An Improved Method for Bounding Stationary Measures of Finite Markov Processes (Extended Version)*

Peter Buchholz
Informatik IV, Universität Dortmund
D-44221 Dortmund, Germany
email: peter.buchholz@udo.edu

Abstract

A new method to compute bounds on stationary results of finite Markov processes in discrete or continuous time is introduced. The method extends previously published approaches using polyhedra of eigenvectors for stochastic matrices with a known lower and upper bound of their elements. Known techniques compute bounds for the elements of the stationary vector with respect to the lower bounds of the matrix elements and another set of bounds with respect to the upper bounds of matrix elements. The resulting bounds are usually not sharp, if lower and upper bounds for the elements are known. The new approach combines lower and upper bounds resulting in sharp bounds which are often much tighter than bounds computed using only one bounding value for the matrix elements.

Keywords: Markov processes; bounding techniques; stationary analysis

1 Introduction

Stationary measures of Markov chains in continuous time (CTMCs) or discrete time (DTMCs) are often used to express performance, dependability or performability measures in various application areas. However, often the transition rates or probabilities of the process result from measurements and are only approximately known in form of lower and upper bounds. In this case, the computation of bounds for the stationary distribution is an alternative to the exact computation of stationary measures from a process where transition rates/probabilities are fixed to some values inside the interval of possible values. An established and widely used technique for bounding the stationary distribution of Markov processes has been published by Courtois and Semal [4, 5] twenty years ago. The method is defined for discrete time Markov processes, also denoted as Markov chains, for which lower or upper bounds for the transition probabilities are known. The stationary distribution is shown to belong to a polyhedron of vectors defined by the normalized rows of an inverse matrix resulting from the lower or upper bound matrix. It is shown in the mentioned papers that the derived bounds are the best possible bounds, if only the lower or upper bounds for transition probabilities are known. The basic method of [4] has been improved and extended until recently. In [13] bounds computed for huge DTMCs via decomposition and aggregation are improved by an iterative approach which computes increasing lower bounds for the transition probabilities of some aggregated DTMC and applies the basic method to those bounding matrices. In [9, 10] the method

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is improved for the computation of bounds for matrices with a block Hessenberg structure which often appears in models for reliability analysis. The application of the method to nearly or quasi lumpable DTMCs is considered in [1, 6] and [2] describes the application of the method for bound computation in stochastic automata networks.

In this paper we introduce a new method for bounding the stationary measures of a finite Markov process by an improved version of the basic bounding method using eigenvector polyhedra [4, 5]. Instead of considering the polyhedron of eigenvectors of all irreducible stochastic matrices which are bounded from below by the lower bound matrix and another polyhedron defined by the set of irreducible stochastic matrices bounded from above by the upper bound matrix, the extended method considers a single set of irreducible stochastic matrices which are bound from below and from above by the lower and upper bound matrix, respectively. We assume that measures can be described by rate based rewards. In all cases where non-trivial lower and upper bounds for the elements of the transition matrix are known, the new method yields tighter bounds than the original approach and for many applications, the width of the bounds is reduced by several orders of magnitude. It is shown that the resulting bounds are sharp. I.e., for every reward vector exists an irreducible stochastic matrix with elements bounded from below by the elements from the lower bound matrix and from above by the upper bound matrix which yields exactly the value of the computed bound.

The outline of the rest of the paper is as follows: In the next section the notation, the basic bounding method for stationary analysis and some of the published extensions are introduced. Section 3 presents an extension of the known approach by considering matrices in the polyhedron defined by the lower and upper bound matrix. Subsequently, a bounding algorithm is introduced and afterwards some examples are analyzed with the new and the known method.

2 Basic Definitions and Known Results For Stationary Analysis

Throughout the paper, boldface capital and lowercase letters are used for matrices and vectors, respectively. Vectors are row vectors, if not stated otherwise. $diag(\mathbf{p})$ for a n-dimensional column vector $\mathbf{p}$ is a $n \times n$ diagonal matrix with $\mathbf{p}(i)$ in position (i, i). $\mathbf{e}$ is a row vector where all elements are 1 and $\mathbf{e}_i$ is a row vector with 1 in position i and 0 elsewhere. $\mathbf{A}^T$ and $\mathbf{a}^T$ are the transposed matrix and vector, respectively. Except $\mathbb{R}$ and $\mathbb{N}$ sets are represented by calligraphic letters. We use $\mathbf{A} < \mathbf{B}$ if $\mathbf{A}(i,j) \leq \mathbf{B}(i,j)$ for all matrix entries and $\mathbf{A} \neq \mathbf{B}$. Similarly we use $\mathbf{A} \leq \mathbf{B}$ for $\mathbf{A} < \mathbf{B}$ or $\mathbf{A} = \mathbf{B}$. If $\mathbf{A} \leq \mathbf{B}$, we denote $\mathbf{A}$ as a lower bound matrix for $\mathbf{B}$ and $\mathbf{B}$ as an upper bound matrix for $\mathbf{A}$.

