

# Efficient Generation of PH-distributed Random Variates

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**Abstract.** Phase-type (PH) distributions are being used to model a wide range of phenomena in performance and dependability evaluation. The resulting models may be employed in analytical as well as in simulation-driven approaches. Simulations require the efficient generation of random variates from PH distributions. PH distributions have different representations and different associated computational costs for random-variate generation. In this paper we study the problem of efficient representation and efficient generation of PH distributed variates.

Key words: PH distribution, pseudo random number generation.

## 1 Introduction

Phase-type (PH) distributions [1] are very useful in modelling interarrival times, failure times, and other phenomena in computer systems. They can be employed in analytical approaches as well as in simulation-based evaluations. When PH distributions are used in simulations, often large sets of random variates must be generated, and thus efficiency of random-variate generation from PH distributions is important. We consider algorithms that ‘play’ the underlying Markov chain. These algorithms provide high accuracy, because they represent each PH sample as a sum of exponential samples, directly following the definition of PH distributions.

PH distributions have different Markovian representations. In [2] we observed that the computational complexity of PH-distributed random-variate generation depends on the representation. This fact poses the research problem of finding the representation that is optimal for random-variate generation.

In [3] we addressed the question by considering the sub-class of Acyclic Phase-type (APH) distributions. For APH distributions the optimal representation is obtained as follows: Starting from any representation the first step is to transform

the representation to the CF-1 canonical form defined in [4]. An APH distribution is in CF-1 form if the generator matrix has a bi-diagonal structure and the transition rates are non-decreasing towards the absorbing state. Transformation to the CF-1 form is always possible because all APH distributions have a CF-1 representation [4]. The second step is to find the optimal ordering of the diagonal (and the associated sub-diagonal) elements. It is shown in [3] that for APH in bi-diagonal form the optimal representation is the reversed CF-1 form if it is Markovian. For the case when the reversed CF-1 form is not Markovian, heuristic search algorithms are proposed to find the optimal ordering of the diagonal elements.

In this paper we generalize the results obtained for the APH class to the PH class. We propose to follow a similar approach. In the first step we transform the representation to a sparse Markovian representation. To the best of our knowledge, the only representation with these properties which is available for the whole PH class is the monocyclic representation proposed by Mocanu and Commault [5]. The monocyclic representation is a natural extension of the CF-1 form, in the sense that the generator matrix remains bi-diagonal, but on the matrix block level. Due to their structures these matrix blocks are referred to as feedback Erlang (FE) blocks. The second step of the proposed procedure is to find the optimal ordering of the FE matrix blocks (and the associated sub-diagonal matrix blocks). We are going to show that in contrast to the APH case the optimal ordering of the FE blocks cannot be predicted in a simple way (e.g., by the associated dominant eigenvalue). As a result, finding the optimal representation composed by FE blocks is based on the use of exhaustive or heuristic search algorithms over the set of possible ordering of the FE blocks.

The method proposed in this paper is composed of two parts, preprocessing and random variate generation. The computational complexity of the sum of both steps should be optimized in general. There are obvious extreme solutions for the cases when very few and extremely large numbers of random samples are required. In the first case the preprocessing phase can be omitted and in the second case arbitrarily large look-up tables can be computed during the preprocessing phase. Our proposed solution is between these extremes. We assume  $10^6 - 10^{10}$  samples, where the cost of the preprocessing phase of our method is negligible in case of moderate size ( $< 15$  states) PH distributions. The cost of the preprocessing phase increases sub-linearly with the size.

The paper is structured as follows. We first describe the notation used throughout the paper and briefly recall the results from [3] in Section 2. In Section 3 we propose an algorithm for generating random variates from general PH distributions with monocyclic representation and discuss the associated computational cost. Section 4 presents the transformation of reordering the FE blocks in the monocyclic representation and discusses its properties. A counterexample is presented to show that the nice ordering rules of APH representations are not applicable in case of general PH distributions. In Section 5 we provide heuristics for efficient search of optimal representation, and Section 6 studies the efficiency of the proposed procedures.

