 + 6\lambda^5 + 15\lambda^4 + 18.6\lambda^3 + 10.8\lambda^2 + 1.8\lambda + 0.05; \quad (2.6)\end{aligned}$$

$$\begin{aligned}\det(\lambda I - U(\mathbf{x},\mathbf{y})) = \lambda^6 &+ \left(\sum_{i=1}^{6} x_i\right)\lambda^5 + \left(\sum_{1\le i<j\le 6} x_i x_j - x_{1,2}y_2\right)\lambda^4\\ &+ \left(\sum_{1\le i<j<k\le 6} x_i x_j x_k - x_{1,2}y_2(x_3+x_4+x_5+x_6) - x_{1,3}y_2y_3\right)\lambda^3\\ &+ c_2(\mathbf{x},\mathbf{y})\lambda^2 + c_1(\mathbf{x},\mathbf{y})\lambda + c_0(\mathbf{x},\mathbf{y}),\end{aligned}$$

where $c_2(\mathbf{x},\mathbf{y})$, $c_1(\mathbf{x},\mathbf{y})$, and $c_0(\mathbf{x},\mathbf{y})$ are polynomial functions of $\mathbf{x}$ and $\mathbf{y}$. Comparing the coefficients of λ^5 and λ^4 on both sides of the equation $\det(\lambda I - T) = \det(\lambda I - U(\mathbf{x},\mathbf{y}))$, yields

$$\begin{aligned}x_1 + x_2 + x_3 + x_4 + x_5 + x_6 &= 6;\\ \sum_{1\le i<j\le 6} x_i x_j - x_{1,2}y_2 &= 15.\end{aligned} \quad (2.7)$$

As all elements of $\mathbf{x}$ and $\mathbf{y}$ are non-negative, the two equalities in equation (2.7) lead to

$$\begin{aligned}36 &= \left(x_1 + x_2 + x_3 + x_4 + x_5 + x_6\right)^2\\ &= x_1^2 + x_2^2 + x_3^2 + x_4^2 + x_5^2 + x_6^2 + 2\sum_{1\le i<j\le 6} x_i x_j\\ &= \frac{1}{5}\sum_{1\le i<j\le 6}(x_i^2 + x_j^2) + 2\sum_{1\le i<j\le 6} x_i x_j\\ &\ge \frac{12}{5}\sum_{1\le i<j\le 6} x_i x_j\\ &= 36 + \frac{12}{5}x_{1,2}y_2, \end{aligned} \quad (2.8)$$

which implies that $x_1 = x_2 = x_3 = x_4 = x_5 = x_6 = 1$ and $x_{1,2}y_2 = 0$. Note that, in equation (2.8), we use the inequality $a^2 + b^2 \geq 2ab$ for any real numbers a and b, where the equality holds if and only if $a = b$. If $y_2 = 0$, then $-x_1 = -1$ is an eigenvalue of $U(\mathbf{x}, \mathbf{y})$, which is impossible since -1 is not an eigenvalues of T. Thus, y_2 must be positive, which implies that $x_{1,2} = 0$.

Comparing the coefficients of λ^3 on both sides of the equation $\det(\lambda I - T) = \det(\lambda I - U(\mathbf{x}, \mathbf{y}))$, yields $x_{1,3}y_2y_3 = 1.4$. Since $0 < y_2 \leq 1$ and $0 \leq y_3 \leq 1$, we have $x_{1,3} = 1.4/(y_2y_3) \geq 1.4 > x_1 = 1$. Thus, $U(\mathbf{x}, \mathbf{y})$ is not a *PH*-generator. Therefore, the *PH*-representation $(\boldsymbol{\alpha}, T)$ has no equivalent generalized unicyclic representation $(\boldsymbol{\beta}, U(\mathbf{x}, \mathbf{y}))$ of order 6. Consequently, the *PH*-representation $(\boldsymbol{\alpha}, T)$ has no equivalent unicyclic representation $(\boldsymbol{\beta}, U(\mathbf{x}))$ of order 6. Note that, since the *PH*-distribution $(\boldsymbol{\alpha}, T)$ has six distinct poles, it cannot have an equivalent (generalized) unicyclic representation of order 1, 2, 3, 4, or 5.

Remark 1. For a different initial probability vector $\boldsymbol{\alpha}$, the *PH*-representation $(\boldsymbol{\alpha}, T)$ (where T is given in equation (2.4)) may have a unicyclic representation of the form $(\boldsymbol{\beta}, U(\mathbf{x}))$. For instance, if $\boldsymbol{\alpha} = (0, 0, 1, 0, 0, 0)$, then $(\boldsymbol{\alpha}, T)$ has a unicyclic representation $((0, 0, 1, 0, 0, 0), U(\mathbf{x}))$ with $\mathbf{x} = (1, 1, 1, 1, 1, 1, 0, 0.5, 0, 0, 0)$.

Remark 2. Using the same method, it can be shown that the *PH*-representation $(\boldsymbol{\alpha}, T)$ with $\boldsymbol{\alpha} = (0, 0, 0.6, 0, 0, 0.4)$ and

$$T = \begin{pmatrix} T_1 & T_3 \\ 0 & T_2 \end{pmatrix}, \quad \text{where} \quad T_3 = \begin{pmatrix} 0.1 & 0.1 & 0.1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{2.9}$$

and T_1 and T_2 are given in equation (2.4), does not have a generalized unicyclic representation of order 6.

Although not all *PH*-representations have an equivalent unicyclic representation of the same order, Cumani[7], He and Zhang[9], and numerical results show that many of them do. Thus, it is interesting and useful to know how to find unicyclic representations for *PH*-distributions. In sections 3 and 4, we develop some algorithms for computing unicyclic representations.