Let X_k be a DTMC with finite state space $\mathcal{S} = \{1, \ldots, n\}$ and irreducible, aperiodic, stochastic transition matrix $\mathbf{P}$. This DTMC has a unique stationary distribution vector $\mathbf{p}$ which equals the left eigenvector for eigenvalue 1 normalized to 1 [14]. In the sequel we implicitly assume that the eigenvector is normalized to 1. Here we are interested in result measures that can be represented as the expectation of a rate based reward measure represented by a non-negative reward value $\mathbf{r}(i) \geq 0.0$ for each $i \in \mathcal{S}$. $\mathbf{r}$ is the column vector of rate rewards. The expectation of the reward is defined as $E[R] = \mathbf{pr}$. Reward values can be used to represent a wide variety of measures for examples see [9]. Now assume that instead of matrix $\mathbf{P}$ only two matrices $\mathbf{0} \leq \mathbf{L} \leq \mathbf{P}$ and $\mathbf{U} \geq \mathbf{P}$ are known. Since $\mathbf{Pe}^T = \mathbf{e}^T$, the relations $\mathbf{Le}^T \leq \mathbf{e}^T$ and $\mathbf{Ue}^T \geq \mathbf{e}^T$ hold. We consider only stochastic matrices, such that knowledge of $\mathbf{L}$ puts some restrictions on the size of the elements of $\mathbf{U}$ and vice versa. Thus, we assume in the sequel that $\mathbf{U}(i,j) \leq 1.0 - \sum_{k \in \mathcal{S} \setminus \{j\}} \mathbf{L}(i,k)$ and $\mathbf{L}(i,j) \geq \max(0.0, 1.0 - \sum_{k \in \mathcal{S} \setminus \{j\}} \mathbf{U}(i,k))$.

Define for $\mathbf{L}$ and $\mathbf{U}$ with $\mathbf{0} \leq \mathbf{L} \leq \mathbf{U}$, $\mathbf{L}\mathbf{e}^T \leq \mathbf{e}^T$ and $\mathbf{U}\mathbf{e}^T \geq \mathbf{e}^T$ the sets of stochastic matrices

$$
\begin{aligned}
&\mathcal{P}_{\mathbf{L}} = \{\mathbf{P} | \mathbf{P} \geq \mathbf{L}, \mathbf{P}\mathbf{e}^T = \mathbf{e}^T, \mathbf{P} \text{ irreducible}\} \ , \\
&\mathcal{P}_{\mathbf{U}} = \{\mathbf{P} | \mathbf{0} < \mathbf{P} \leq \mathbf{U}, \mathbf{P}\mathbf{e}^T = \mathbf{e}^T, \mathbf{P} \text{ irreducible } \} \text{ and} \\
&\mathcal{P}_{\mathbf{L},\mathbf{U}} = \mathcal{P}_{\mathbf{L}} \cap \mathcal{P}_{\mathbf{U}} \ .
\end{aligned}
$$

We assume in the sequel that the matrices $\mathbf{L}$ and $\mathbf{U}$ are such that the sets are non-empty. According to [5] $\mathcal{P}_{\mathbf{L}} \neq \{\mathbf{P}\}$ for irreducible matrices $\mathbf{L}$, if and only if $\rho(\mathbf{L}) < 1$ where $\rho(\mathbf{L})$ is the spectral radius of $\mathbf{L}$. If $\rho(\mathbf{L}) = 1$ and $\mathbf{L}$ is irreducible, then $\mathcal{P}_{\mathbf{L}} = \{\mathbf{L}\}$. In the sequel we assume that $\mathbf{L}$ is irreducible and $\rho(\mathbf{L}) \leq 1$. The matrices in the sets $\mathcal{P}_{\mathbf{L}}$ and $\mathcal{P}_{\mathbf{U}}$ define the following sets of left eigenvectors