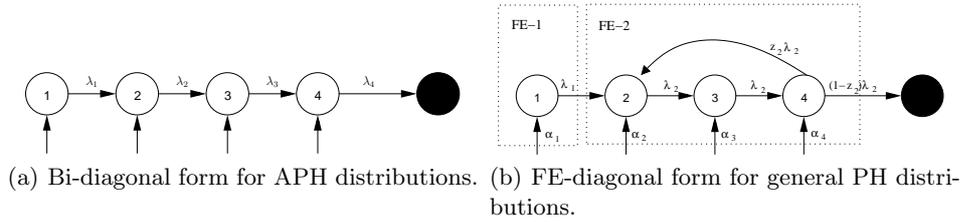


Fig. 1. Comparison of bi-diagonal and FE-diagonal forms for PH distributions.

## 2 Notation and Previous Results

A PH distribution of size  $n$  is described by an initial probability vector  $\alpha \in \mathbb{R}^n$  and a sub-generator matrix  $\mathbf{Q} \in \mathbb{R}^{n \times n}$  with entries  $q_{ij}$  such that  $q_{ii} < 0$  and  $q_{ij} \geq 0$  for  $i \neq j$ . In this case the cumulative distribution function (CDF) is

$$F(x) = 1 - \alpha e^{\mathbf{Q}x} \mathbf{1},$$

where  $\mathbf{1}$  is the column vector of ones of appropriate size. The representation  $(\alpha, \mathbf{Q})$  is not unique.

**Definition 1.** *If  $\mathbf{P}$  is invertible and  $\mathbf{P}\mathbf{1} = \mathbf{1}$ , then the similarity transformation  $(\alpha\mathbf{P}, \mathbf{P}^{-1}\mathbf{Q}\mathbf{P})$  provides another representation of the same distribution, since its CDF is*

$$1 - \alpha\mathbf{P}e^{\mathbf{P}^{-1}\mathbf{Q}\mathbf{P}t}\mathbf{1} = 1 - \alpha\mathbf{P}\mathbf{P}^{-1}e^{\mathbf{Q}t}\mathbf{P}\mathbf{1} = 1 - \alpha e^{\mathbf{Q}t}\mathbf{1}.$$

The representation  $(\alpha, \mathbf{Q})$  is called *Markovian* if  $\forall i : \alpha_i \geq 0$  and  $\alpha\mathbf{1} = 1$  and  $\mathbf{Q}_{ii} < 0$ ,  $\mathbf{Q}_{ij} \geq 0$ ,  $i \neq j$ . With a Markovian representation, we refer to  $\alpha$  as the initial probability vector and to  $\mathbf{Q}$  as the sub-generator matrix.

The computational complexity of PH-distributed random-variate generation depends on the representation [2]. Our goal is to find the representation with the lowest computational complexity. The optimization of APH representations is based on bi-diagonal representations of APH distributions in [3]. In these representations, the only non-zero entries of the sub-generator matrix  $\mathbf{Q}$  are on the diagonal and on the upper diagonal, with  $q_{i,i+1} = -q_{ii}$ . Bi-diagonal representations can be conveniently specified by the vector  $\lambda = (\lambda_1, \dots, \lambda_n)$ , where  $\lambda_i = -q_{ii}$  for  $i = 1, \dots, n$ . Figure 1(a) shows the CTMC of an APH distribution with size  $n = 4$  in bi-diagonal form. All APH distributions have at least one bi-diagonal representation with Markovian initialisation vector [4]. The bi-diagonal representation with non-decreasing  $\lambda$  is referred to as CF-1 form.

Bi-diagonal Markovian representations are only available if all eigenvalues of the sub-generator matrix  $\mathbf{Q}$  (i.e. all poles of the Laplace-Stieltjes Transform of the distribution) are real. As general PH distributions may have complex poles, [5] proposed the use of Feedback-Erlang (FE) blocks to represent pairs of complex eigenvalues:

**Definition 2.** [5] A Feedback-Erlang (FE) block with parameters  $(b, q, z)$  is a chain of  $b$  states with transition rate  $q$  and one transition from the  $b$ th state to the first state, with rate  $zq$ . The probability  $z \in [0, 1)$  is called the feedback probability.