3. UNICYCLIC REPRESENTATIONS FOR *PH*-REPRESENTATIONS OF ORDER 3

It was noted in O'Cinneide[21] that every *PH*-representation of order 3 has a unicyclic representation of order 3. However, no formal proof was given there. In addition, no algorithm was introduced for computing unicyclic representations. In this section, we give a proof to that claim and introduce an algorithm for computing unicyclic representations. The results obtained in this section are stronger in the sense that we find a unicyclic generator of order 3 that PH-majorizes the original PH-generator.

To find a unicyclic representation for a PH-distribution $(\boldsymbol{\alpha}, T)$ of order 3, we first find a unicyclic generator $U(\mathbf{x})$ of order 3 that *PH-majorizes* T (denoted as $PH(T) \subseteq PH(U(\mathbf{x}))$), i.e., for any PH-representation $(\boldsymbol{\alpha}, T)$, there exists a probability vector $\boldsymbol{\beta}$ such that $(\boldsymbol{\beta}, U(\mathbf{x}))$ and $(\boldsymbol{\alpha}, T)$ represent the same probability distribution. According to O'Cinneide[17], $U(\mathbf{x})$ PH-majorizes T if and only if there exists a nonnegative matrix P with unit row sums such that $TP = PU(\mathbf{x})$. Then the PH-representation $(\boldsymbol{\alpha}, T)$ has an equivalent unicyclic representation $(\boldsymbol{\alpha}P, U(\mathbf{x}))$.

Denote by $\{-\lambda_1, -\lambda_2, -\lambda_3\}$ the eigenvalues of T (counting multiplicity). We assume that $-\lambda_3$ is the Perron-Frobenius eigenvalue of T, i.e., the eigenvalue with the largest real part, which is real (see Minc[13]). For any PH-generator T, λ_3 is positive. If all eigenvalues are real, we assume that $\lambda_1 \geq \lambda_2 \geq \lambda_3$. Denote by $f_T(\lambda)$ the characteristic polynomial of T. Then we have

$$f_T(\lambda) = \det(\lambda I - T) = (\lambda + \lambda_1)(\lambda + \lambda_2)(\lambda + \lambda_3) = \lambda^3 + a_2\lambda^2 + a_1\lambda + a_0, \tag{3.1}$$

where

$$\begin{aligned} a_0 &= -\det(T) = \lambda_1\lambda_2\lambda_3; \\ a_1 &= t_{1,1}t_{2,2} + t_{2,2}t_{3,3} + t_{3,3}t_{1,1} - t_{1,2}t_{2,1} - t_{1,3}t_{3,1} - t_{2,3}t_{3,2} = \lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_1\lambda_3; \\ a_2 &= -(t_{1,1} + t_{2,2} + t_{3,3}) = \lambda_1 + \lambda_2 + \lambda_3. \end{aligned} \tag{3.2}$$

Note that a_0, a_1, and a_2 are all positive. Also note that if one of λ_1 and λ_2 is not real, the other is not real and the two are conjugate numbers.

Numerical examples demonstrate that the equivalent unicyclic representation of the same order may not be unique. Thus, we require that $U(\mathbf{x})$ and T have the same characteristic polynomial so that we can find the elements of $U(\mathbf{x})$ explicitly. We also assume that $x_{1,2} = 0$. Because of the constraint $x_{1,2} = 0$, the solution found in this section has a *generalized feedback Erlang generator,* which is a special unicyclic generator. By the structure of $U(\mathbf{x})$, the equation $\det(\lambda I - T) = \det(\lambda I - U(\mathbf{x}))$ is equivalent to

$$\begin{aligned} a_0 &= (x_1 - x_{1,3})x_2x_3; \\ a_1 &= x_1x_2 + x_2x_3 + x_3x_1; \\ a_2 &= x_1 + x_2 + x_3. \end{aligned} \tag{3.3}$$

Suppose that x_1 is to be determined later. By solving equation (3.3), we obtain $x_{1,3}$, x_2, and x_3 in terms of x_1 and $\{a_0, a_1, a_2\}$ as follows:

$$\begin{aligned} x_{1,3} &= \frac{-f_T(-x_1)}{a_0 - f_T(-x_1)} x_1; \\ x_2 &= \frac{a_2 - x_1 + \sqrt{(a_2 - x_1)^2 - 4(x_1^2 - a_2 x_1 + a_1)}}{2}; \\ x_3 &= \frac{a_2 - x_1 - \sqrt{(a_2 - x_1)^2 - 4(x_1^2 - a_2 x_1 + a_1)}}{2}. \end{aligned} \tag{3.4}$$

For the matrix $U(\mathbf{x})$ to be a *PH*-generator, we must have $x_1 > x_{1,3} \geq 0$, $x_2 > 0$, and $x_3 > 0$. According to equation (3.4), the following conditions must be satisfied:

$$\begin{aligned} &0 < x_1; \\ &0 \leq -f_T(-x_1); \\ &0 < a_2 - x_1; \\ &0 < x_1^2 - a_2 x_1 + a_1; \\ &0 \leq (a_2 - x_1)^2 - 4(x_1^2 - a_2 x_1 + a_1). \end{aligned} \tag{3.5}$$

Apparently, if inequalities in equation (3.5) are satisfied, $\mathbf{x}$ is non-negative. Next, we identify conditions on x_1 so that all inequalities in equation (3.5) hold. Denote by

$$\begin{aligned} \gamma_U &= \frac{1}{3}\left(a_2 + 2\sqrt{a_2^2 - 3a_1}\right); \\ \gamma_0 &= \frac{1}{3}\left(a_2 + \sqrt{a_2^2 - 3a_1}\right); \\ \gamma_L &= \begin{cases} \lambda_1, & \text{if } \lambda_1 \text{ is real;} \\ \gamma_0, & \text{otherwise.} \end{cases} \end{aligned} \tag{3.6}$$

Lemma 1. *The three constants γ_L, γ_0, and γ_U are positive. We have*

i) $\gamma_U \geq \gamma_0 \geq \lambda_3$;
ii) $a_2 > \gamma_U \geq \gamma_L$;
iii) $f_T'(-\gamma_0) = 0$;
iv) $\gamma_U \geq \lambda_1 \geq \gamma_0$ *if* λ_1 *is real; and*
v) $f_T'(-\gamma_U) = a_2^2 - 3a_1$.