$$
\begin{aligned}
&\mathcal{V}_{\mathbf{L}} = \{\mathbf{v} \geq \mathbf{0} | \exists \mathbf{P} \in \mathcal{P}_{\mathbf{L}}, \mathbf{v}\mathbf{P} = \mathbf{v}, \mathbf{v}\mathbf{e}^T = 1\} \ , \\
&\mathcal{V}_{\mathbf{U}} = \{\mathbf{v} \geq \mathbf{0} | \exists \mathbf{P} \in \mathcal{P}_{\mathbf{U}}, \mathbf{v}\mathbf{P} = \mathbf{v}, \mathbf{v}\mathbf{e}^T = 1\} \text{ and} \\
&\mathcal{V}_{\mathbf{L},\mathbf{U}} = \{\mathbf{v} \geq \mathbf{0} | \exists \mathbf{P} \in \mathcal{P}_{\mathbf{L},\mathbf{U}}, \mathbf{v}\mathbf{P} = \mathbf{v}, \mathbf{v}\mathbf{e}^T = 1\} \ .
\end{aligned}
$$

For the computation of the bounds, the set of columns where $\mathbf{L}$ and $\mathbf{U}$ differ is required. This set is defined as $\mathcal{C}_{\mathbf{L},\mathbf{U}} = \{j | \exists i \in \mathcal{S} : \mathbf{L}(i,j) < \mathbf{U}(i,j)\}$. Knowing only $\mathbf{L}$, $\mathbf{U}$ or both, lower and upper bounds for $E[R]$ and $\mathbf{p}(i)$ can be defined by choosing the minimal and maximal value which is reachable by multiplying an vector from $\mathcal{V}_{\mathbf{L}}$, $\mathcal{V}_{\mathbf{U}}$ or $\mathcal{V}_{\mathbf{L},\mathbf{U}}$ with $\mathbf{r}$ where $\mathbf{r}$ equals $(\mathbf{e}_i)^T$ to compute bounds for $\mathbf{p}(i)$.

$$
\begin{aligned}
E_{\mathcal{V}}^{-}[R] = \min_{\mathbf{v} \in \mathcal{V}} \mathbf{v}\mathbf{r} \leq E[R] \leq \max_{\mathbf{v} \in \mathcal{V}} \mathbf{v}\mathbf{r} = E_{\mathcal{V}}^{+}[R] \\
\mathbf{p}_{\mathcal{V}}^{-}(i) = \min_{\mathbf{v} \in \mathcal{V}} \mathbf{v}(i) \leq \mathbf{p}(i) \leq \max_{\mathbf{v} \in \mathcal{V}} \mathbf{v}(i) = \mathbf{p}_{\mathcal{V}}^{+}(i)
\end{aligned}
\tag{1}
$$

where $\mathcal{V} \in \{\mathcal{V}_{\mathbf{L}}, \mathcal{V}_{\mathbf{U}}, \mathcal{V}_{\mathbf{L},\mathbf{U}}\}$ in both equations. The bounds are the tightest bounds which can be computed knowing only the corresponding sets of matrices. Bounds reduce to the exact results, if the sets contain only a single matrix which means that $\rho(\mathbf{L}) = 1$ with the consequence that $\mathbf{U} = \mathbf{L}$. In this case $\mathcal{V}_{\mathbf{L}} = \{\mathbf{v}\}$ where $\mathbf{v}$ is the left eigenvector of $\mathbf{L}$. If $\rho(\mathbf{L}) < 1$, then the sets contain more than one matrix and the following theorem shows how to compute bounds from $\mathcal{V}_{\mathbf{L}}$.

Theorem 2.1 ([4]) *Let $\mathbf{L} \geq \mathbf{0}$, $\mathbf{L}\mathbf{e}^T \leq \mathbf{e}^T$, $\rho(\mathbf{L}) < 1$ and let $\mathbf{L}$ be irreducible, then*