The dominant eigenvalue of the FE block with parameters  $(b, q, z)$  is always real and given by  $r = -q(1 - z^{1/b})$  [5]. Feedback-Erlang blocks with length  $b = 1$  or feedback probability  $z = 0$  are called *degenerate* FE blocks. Note that an FE block  $(b, q, z)$  with length  $b = 1$  corresponds to an exponential distribution with rate  $q$ , while  $z = 0$  gives the Erlang- $b$  distribution with rate  $q$  (the sum of  $b$  independent exponentially distributed random variables with parameter  $q$ ). In both cases, the dominant eigenvalue is  $-q$ . Analogously to the approach for the APH class, we consider representations with a diagonal structure of the sub-generator:

**Definition 3.** An FE-diagonal representation consisting of  $m$  Feedback-Erlang blocks  $(b_i, q_i, z_i), i = 1, \dots, m$  has a sub-generator matrix  $\mathbf{Q}$  where the only non-zero entries are in the FE blocks along the diagonal and the transition rates from the last state of a Feedback-Erlang block to the first state of the next one. The size of the representation is  $n = \sum_{i=1}^m b_i$ .

Where appropriate, we also use the vector notation

$$\Upsilon = \{(b_1, q_1, z_1), \dots, (b_m, q_m, z_m)\},$$

to describe the structure of the sub-generator matrix. Figure 1(b) shows an example of the CTMC of a general PH distribution in FE-diagonal form. In this representation there are two FE blocks, one of length  $b_1 = 1$  with rate  $q_1 = \lambda_1$ , and one of length  $b_2 = 3$  with rate  $q_2 = \lambda_2$  and feedback probability  $z_2$ . The following theorem, restated from [5], ensures that every PH distribution has at least one Markovian FE-diagonal representation:

**Theorem 1.** [5] Every PH distribution has a monocylic representation with Markovian initial vector. A monocylic representation is an FE-diagonal representation

$$\Upsilon = \{(b_1, q_1, z_1), \dots, (b_m, q_m, z_m)\}$$

such that the dominant eigenvalues of the FE blocks are ordered by increasing absolute value,  $|r_i| \leq |r_j|$ , for  $1 \leq i \leq j \leq m$ .

The monocylic form can be computed using, e.g., the implementations available in the Butools library [6]. Note that for APH distributions the feedback probabilities are zero for all blocks, i.e. FE-diagonal forms for APH distributions consist of degenerate FE blocks. For the APH class the FE diagonal form thus corresponds to the bi-diagonal form defined in [3], and the monocylic form is equivalent to the CF-1 form. The next section discusses an algorithm for generating random variates from a general PH distribution in FE-diagonal form.

### 3 Random-Variate Generation from FE-diagonal Representations

Given a PH distribution with representation  $(\boldsymbol{\alpha}, \mathbf{Q})$  in FE-diagonal form with FE-block vector  $\boldsymbol{\mathcal{Y}} = \{(b_1, q_1, z_1), \dots, (b_m, q_m, z_m)\}$ , random variates can be generated by the following algorithm:

Procedure **FE-diagonal**:

Let  $x := 0$

Draw an  $\boldsymbol{\alpha}$ -distributed discrete sample for the initial state.

The chain is in block  $i$  and has to traverse  $l$  states until the block may be left (e.g., for the left-most state of the  $i$ th block,  $l = b_i$ ).

**while**  $i \leq m$  **do**

$c = \text{Geo}(z_i)$

$x+ = \text{Erl}(cb_i + l, q_i)$

$i++$

$l = b_i$

**end while**

Return( $x$ )

This algorithm was proposed as **Procedure Monocyclic** in [2], but can of course also be applied to FE-diagonal representations. The algorithm uses the

$$\text{Geo}(p) = \left\lfloor \frac{\ln U}{\ln p} \right\rfloor \quad \text{and} \quad \text{Erl}(b, q) = -\frac{1}{q} \ln \left( \prod_{i=1}^b U_i \right) \quad (1)$$

operations for drawing a random variate from the Geometric distribution with parameter  $p$  and support  $0, 1, \dots$ , or the Erlang- $b$  with rate  $q$ , respectively. In both cases,  $U$  denotes a uniformly distributed pseudo random number on  $(0, 1)$ .