Consequently, if $\gamma_L \leq x_1 \leq \gamma_U$, then $\{x_1, x_{1,3}, x_2, x_3\}$ are non-negative, $x_1 > x_{1,3}$, $x_2 \geq x_3 > 0$, and $U(\mathbf{x})$ is a *PH*-generator.

Proof. In view of (3.2), we have

$$a_2^2 - 3a_1 = \frac{1}{2}\left[(t_{11} - t_{2,2})^2 + (t_{2,2} - t_{3,3})^2 + (t_{3,3} - t_{1,1})^2\right] \\ + 3(t_{1,2}t_{2,1} + t_{2,3}t_{3,2} + t_{3,1}t_{1,3}), \tag{3.7}$$

which implies that $a_2^2 - 3a_1$ is non-negative. Thus, γ_0 and γ_U are real and positive and $\gamma_U \geq \gamma_0$. Since $-\lambda_3$ is the eigenvalue of T with the largest real part, we have $\gamma_0 \geq a_2/3 \geq \lambda_3$. We have proved i).

Because $a_1 > 0$, it is easy to see that $\gamma_U < a_2$. If λ_1 is real, λ_2 is also real. By the definitions in equations (3.2) and (3.6), $\gamma_U \geq \lambda_1$ is equivalent to $(\lambda_2 - \lambda_3)^2 \geq 0$. Thus, if λ_1 is real, $\gamma_U \geq \lambda_1$ must be true. If λ_1 is not real, we have $\gamma_U \geq \gamma_0 = \gamma_L$. Hence, $\gamma_U \geq \gamma_L$ holds. We have proved ii).

It is easy to obtain $f_T'(x) = 3x^2 + 2a_2x + a_1$. By routine calculations, we find that $f_T'(x) = 0$ is attained at $-\left(a_2 \pm \sqrt{a_2^2 - 3a_1}\right)/3$, which implies

$$f_T'(-\gamma_0) = 0. \tag{3.8}$$

Consequently, we have iii). Further, equation (3.8) implies that $f_T(x)$ is nondecreasing in $(-\infty, -\gamma_0]$. If λ_1 is real, by routine calculations, it can be shown that $\lambda_1 \geq \gamma_0$ is equivalent to $3(\lambda_1 - \lambda_2)(\lambda_1 - \lambda_3) \geq 0$. Thus, if λ_1 is real, $\lambda_1 \geq \gamma_0$ holds. We have proved iv). Part v) can be verified directly.

If λ_1 is real, then $f_T(-\gamma_L) = 0$. If λ_1 is not real, $-\lambda_3$ is the only real zero point of $f_T(x)$. Then, $f_T(-\gamma_L) \leq 0$ since $\gamma_L \geq \lambda_3$. Therefore, we have $f_T(-\gamma_L) \leq 0$ for all cases. Since $f_T(-\gamma_L) \leq 0$, $f_T(x)$ is nonpositive for x in $[-\gamma_U, -\gamma_L]$. Thus, the second inequality in equation (3.5) is satisfied, which implies $x_1 > x_{1,3} \geq 0$. As

$$\begin{aligned} &x_1^2 - a_2x_1 + a_1 = \frac{a_0 - f_T(-x_1)}{x_1}; \\ &(a_2 - x_1)^2 - 4\left(x_1^2 - a_2x_1 + a_1\right) = a_2^2 - 3a_1 - f_T'(x)|_{x=-x_1}, \end{aligned} \tag{3.9}$$

for $x \leq -\gamma_L$, we have $x^2 + a_2x + a_1 > 0$. Since the second expression in equation (3.9) becomes zero at $x_1 = \gamma_U$, that expression is non-negative if $\gamma_L \leq x_1 \leq \gamma_U$. Therefore, if $\gamma_L \leq x_1 \leq \gamma_U$, then x_2 and x_3 are real and $x_2 \geq x_3 > 0$. Consequently, $U(\mathbf{x})$ is a *PH*-generator. This completes the proof of Lemma 1.