The algorithm works as follows: An initial state is chosen according to the initial probability vector  $\boldsymbol{\alpha}$ . We assume that this state belongs to FE block  $i$ , and there are  $1 \leq l \leq b_i$  states to traverse before the chain may enter the next block. Since all rates in the given FE block are equal ( $q_i$ ), this corresponds to an Erlang- $l$  distribution with rate  $q_i$ . When the last state of the block is reached, one may either enter the next block or follow the feedback-loop to the first state of the current block. The number of loops  $c = 0, 1, \dots$  within the  $i$ th block follows a geometric distribution with parameter  $z_i$ . The random variate corresponding to the loop is Erlang- $c$ -distributed, again with rate  $q_i$ . Consequently, for the block entered upon initialisation the algorithm draws a random variate from an Erlang- $(cb_i + l)$  distribution. All the remaining blocks until absorption are entered at the first state, and thus the respective random variates for the  $j$ th block ( $j = i+1, \dots, m$ ) are distributed according to  $(\mathbf{e}_1, \mathbf{F}_j)$  distributions, where  $\mathbf{e}_1$  is the row vector with 1 at position 1 and zero everywhere else and  $\mathbf{F}_j$  is the sub-generator corresponding to the  $j$ th FE block. Following the argument for the initial step, random variates from these distributions are generated from Erlang- $(c_j b_j + l_j)$  distributions, where  $c_j$  is the number of loops and  $l_j = b_j$  (since each block is entered at the beginning and has to be traversed at least once).

In a preliminary measurement study we observed that the computational cost of computing logarithms dominates the cost of generating PH-distributed random variates. Further performance measures have been considered in [2]. Although the exact cost ratio depends on hardware and software specifics, optimisation for the number of logarithm operations appears to be an effective approach. The number of logarithm operations depends on the distribution of the initial probability mass over the Feedback-Erlang blocks and is independent of both the distribution within the blocks and the length of the blocks. Computation of the expected number of logarithms is straightforward:

$$n^*(\boldsymbol{\alpha}, \boldsymbol{\mathcal{Y}}) = 3\boldsymbol{\beta}\boldsymbol{\nu}^\top,$$

where  $\boldsymbol{\beta} = \left(\sum_{i=1}^{b_1} \alpha_i, \sum_{i=b_1+1}^{b_1+b_2} \alpha_i, \dots, \sum_{i=n-b_m+1}^n \alpha_i\right)$  is the vector of initial probabilities for each FE block, and the entries of  $\boldsymbol{\nu} = (m, m-1, \dots, 1)$  give the number of blocks to traverse when entering the  $i$ th FE block. The result is multiplied by 3, because 3 logarithm operations are required for the computation of the geometric and Erlang samples.

Usually, the **FE-diagonal** algorithm is more efficient than the algorithms that simply ‘play’ the CTMC by selecting a sequence of states, due to the special block bi-diagonal structure of the representation. When a general representation is allowed, random selection of the next state is required in each step. This is eliminated in the **FE-diagonal** algorithm, since the next FE block is uniquely determined by the chain structure of the representation. Therefore, we consider the optimisation of representations in FE-diagonal form, and we present numerical results about the computational gain of the **FE-diagonal** algorithm in Section 6.

## 4 Optimisation for FE-diagonal Representations of the PH Class

The optimal representation of an APH for random-variate generation is the reversed CF-1 form (non-increasing  $\boldsymbol{\Lambda}$ ), if the reversed CF-1 is Markovian [3]. This result was obtained by an analysis of the properties of the **Swap** operator, which exchanges two adjacent entries of the vector  $\boldsymbol{\Lambda}$ . The monocyclic representation of the PH class is the generalization of the CF-1 form used for the APH class. The obvious similarity between both forms raises the question whether the result obtained for the APH class can be generalized to the PH class in FE diagonal representation. To answer this question we introduce the similarity transformation matrix  $\mathbf{P}$  that swaps two adjacent FE blocks and produces the new initial probability vector  $\boldsymbol{\alpha}' = \boldsymbol{\alpha}\mathbf{P}$ .

**Definition 4.** *The  $\mathbf{G}\mathbf{S}\mathbf{w}\mathbf{a}\mathbf{p}(\boldsymbol{\alpha}, \mathbf{A}, i)$  operator exchanges the  $i$ th FE block with the  $(i+1)$ th FE block ( $1 \leq i \leq m-1$ ) on the diagonal in a block-bi-diagonal representation by swapping the  $i$ th and  $(i+1)$ th entry in the vector  $\boldsymbol{\mathcal{Y}}$  (or, equivalently, by swapping the block matrices associated with the FE blocks in the sub-generator).*





Now consider the two initial vectors

$$\boldsymbol{\alpha}_1 = (0.09 \mid 0.1, 0.3, 0.31 \mid 0.1, 0.1, 0),$$

and

$$\boldsymbol{\alpha}_2 = (0.09 \mid 0.1, 0.3, 0.31 \mid 0.2, 0, 0)$$

whose only difference is the distribution of the probability mass assigned to the third FE block. The costs for random-variate generation from  $(\boldsymbol{\alpha}_1, \mathbf{Q})$  and  $(\boldsymbol{\alpha}_2, \mathbf{Q})$ , are

$$n^*(\boldsymbol{\alpha}_1, \mathbf{Q}) = n^*(\boldsymbol{\alpha}_2, \mathbf{Q}) = 3 \cdot (0.09 \cdot 3 + 0.71 \cdot 2 + 0.2) = 5.67.$$

After swapping the two blocks using  $\mathbf{P}$  the resulting initial probability vectors are

$$\boldsymbol{\alpha}'_1 = \boldsymbol{\alpha}_1 \mathbf{P} = (0.09 \mid 0.141852, 0.28963, 0.271111 \mid 0.118519, 0.0888889, 0)$$

and

$$\boldsymbol{\alpha}'_2 = \boldsymbol{\alpha}_2 \mathbf{P} = (0.09 \mid 0.0492593, 0.426667, 0.315556 \mid 0.118519, 0, 0)$$

respectively. Note that in  $\boldsymbol{\alpha}'_1$  the initial probability mass assigned to the third FE block increased from 0.2 to 0.207407, while in  $\boldsymbol{\alpha}'_2$  the probability mass decreased from 0.2 to 0.118519. The costs of random-variate generation changed as follows:

$$\begin{aligned} n^*(\boldsymbol{\alpha}'_1, \mathbf{Q}') &= 3 \cdot 1.8825939 = 5.6477817, \\ n^*(\boldsymbol{\alpha}'_2, \mathbf{Q}') &= 3 \cdot 1.9714836 = 5.9144508. \end{aligned}$$

That is, with  $\boldsymbol{\alpha}_1$  swapping the blocks resulted in a cost decrease, while with  $\boldsymbol{\alpha}_2$  costs increased.

The example illustrates that with true FE-diagonal representations (i.e. those with non-degenerate FE blocks) the effect of swapping two consecutive FE blocks may depend not only on the properties of the sub-generator of the distribution, but also on the distribution in the initial probability vector. Consequently, the procedures proposed for finding the optimal representation of APH distributions in [3] cannot be used for the PH class.

## 5 Algorithms for Monocyclic Optimisation

Example 1 shows that the reversed Monocyclic form of a true PH distribution is not guaranteed to be optimal, even if the initialisation vector is Markovian. Hence the efficient optimisation methods developed for the APH class cannot be applied to the PH class, since, first, there is no general optimum that only needs to be checked for non-negativity of the initialisation vector, and, second, the direction in which to search for the optimum cannot be derived from the sub-generator alone. On the other hand, Example 1 is not just bad news, since