Next, for $\mathbf{x}$ satisfying equation (3.3), we introduce a matrix P satisfying $TP = PU(\mathbf{x})$ and $P\mathbf{e} = \mathbf{e}$. For more about the matrix P, we refer to He and Zhang[9]. Denote by

$$\begin{aligned} \mathbf{p}_1 &= -T\mathbf{e}/(x_1 - x_{1,3}); \\ \mathbf{p}_2 &= -(x_1I + T)T\mathbf{e}/((x_1 - x_{1,3})x_2); \\ \mathbf{p}_3 &= -(x_2I + T)(x_1I + T)T\mathbf{e}/((x_1 - x_{1,3})x_2x_3). \end{aligned} \tag{3.10}$$

It is easy to verify that $T\mathbf{p}_1 = -x_1\mathbf{p}_1 + x_2\mathbf{p}_2$ and $T\mathbf{p}_2 = -x_2\mathbf{p}_2 + x_3\mathbf{p}_3$. By Cayley-Hamilton Theorem (Lancaster and Tismenetsky[12]), we have $\det(\lambda I - U(\mathbf{x}))|_{\lambda=T} = 0$, which is equivalent to

$$-x_{1,3}x_2x_3I + x_3(x_2I + T)(x_1I + T) + (x_2I + T)(x_1I + T)T = 0. \tag{3.11}$$

Equation (3.11) leads to $T\mathbf{p}_3 = -x_3\mathbf{p}_3 + x_{1,3}\mathbf{p}_1$. Define $P = (\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3)$. It can be shown that $TP = PU(\mathbf{x})$ and $P\mathbf{e} = \mathbf{e}$ if and only if P is given by equation (3.10).

According to Theorem 2 in O'Cinneide[17], finding $U(\mathbf{x})$ such that $U(\mathbf{x})$ *PH*-majorizes T is equivalent to finding x_1 such that the matrix $U(\mathbf{x})$ is a *PH*-generator and the matrix P is non-negative. According to Lemma 1, if $\gamma_L \le x_1 \le \gamma_U$, $U(\mathbf{x})$ is a *PH*-generator. By Lemma 1 and the expression of $\mathbf{p}_1$ in equation (3.10), $\mathbf{p}_1$ is non-negative if $\gamma_L \le x_1 \le \gamma_U$. In order to choose x_1 such that $\mathbf{p}_2$ and $\mathbf{p}_3$ are also non-negative, we define

$$\phi = \max\{-t_{1,1}, -t_{2,2}, -t_{3,3}\}. \tag{3.12}$$

Lemma 2. *We have $\phi \le \gamma_U$. If $x_1 = \phi = -t_{k,k}$, then $x_2 + t_{i,i} \ge 0$, for $i \ne k$. If $x_1 = \gamma_0$, then $x_2 = x_1$.*

Proof. Suppose that $-t_{1,1} \ge -t_{2,2} \ge -t_{3,3}$. First note that, by equations (3.2) and (3.6), $\gamma_U \ge -t_{1,1}$ is equivalent to

$$\begin{aligned} &\frac{1}{3}\left(a_2 + 2\sqrt{a_2^2 - 3a_1}\right) \ge -t_{1,1} \\ &\quad \Leftrightarrow 4(a_2^2 - 3a_1) \ge (-2t_{1,1} + t_{2,2} + t_{3,3})^2 \\ &\quad \Leftrightarrow 3(t_{2,2} - t_{3,3})^2 + 12(t_{2,1}t_{1,2} + t_{1,3}t_{3,1} + t_{2,3}t_{3,2}) \ge 0. \end{aligned} \tag{3.13}$$

Thus, we have $\gamma_U \ge -t_{1,1}$. Consequently, we have $\phi \le \gamma_U$.

To prove the second part, for simplicity, we assume that $k = 1$. By equation (3.4), we have

$$\begin{aligned} x_2 &= \frac{a_2 + t_{1,1} + \sqrt{(a_2 + t_{1,1})^2 - 4(t_{1,1}^2 + a_2t_{1,1} + a_1)}}{2} \\ &= \frac{-t_{2,2} - t_{3,3} + \sqrt{(t_{2,2} - t_{3,3})^2 + 4(t_{1,2}t_{2,1} + t_{2,3}t_{3,2} + t_{3,1}t_{1,3})}}{2} \\ &\ge \frac{-t_{2,2} - t_{3,3} + \sqrt{(t_{2,2} - t_{3,3})^2}}{2} = \max\{-t_{2,2}, -t_{3,3}\}, \end{aligned} \tag{3.14}$$

which leads to the desired results.

Lastly, if $x_1 = \gamma_0$, we have $f_T'(-x_1) = f_T'(-\gamma_0) = 0$ by equation (3.8). Then

$$x_2 = \frac{a_2 - \gamma_0 + \sqrt{a_2^2 - 3a_1 - f_T'(-\gamma_0)}}{2}$$
$$= \frac{1}{2}\left[a_2 - \frac{a_2 + \sqrt{a_2^2 - 3a_1}}{3} + \sqrt{a_2^2 - 3a_1}\right]$$
$$= \frac{a_2 + \sqrt{a_2^2 - 3a_1}}{3} = \gamma_0 = x_1. \tag{3.15}$$

This completes the proof of Lemma 2.

Now, we are ready to choose a value for x_1 such that $U(\mathbf{x})$ is a *PH*-generator and $U(\mathbf{x})$ *PH*-majorizes T (i.e., P is non-negative). Denote by

$$x_1^* = \begin{cases} \max\{\phi, \lambda_1\}, & \text{if } \lambda_1 \text{ is real;} \\ \max\{\phi, \gamma_0\}, & \text{otherwise.} \end{cases} \tag{3.16}$$

Theorem 3.1. *If $x_1 = x_1^*$, where x_1^* is given in equation* (3.16)*, we have the following conclusions:*

1) $U(\mathbf{x})$ *is a unicyclic generator;*
2) P *is non-negative;*
3) $PH(T) \subseteq PH(U(\mathbf{x}))$*; and*
4) $(\boldsymbol{\alpha}P, U(\mathbf{x}))$ *is an equivalent unicyclic representation of PH-representation* $(\boldsymbol{\alpha}, T)$.