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Algorithm GBubbleSortOptimise( $\alpha, \mathcal{Y}$ ):
for  $i = 1, \dots, m - 1$  do
  for  $j = 1, \dots, m - 1$  do
    ( $\alpha', \mathcal{Y}'$ ) := GSwap( $\alpha, \mathcal{Y}, i$ )
    if ComparisonHeuristic( $\alpha, \mathcal{Y}, j$ ) = true  $\wedge$   $\alpha' \geq \mathbf{0}$  then
      ( $\alpha, \mathcal{Y}$ ) := ( $\alpha', \mathcal{Y}'$ )
    else
      break
    end if
  end for
end for
return ( $\alpha, \mathcal{Y}$ )

```

**Fig. 2.** GBubbleSortOptimise attempts to re-order phases such that the global ordering imposed by ComparisonHeuristic is generated.

it also shows that a cost reduction by swapping adjacent FE blocks is indeed possible.

The optimum for the FE-diagonal representation of a PH distribution can be found by an optimisation of the costs over the set of all permutations of the FE blocks. This exhaustive approach is guaranteed to find the optimum with respect to all permutations, but involves generating and checking  $m!$  representations. The approach may be feasible if neither the number of FE blocks  $m$  nor the block lengths are too large, but running-times become prohibitive for large  $m$  or large FE blocks. Large  $m$  require a large number of permutations to be checked, while large FE blocks imply large  $\hat{\mathbf{P}}$ , and thus higher costs for solving (2) and (3).

Therefore, we propose extensions of the algorithms for efficient APH optimisation. We need to replace the strict ordering criterion available for the bi-diagonal form of APH distributions with efficient heuristics. The general approach of the algorithms GBubbleSortOptimise in Figure 2 and GFindMarkovian in Figure 3 are identical to those for APH optimization. In both algorithms, the comparison of two adjacent rates has been replaced by a call to the generic routine ComparisonHeuristic, which returns **true** or **false**, depending on whether the two Feedback-Erlang blocks given as its arguments are in the order imposed by the heuristic. The GBubbleSortOptimise algorithm is guaranteed to always find a Markovian representation, since it does not leave the region of orderings with Markovian initialisation vectors. The GFindMarkovian algorithm, on the other hand, may terminate without finding a Markovian representation. It is guaranteed to terminate with a Markovian representation only with the eigenvalue heuristic discussed below.

In the following we discuss four heuristics that can be used as ComparisonHeuristic in either algorithm. The heuristics presented here have been derived based on the following argument: In Lemma 1 of [3] we showed that the optimal ordering for the APH case is obtained if the ordering of the elements of the diagonal of the CF-1 form is reversed (provided that this ordering is Markovian). Due to the simplicity of the CF-1 form, this re-ordering can be seen equivalently

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Algorithm GFindMarkovian( $\alpha, \mathcal{Y}$ ):
Let  $(\alpha', \mathcal{Y}')$  be the reversed Monocyclic form of  $(\alpha, \mathcal{Y})$ 
r:=0
while  $\neg(\alpha' \geq \mathbf{0})$  do
   $i := \max\{2, \operatorname{argmin}_i \{\alpha'_i < 0\}\}$ 
  while  $\neg(\alpha' \geq \mathbf{0}) \wedge \exists k : \operatorname{ComparisonHeuristic}(\mathcal{Y}[k], \mathcal{Y}[k+1]) = \text{false}$  do
     $k := \operatorname{argmin}_j \{j \mid i-1 \leq j \leq m-1 \wedge \mathcal{Y}[j] \geq \mathcal{Y}[j+1]\}$ 
     $(\alpha', \mathcal{Y}') := \operatorname{GSwap}(\alpha', \mathcal{Y}', k)$ 
    if  $(\alpha', \mathcal{Y}')$  is a new representation then
       $r++$ 
    end if
    if  $r = m!$  then
      goto END
    end if
  end while
end while
END:
return  $(\alpha', \mathcal{Y}')$ 

```

**Fig. 3.** GFindMarkovian starts from the possibly non-Markovian reversed Monocyclic form and searches for a Markovian representation by re-ordering phases such that the reversed ordering imposed by ComparisonHeuristic is produced.

as a re-ordering of the dominant eigenvalues, of the means, and of the exit rates. Furthermore, property (3) in [3] corresponds to the determinant of the swap matrix being larger than 1. These four criteria differ from each other if true Feedback-Erlang blocks are compared.

**Eigenvalues Heuristic.** The eigenvalues heuristic relates to the CF-1 case most directly. Recall that the monocyclic representation is defined such that the Feedback Erlang blocks are ordered along the diagonal according to increasing absolute value of their dominant eigenvalues. The eigenvalues heuristic directly applies the observation from the CF-1 case that swapping two blocks may move probability mass to the right iff the eigenvalue of the right phase is larger than that of the left phase. Equivalently, in the monocyclic case probability mass may be moved to the right if the dominant eigenvalue of the right FE block is larger than that of the left FE block. We define the Eigenvalues heuristic as follows:

$$\operatorname{EigenvaluesHeuristic}(\alpha, \mathcal{Y}, i) = \begin{cases} \text{true} & |r_i| < |r_{i+1}|, \\ \text{false} & \text{else,} \end{cases}$$

that is, the heuristic returns true if the absolute value of the dominant eigenvalue of the  $i$ th block is larger than that of the  $(i+1)$ th block.

**Mean Heuristic.** The mean heuristic stems from the following observation for the CF-1 case: Re-ordering phases directly relates to re-ordering the means of the associated distributions. I.e., swapping two phases such that the one with higher rate is moved to the left is equivalent to swapping them such that the one with the lower mean moves to the left. This idea can be applied to the

monocyclic case as follows. First, we have to assign a mean to each FE block. While this is unambiguous in the CF-1 case (where FE blocks are of length 1), in the monocyclic case probability mass may be assigned to all phases of a block, rendering the mean dependent on the distribution of the mass. The most straightforward approach is then to assign probability mass of 1 to the first entry of the block. The mean of a Feedback-Erlang block  $(b_i, q_i, z_i)$  with sub-generator matrix  $\mathbf{F}_i$  and probability mass 1 at the first entry is  $\hat{M}_i = \mathbf{e}_1(-\mathbf{F}_i)^{-1}\mathbf{1}$ . The mean heuristic is then defined as

$$\text{MeanHeuristic}(\boldsymbol{\alpha}, \boldsymbol{\mathcal{Y}}, i) = \begin{cases} \text{true} & \hat{M}_i > \hat{M}_{i+1}, \\ \text{false} & \text{else.} \end{cases}$$