Proof. By definition, it is clear from Lemmas 1 and 2 that $\gamma_L \leq x_1^* \leq \gamma_U$ and $\phi \leq x_1^*$. Therefore, for $x_1 = x_1^*$, $U(\mathbf{x})$ is a *PH*-generator. As we have mentioned, $\mathbf{p}_1$ is non-negative. Since $x_1^* \geq \phi$, $x_1 I + T$ is non-negative. Thus, vector $\mathbf{p}_2$ is non-negative. In the rest of the proof, we show that, if $x_1 = x_1^*$, the corresponding vector $\mathbf{p}_3$ is non-negative. For that purpose, we consider three cases: a) $x_1^* = \lambda_1$; b) $x_1^* = \phi$; and c) $x_1^* = \gamma_0$.

For case a), in view of equation (3.3), it is clear that $U(\mathbf{x})$ is an ordered Coxian generator with $x_1 = \lambda_1$, $x_2 = \lambda_2$, $x_3 = \lambda_3$, $x_{1,3} = 0$. By Cayley-Hamilton Theorem (Lancaster and Tismenetsky[12]) and $\lambda_1 \geq \lambda_2 \geq \lambda_3$, $\mathbf{p}_3$ is a Perron-Frobenius eigenvector of T and is non-negative (see Property 4.1 in He and Zhang[9]).

For case b), without loss of generality, we assume that $x_1 = x_1^* = -t_{1,1}$. Then the matrix $x_1 I + T$ is non-negative. By Theorem 3.1, we have

$x_2 \geq -t_{2,2}$ and $x_2 \geq -t_{3,3}$. Then all elements of the matrix $x_2 I + T$ are non-negative, except the element in the (1, 1)-th position. That implies that elements of the second and the third rows of the matrix $(x_2 I + T)(x_1 I + T)$ are non-negative. By routine calculations, we have

$$
\begin{aligned}
&(x_2 I + T)(x_1 I + T)\\
&= \begin{pmatrix} t_{1,2}t_{2,1} + t_{1,3}t_{3,1} & t_{1,2}(x_2 + t_{2,2}) + t_{1,3}t_{3,2} & t_{1,3}(x_2 + t_{3,3}) + t_{1,2}t_{2,3} \\ * & * & * \\ * & * & * \end{pmatrix}.
\end{aligned} \tag{3.17}
$$

Thus, the first row of the matrix $(x_2 I + T)(x_1 I + T)$ is non-negative. Therefore, the matrix $(x_2 I + T)(x_1 I + T)$ is non-negative. Consequently, $-(x_2 I + T)(x_1 I + T)T\mathbf{e}$ is a non-negative vector. Since $\mathbf{p}_3 = -(x_2 I + T)(x_1 I + T)T\mathbf{e}/((x_1 - x_{1,3})x_2 x_3)$, we have shown that $\mathbf{p}_3$ is non-negative.

For case c), we know that $x_1 > \phi$. By Lemma 2, $x_2 = x_1 > \phi$. That implies that the matrices $x_2 I + T$ and $(x_2 I + T)(x_1 I + T)$ are non-negative. Therefore, $\mathbf{p}_3$ is non-negative.

In summary, if $x_1 = x_1^*$, $U(\mathbf{x})$ is a unicyclic generator and P is non-negative. Other results follow immediately. This completes the proof of Theorem 3.1.

We summarize the procedure for computing an equivalent unicyclic representation for a *PH*-representation $(\boldsymbol{\alpha}, T)$ of order 3 as follows.

1. Find $\{a_0, a_1, a_2\}$ and $\{-\lambda_1, -\lambda_2, -\lambda_3\}$ for T.
2. Compute γ_0 and ϕ by equations (3.6) and (3.12).
3. Compute x_1^* and $\{x_{1,3}, x_2, x_3\}$ by equations (3.16) and (3.4).
4. Compute the matrix P by equation (3.10) and $\boldsymbol{\beta} = \boldsymbol{\alpha} P$.

Then $(\boldsymbol{\beta}, U(\mathbf{x}))$ is an equivalent unicyclic representation of $(\boldsymbol{\alpha}, T)$.

In He and Zhang[9], it was shown that, if all the eigenvalues of T are real, it is possible that T is *PH*-majorized by an ordered Coxian generator (i.e., $x_{1,2} = x_{1,3} = 0$). As a byproduct, we find a necessary and sufficient condition for T to be *PH*-majorized by an ordered Coxian generator.

Property 3.1. A *PH*-generator T of order 3 is *PH*-majorized by an ordered Coxian generator $U(\mathbf{x})$ with $\mathbf{x} = (\lambda_1, \lambda_2, \lambda_3, 0, 0)$ if and only if $\{-\lambda_1, -\lambda_2, -\lambda_3\}$ are all real and $\max\{\lambda_1, \lambda_2, \lambda_3\} \geq \eta$, where

$$
\eta = \max_{k=1,2,3} \left\{ \frac{\sum_{i=1}^{3} \sum_{j=1}^{3} t_{k,i} t_{i,j}}{-\sum_{i=1}^{3} t_{k,i}} \right\}, \tag{3.18}
$$

with the convenience $(\sum_{i=1}^{3} \sum_{j=1}^{3} t_{k,i} t_{i,j})(-\sum_{j=1}^{3} t_{k,j})^{-1} = -\infty$ if $\sum_{j=1}^{3} t_{k,j} = 0$.

Proof. First note that the vector $-T\mathbf{e}$ is non-negative. Since

$$\sum_{i=1}^{3}\sum_{j=1}^{3} t_{k,i}t_{i,j} = t_{k,k}\sum_{j=1}^{3} t_{k,j} + \sum_{i\neq k} t_{k,i}\left(\sum_{j=1}^{3} t_{i,j}\right), \tag{3.19}$$

we have $\eta \leq \phi$. By the definition of T, $\max\{-(t_{k,1}+t_{k,2}+t_{k,3}),\ k=1,2,3\} > 0$, which implies $\eta \geq 0$. It is easy to see that for any $x \geq \eta, -(xI+T)T\mathbf{e} \geq 0$. If all eigenvalues are real, by Property 4.1 in He and Zhang[9], $\mathbf{p}_3$ is nonnegative if $\mathbf{x} = (\lambda_1, \lambda_2, \lambda_3, 0, 0)$ and $\lambda_1 \geq \lambda_2 \geq \lambda_3$. Since $\mathbf{p}_1$ is non-negative, we only need to show that $\mathbf{p}_2$ is non-negative. Since $x_1 = \lambda_1 \geq \eta$, $\mathbf{p}_2 = -(x_1 I + T)T\mathbf{e}/((x_1 - x_{1,3})x_2)$ is non-negative. Therefore, $PH(T) \subseteq PH(U(\mathbf{x}))$.

On the other hand, if $PH(T) \subseteq PH(U(\mathbf{x}))$, according to O'Cinneide[17], the corresponding matrix P must be nonnegative. By Property 5.1 in He and Zhang[9], the matrix P is non-negative if $\mathbf{x} = (\lambda_1, \lambda_2, \lambda_3, 0, 0)$ and $\lambda_1 \geq \lambda_2 \geq \lambda_3$. Consequently, $\mathbf{p}_2$ is non-negative, which implies $\max\{\lambda_1, \lambda_2, \lambda_3\} = \lambda_1 = x_1 \geq \eta$. This completes the proof of Property 3.1.

Remark 3. The unicyclic representation of a *PH*-representation of order 3 may not be unique. For instance, if $\eta \geq \lambda_1$, we choose $x_1 = \eta$. Numerically, an equivalent unicyclic representation can be obtained for $x_1 = \eta$. Furthermore, define $x_U = \max\{x_1 : -(x_2 I + T)(x_1 I + T)T\mathbf{e}$ is non-negative$\}$. Then any x_1 in the interval $[x_1^*, x_U]$ corresponds to an equivalent unicyclic representation.

Example 1. Consider four *PH*-generators T_1, T_2, T_3, and T_4 given in equation (3.20).

$$T_1 = \begin{pmatrix} -5 & 1 & 1.2 \\ 3.8 & -4 & 0 \\ 0.1 & 1 & -1.5 \end{pmatrix}, \quad T_2 = \begin{pmatrix} -5 & 0.1 & 2.5 \\ 1.4 & -1.5 & 0 \\ 0.1 & 1.3 & -1.5 \end{pmatrix},$$
$$T_3 = \begin{pmatrix} -5 & 0 & 1.2 \\ 3.8 & -4 & 0 \\ 0.1 & 3 & -3.5 \end{pmatrix}, \quad T_4 = \begin{pmatrix} -5 & 1 & 1.2 \\ 3.8 & -4 & 0 \\ 0.1 & 3 & -3.5 \end{pmatrix}. \tag{3.20}$$

For T_1, all eigenvalues are real, $\lambda_1 = 6.2755$, and $\phi = 5$. For this case, $x_1^* = \lambda_1 = 6.2755$. For T_2, all eigenvalues are real, $\lambda_1 = 4.6703$, and $\phi = 5$. For this case, $x_1^* = \phi = 5$. For T_3, two eigenvalues are not real, $\gamma_0 = 4.6509$, and $\phi = 5$. For this case, $x_1^* = \phi = 5$. For T_4, two eigenvalues are not real, $\gamma_0 = 5.3919$, and $\phi = 5$. For this case, $x_1^* = \gamma_0 = 5.3919$. This example shows that all four cases considered in Theorem 3.1 may occur.

In the next example, we give a geometric explanation to the construction of the unicyclic *PH*-generator $U(\mathbf{x})$.

Example 2. We consider T_2 defined in equation (3.20). By using the algorithm, we find $T_2P = PU(\mathbf{x})$ and $P\mathbf{e} = \mathbf{e}$ with $\mathbf{x} = (5,\ 2.1245,\ 0.8755,\ 0,\ 1.7124)$. Let $Q = P^{-1}$. Then $QT_2 = U(\mathbf{x})Q$. Let $\{\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3\}$ be the first, second, and third rows of Q, respectively. Then the polytope $\text{conv}\{\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3\}$ is called a *PH*-invariant polytope under T_2 corresponding to $U(\mathbf{x})$. Let $\mathbf{e}_1 = (1, 0, 0)$, $\mathbf{e}_2 = (0, 1, 0)$, and $\mathbf{e}_3 = (0, 0, 1)$. Then $\text{conv}\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ is the probability vector polytope. Geometrically, $PH(T_2) \subseteq PH(U(\mathbf{x}))$ is equivalent to $\text{conv}\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\} \subseteq \text{conv}\{\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3\}$, as shown in Figure 1.