**Exit-Rates Heuristic** The exit-rates heuristic compares the exit rates  $(1 - z_i)q_i, (1 - z_{i+1})q_{i+1}$  of neighbouring FE blocks. Based on the result for the CF-1 case, optimisation then consists in re-ordering blocks such that the highest exit rates (i.e. largest rates  $q_i$  in the CF-1 case) move to the left. The heuristic is defined as follows:

$$\text{ExitRatesHeuristic}(\boldsymbol{\alpha}, \boldsymbol{\mathcal{Y}}, i) := \begin{cases} \text{true} & (1 - z_i)q_i < (1 - z_{i+1})q_{i+1}, \\ \text{false} & \text{else.} \end{cases}$$

**Determinant Heuristic** For the APH case, the similarity transformation matrix  $\hat{\mathbf{P}}$  has the following explicit structure [3]:

$$\hat{\mathbf{P}} = \begin{pmatrix} 1 & 0 \\ \frac{q_i - q_{i+1}}{q_i} & \frac{q_{i+1}}{q_i} \end{pmatrix} \quad (6)$$

with determinant  $|\hat{\mathbf{P}}| = q_{i+1}/q_i$ . In this case, swapping two adjacent rates moves probability mass to the right iff  $q_{i+1} > q_i$ , or, equivalently, if  $|\hat{\mathbf{P}}| > 1$ . The determinant heuristic, defined as

$$\text{DeterminantHeuristic}(\boldsymbol{\alpha}, \boldsymbol{\mathcal{Y}}, i) := \begin{cases} \text{true} & |\hat{\mathbf{P}}| > 1, \\ \text{false} & \text{else.} \end{cases}$$

generalizes this criterion to the general case.

## 5.1 Discussion

While these heuristics are exact for degenerate FE blocks, they may be misleading with non-degenerate FE blocks, as can be illustrated using Example 1. Table 1 shows the relevant properties considered by the eigenvalues, mean, and exit rates heuristics. The determinant of the swap matrix  $\hat{\mathbf{P}}$  is  $|\hat{\mathbf{P}}| = 0.208$ . Observe that the eigenvalues, mean, and exit rates heuristics would recommend to swap the two blocks. As we saw in the counterexample, this is correct for  $\boldsymbol{\alpha}_1$ , but incorrect for  $\boldsymbol{\alpha}_2$ . Likewise, the prediction by the determinant heuristic that swapping would not move probability mass to the right is wrong for  $\boldsymbol{\alpha}_1$ , but correct for  $\boldsymbol{\alpha}_2$ .

	$\mathbf{F}_1$	$\mathbf{F}_2$
Dominant eigenvalue	$r_2 = -0.3095$	$r_1 = -1$
Mean with mass 1 at first state	$\hat{M}_2 = 4$	$\hat{M}_1 = 3$
Mean with normalised mass ( $\alpha_1$ )	$M_2 = 4$	$M_1 = 1.7042$
Mean with normalised mass ( $\alpha_2$ )	$M_2 = 2.5$	$M_1 = 1.7042$
Exit rate	0.75	1

**Table 1.** Properties of the FE blocks in Example 1.

## 6 Application of the Algorithms

We have implemented the proposed representation optimization methods in Mathematica. To test their efficiency we also implemented a random general PH representation generator. For a given size  $n$ , we first draw uniformly distributed samples for the initial distribution, which are normalized later. We then draw uniformly distributed samples for the off-diagonal elements of the generator matrix and for the transition rates to the absorbing state of the PH distribution. The mean ratio of the off-diagonal elements of the generator matrix and the transition rates to the absorbing state has a significant effect on the cost of random-variate generation. This ratio is referred to as *termination rate* below.