If we choose $z_1 = \lambda_1 = 4.6703$, $z_2 = \lambda_2 = 2.8741$, and $z_3 = \lambda_3 = 0.4556$, then the corresponding $U(\mathbf{z})$ is an ordered Coxian generator with $\mathbf{z} = (4.6703, 2.8741, 0.4556, 0, 0)$. Using equation (3.10), we find matrix W for $WT_2 = U(\mathbf{z})W$ and $W\mathbf{e} = \mathbf{e}$. Let $\{\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3\}$ be the first, second, and third rows of W. Then the polytope $\text{conv}\{\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3\}$ is a *PH*-invariant polytope under T_2 corresponding to $U(\mathbf{z})$. The polytope $\{\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3\}$ is plotted in Figure 1. Apparently, $\text{conv}\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\} \not\subset \text{conv}\{\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3\}$, i.e., $PH(T_2) \not\subset PH(U(\mathbf{z}))$. According to Figure 1, for some *PH*-representation $(\boldsymbol{\alpha}, T_2)$ (e.g., $\boldsymbol{\alpha} = \mathbf{e}_2$ and $\boldsymbol{\alpha} = \mathbf{e}_3$), it has an equivalent Coxian representation of order 3. For some other *PH*-representation $(\boldsymbol{\alpha}, T_2)$ (e.g., $\boldsymbol{\alpha} = \mathbf{e}_1$), there exists no equivalent Coxian representation of order 3.

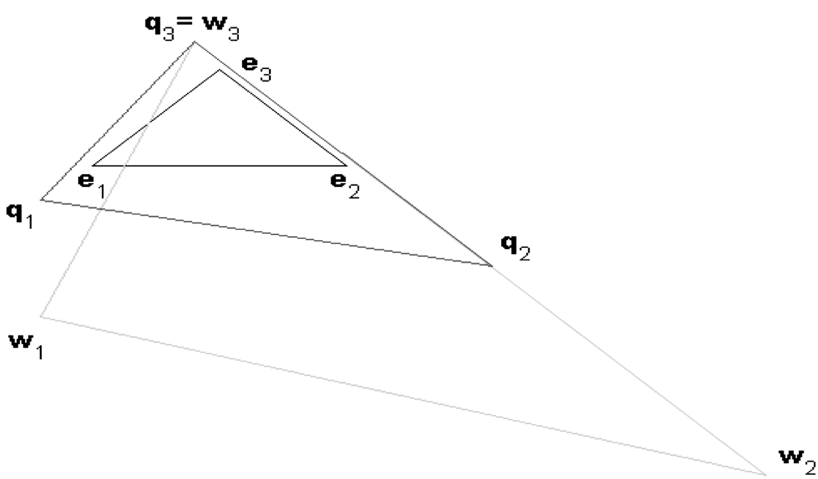

FIGURE 1 *PH*-invariant polytopes for Example 2.

4. AN NLP APPROACH FOR COMPUTING UNICYCLIC REPRESENTATIONS

In this section, we introduce an algorithm for computing unicyclic representations for a *PH*-representation $(\boldsymbol{\alpha}, T)$ of order m. A nonlinear program approach is taken. The algorithm is based on the following property.

Property 4.1. a) For any *PH*-generator T, if there exists $\mathbf{x}$ such that $TP = PU(\mathbf{x})$, where $U(\mathbf{x})$ is a *PH*-generator of order m and P is a non-negative matrix with unit row sums, then we have $PH(T) \subseteq PH(U(\mathbf{x}))$. b) For any *PH*-representation $(\boldsymbol{\alpha}, T)$, if there exists $\mathbf{x}$ such that $TP = PU(\mathbf{x})$, where $U(\mathbf{x})$ is a *PH*-generator of order m, P has unit row sums, and $\boldsymbol{\beta} = \boldsymbol{\alpha} P$ is non-negative, then $(\boldsymbol{\beta}, U(\mathbf{x}))$ is an equivalent unicyclic representation of $(\boldsymbol{\alpha}, T)$.

Proof. The results can be obtained by Theorem 2 in O'Cinneide[17]. This completes the proof of Property 4.1.

Now, we introduce the following nonlinear program

$$\begin{aligned} &\min_{(\mathbf{X},P)} \left\{ \sum_{i=2}^{N} x_{1,i} \right\} \\ &s.\,t. \quad TP = PU(\mathbf{x}); \\ &x_1 - x_{1,2} - \cdots - x_{1,N} > 0; \\ &\boldsymbol{\alpha} P \geq 0, \quad P\mathbf{e} = \mathbf{e}, \quad \mathbf{x} \geq 0, \end{aligned} \tag{4.1}$$

where $\mathbf{x} = (x_1, x_2, \ldots, x_N, x_{1,2}, \ldots, x_{1,N})$, P is an $m \times N$ matrix, and N is a positive integer.

If nonlinear program (4.1) has a solution $(\mathbf{x}, P)$, then $U(\mathbf{x})$ is a *PH*-generator and $(\boldsymbol{\alpha} P, U(\mathbf{x}))$ is an equivalent unicyclic representation of $(\boldsymbol{\alpha}, T)$. If nonlinear program (4.1) does not have a solution, we choose a different N and solve the nonlinear program again. If we want to find a $U(\mathbf{x})$ such that $U(\mathbf{x})$ *PH*-majorizes T, we replace the constraint $\boldsymbol{\alpha} P \geq 0$ by $P \geq 0$ in equation (4.1).

Remark 4. If $m = 3$, by using the algorithm developed in section 3, we can find an equivalent unicyclic representation without solving (4.1). If T is triangular or symmetric, then T is *PH*-majorized by an ordered Coxian generator that can be found without solving (4.1) (see He and Zhang[9]). Unfortunately, for a general case with $m > 3$, we need the nonlinear program to find $\mathbf{x}$ for a unicyclic *PH*-generator (if exists).

Next, we propose an algorithm for computing an equivalent unicyclic representation of a *PH*-representation $(\boldsymbol{\alpha}, T)$. Denote by N_0 a positive integer.

Step 1: Set $N = 1$.
Step 2: Solve nonlinear program (4.1).
Step 3: If (4.1) has a solution, go to Step 4. Otherwise, set $N =: N + 1$. If $N > N_0$, go to Step 5; otherwise, go to Step 2.
Step 4: An equivalent unicyclic representation $(\boldsymbol{\alpha}P, U(\mathbf{x}))$ of order N has been found.
Step 5: No solution in the range $N \le N_0$ is found. The program is terminated.

Note that, since we do not know whether or not $(\boldsymbol{\alpha}, T)$ has an equivalent unicyclic representation (of any order), we need to introduce N_0 to terminate the program.

Example 3. Consider a *PH*-representation $(\boldsymbol{\alpha}, T)$ of order 4 with $\boldsymbol{\alpha} = (0.2, 0, 0, 0.8)$ and

$$T = \begin{pmatrix} -1 & 0 \\ 0 & T_1 \end{pmatrix}, \quad \text{where} \quad T_1 = \begin{pmatrix} -1 & 0 & 0.5 \\ 1 & -1 & 0 \\ 0 & 1 & -1 \end{pmatrix}. \tag{4.2}$$

Using the method in section 2, it can be shown that the *PH*-representation $(\boldsymbol{\alpha}, T)$ does not have an equivalent unicyclic representation order 4. By using the above algorithm, we find an equivalent unicyclic representation $(\boldsymbol{\beta}, U(\mathbf{x}))$ of order 5, where

$$\boldsymbol{\beta} = (0.1765, 0.0560, 0.1824, 0.1623, 0.4228);$$

$$U(\mathbf{x}) = \begin{pmatrix} -1.4642 & 0 & 0 & 0.1109 & 0.2203 \\ 1.4642 & -1.4642 & 0 & 0 & 0 \\ 0 & 1.4642 & -1.4642 & 0 & 0 \\ 0 & 0 & 1.4642 & -1.4642 & 0 \\ 0 & 0 & 0 & 0.3038 & -0.3038 \end{pmatrix}. \tag{4.3}$$

Example 4. Consider the *PH*-generator T given in equation (4.4). We are interested in finding an equivalent unicyclic representation $(\boldsymbol{\beta}, U(\mathbf{x}))$ of order 4 for *PH*-distribution $(\boldsymbol{\alpha}, T)$. By using the above algorithm, it is found that $\mathbf{x} = (3.5219, 3.5219, 3.5219, 0.4343, 0, 0.0557, 1.0307)$ and P is given in equation (4.4).

$$T = \begin{pmatrix} -4 & 0 & 0 & 2 \\ 1 & -4 & 0 & 2.7 \\ 0 & 1.5 & -2 & 0 \\ 0.1 & 0 & 0.9 & -1 \end{pmatrix} \quad \text{and}$$
$$P = \begin{pmatrix} 0.8212 & -0.1115 & 0.0582 & 0.2321 \\ 0.1232 & 0.2164 & -0.0029 & 0.6633 \\ 0.2053 & 0.1412 & 0.1532 & 0.5003 \\ 0 & 0.0758 & 0.0872 & 0.8371 \end{pmatrix}. \tag{4.4}$$

Since the matrix P is not nonnegative, $PH(T) \subseteq PH(U(\mathbf{x}))$ is not true. For instance, if $\boldsymbol{\alpha} = (1, 0, 0, 0)$, $(\boldsymbol{\alpha}P,\ U(\mathbf{x}))$ is not a PH-representation.

However, the PH-representation $((1, 0, 0, 0), T)$ actually has an equivalent unicyclic representation of order 4, which can be obtained as follows. Applying the above algorithm with the constraint $\boldsymbol{\alpha}P \geq 0$ being replaced by $P \geq 0$, we obtain

$$U(\mathrm{z}) = \begin{pmatrix} -4 & 0 & 0.1215 & 1.3749 \\ 3.2523 & -3.2523 & 0 & 0 \\ 0 & 3.2523 & -3.2523 & 0 \\ 0 & 0 & 0.4955 & -0.4955 \end{pmatrix};$$
$$P = \begin{pmatrix} 0.7989 & 0.0000 & 0.0491 & 0.1520 \\ 0.1198 & 0.2456 & 0.0098 & 0.6247 \\ 0.1997 & 0.1781 & 0.1819 & 0.4403 \\ 0.0000 & 0.0786 & 0.1046 & 0.8156 \end{pmatrix}. \tag{4.5}$$

Apparently, $U(\mathbf{z})$ is a PH-generator. Since P is non-negative, we have $PH(T) \subseteq PH(U(\mathbf{z}))$. Consequently, ((1, 0, 0, 0), T) has an equivalent unicyclic representation ((0.7989, 0, 0.0491, 0.1520), $U(\mathbf{z})$).

Similar to Example 2, geometrically, to find a $U(\mathbf{x})$ that PH-majorizes T is equivalent to finding a PH-invariant polytope under T that includes the probability vector polytope.

5. DISCUSSION

To end this note, we would like to point out that, since not all PH-representations have an equivalent unicyclic representation of the same order, it is interesting to identify classes of PH-representations that have an equivalent unicyclic representation of the same order. Section 3 showed that the class of *PH*-representations of order 3 (i.e., $m = 3$) has that property. In Cumani[7], Dehon and Latouche[8], He and Zhang[9], and O'Cinneide[19], it has been shown that *PH*-representations with a triangular or symmetric *PH*-generator have an equivalent ordered Coxian representation of the same or a smaller order, which is a special form of the unicyclic representation. Those results indicate that more work can be done in this direction. Future research topics include finding necessary and sufficient conditions for a *PH*-representation to have an equivalent unicyclic representation of the same order, proving or disproving that every *PH*-distribution has a unicyclic representation of some order, and etc. It is even more interesting to address those issues for the generalized unicyclic representation defined in equation (2.3).

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