Having a random general PH representation we first compute the monocyclic representation of the same distribution and then we optimize the representation using the introduced heuristic approaches and an exhaustive search method by interchanging the FE block of the representation. The exhaustive search method evaluates all permutations of the FE blocks. The computational complexity of the exhaustive search method becomes significant at  $n > 6$ . The heuristic search algorithms perform a negligible number of **GSwap** operations compared to the exhaustive search method and find suboptimal representations in the majority of the cases. Table 2 shows the cost of generating PH-distributed random variates based on the obtained representations. When the termination rate is equal to 1 and  $n = 6$  there is a gain of  $\sim 60\%$  due to the transformation to the monocyclic representation. A further  $\sim 40\%$  gain comes from heuristic optimisation of the FE blocks. The results of the exhaustive search method indicates that the suboptimal representation of the eigenvalue, the mean and the exit rate heuristics are very close to the global optimum obtained by the exhaustive search method.

The rows of Table 2 demonstrate the effect of the termination rate. The higher the transition rate to the absorbing state, the lower the number of state transitions before absorption. In case of fast transitions to the absorbing state the simple simulation which ‘plays’ the transitions of the Markov chain until absorption is an efficient simulation method due to the low number of state transitions. In this case the transformation to the monocyclic representation and the additional optimization cannot reduce the cost of random-variate generation. For both order 6 (Table 2) and order 10 (Table 3) the turning point is around termination rate  $\sim 10$ : For higher termination rate the direct simulation is more efficient, and vice versa for lower termination rate.

termination rate	random PH	mono cyclic	eigenvalue	mean heuristic	exitrate	determinant	exhaustive search
0.033	332.008	5.07253	3.06384	3.06234	3.12738	5.07174	3.02422
0.1	102.696	5.03166	3.02877	3.05235	3.11337	5.02784	3.01783
0.33	33.308	4.98996	3.08534	3.09713	3.15197	4.98222	3.01082
1	11.6818	4.24592	2.6476	2.61502	2.77029	4.2132	2.53818
3.3	4.53882	3.38355	2.23615	2.18118	2.25545	3.37198	2.11419
10	2.2624	2.7238	1.9441	1.92582	1.9441	2.72091	1.85605
33	1.50076	2.39407	1.91512	1.91488	1.91512	2.39407	1.83054

**Table 2.** Average simulation costs (number of logarithms) for order 6 PH distribution based on 100 samples

termination rate	random PH	mono cyclic	eigenvalue	mean heuristic	exitrate	determinant
0.033	561.077	8.64065	8.62078	8.62078	8.62078	8.64065
0.1	186.376	8.18222	8.17221	8.17221	8.17221	8.18222
0.33	58.8492	7.97052	7.9417	7.94135	7.94203	7.97014
1	19.4483	6.52973	6.47238	6.47238	6.47238	6.52973
3.3	7.07673	5.45818	5.38195	5.38257	5.38397	5.45661
10	3.15833	4.98105	4.96477	4.96336	4.96477	4.98105
33	1.77828	3.06237	3.05572	3.05572	3.05572	3.06237

**Table 3.** Average simulation costs (number of logarithms) for order 10 PH distribution based on 100 samples

It is interesting to see how the proposed transformation reduces the dynamics of the cost. In the evaluated range of termination rates between 0.033 and 33, the cost of random-variate generation with direct simulation varies from 1.5 to 332, while the cost of random-variate generation with optimized representation varies from 1.8 to 3, and a bit larger dynamics reduction appears in Table 3.

Comparing the performance of heuristic optimization methods we obtain that the eigenvalue and mean heuristics perform better than the exit-rate and determinant heuristics. Based on the average performance in Tables 2 and 3, the order of the heuristics is eigenvalue, mean, exit rate and determinant, and there are only a few cases where the mean heuristic performs better than the eigenvalue heuristic. The results of this section are computed by the `GBubbleSortOptimise` procedure, which always terminates with Markovian initial vector.

## 7 Conclusion

In this paper we considered the optimization of phase-type distributions for random-variate generation. We propose to use the FE-diagonal representations. We studied optimization of the costs involved with random-variate generation and showed by a counterexample that the nice ordering property of the APH class does not generalize to the PH class with FE-diagonal form. We developed

different heuristic algorithms for optimisation of the PH representation and studied the quality of the heuristics compared to the exhaustive search. The structure of the original PH representation affects the gain of representation optimisation. In a wide range of cases (termination rate  $< 10$ ) the proposed procedure reduces the cost of random-variate generation. Additionally, the proposed procedure significantly reduces the dependence of the cost on the structure of the original PH representation.

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