1. $(\mathbf{I} - \mathbf{L})$ *is nonsingular,*
2. $\mathbf{N} = (\mathbf{I} - \mathbf{L})^{-1} \geq \mathbf{0}$,
3. $\forall \mathbf{v} \in \mathcal{V}_{\mathbf{L}} \exists \mathbf{a} \geq \mathbf{0}, \mathbf{a}\mathbf{e}^T = 1.0$ *such that* $\mathbf{a}\mathbf{Z} = \mathbf{v}$ *where* $\mathbf{Z} = \left(diag(\mathbf{N}\mathbf{e}^T)\right)^{-1} \mathbf{N}$,
4. $\mathbf{p}_{\mathcal{V}_{\mathbf{L}}}^{-}(i) = \min_{j \in \mathcal{S}} \mathbf{Z}(j,i) \leq \mathbf{v}(i) \leq \max_{j \in \mathcal{S}} \mathbf{Z}(j,i) = \mathbf{Z}(i,i) = \mathbf{p}_{\mathcal{V}_{\mathbf{L}}}^{+}(i)$,
5. $E_{\mathcal{V}_{\mathbf{L}}}^{-}[R] = \min_{i \in \mathcal{S}} \mathbf{e}_i \mathbf{Z}\mathbf{r} \leq E[R] \leq \max_{i \in \mathcal{S}} \mathbf{e}_i \mathbf{Z}\mathbf{r} = E_{\mathcal{V}_{\mathbf{L}}}^{+}[R]$

Similar bounds under more restricted conditions can be computed for the upper bound matrix $\mathbf{U}$.

Theorem 2.2 ([4]) *Let $\mathbf{U} \geq \mathbf{0}$ and $\mathbf{U}\mathbf{e}^T \geq \mathbf{e}^T$. If the inverse matrix $\mathbf{M} = (\mathbf{I} - \mathbf{U})^{-1}$ exists and satisfies $\mathbf{M}\mathbf{e}^T < \mathbf{0}$ and $\mathbf{e}\mathbf{M} < \mathbf{0}$, then*

1. $\forall \mathbf{v} \in \mathcal{V}_{\mathbf{U}} \exists \mathbf{a} \geq \mathbf{0}, \mathbf{a}\mathbf{e}^T = 1.0$ *such that* $\mathbf{a}\mathbf{Y} = \mathbf{v}$ *where* $\mathbf{Y} = \left(diag(\mathbf{M}\mathbf{e}^T\right)^{-1} \mathbf{M}$,
2. $\mathbf{p}_{\mathcal{V}_{\mathbf{U}}}^{-}(i) = \min_{j \in \mathcal{S}} \mathbf{Y}(j,i) \leq \mathbf{v}(i) \leq \max_{j \in \mathcal{S}} \mathbf{Y}(j,i) = \mathbf{Y}(i,i) = \mathbf{p}_{\mathcal{V}_{\mathbf{U}}}^{+}(i)$,
3. $E_{\mathcal{V}_{\mathbf{U}}}^{-}[R] = \min_{i \in \mathcal{S}}(\mathbf{e}_i \mathbf{Y}\mathbf{r}) \leq E[R] \leq \max_{i \in \mathcal{S}}(\mathbf{e}_i \mathbf{Y}\mathbf{r}) = E_{\mathcal{V}_{\mathbf{U}}}^{+}[R]$.

The minimum and maximum values computed in step 4 and 5 (2 and 3) of the theorems can be improved by building the minimum/maximum according to the elements in $\mathcal{C}_{\mathbf{L},\mathbf{U}}$ if both matrices $\mathbf{L}$ and $\mathbf{U}$ are known. In this case we get the following bounds for $\mathbf{p}(i)$

$$\begin{aligned} \mathbf{p}^{-}_{\mathcal{V}_{\mathbf{L}},\mathcal{V}_{\mathbf{U}}}(i) &= \max\left(\min_{j\in\mathcal{C}_{\mathbf{L},\mathbf{U}}} \mathbf{Z}(j,i),\ \min_{k\in\mathcal{C}_{\mathbf{L},\mathbf{U}}} \mathbf{Y}(k,i)\right) \leq \mathbf{p}(i) \text{ and} \\ \mathbf{p}^{+}_{\mathcal{V}_{\mathbf{L}},\mathcal{V}_{\mathbf{U}}}(i) &= \min\left(\max_{j\in\mathcal{C}_{\mathbf{L},\mathbf{U}}} \mathbf{Z}(j,i),\ \max_{k\in\mathcal{C}_{\mathbf{L},\mathbf{U}}} \mathbf{Y}(k,i)\right) \geq \mathbf{p}(i) \end{aligned} \tag{2}$$

and similar bounds for $E[R]$

$$\begin{aligned} E^{-}_{\mathcal{V}_{\mathbf{L}},\mathcal{V}_{\mathbf{U}}}[R] &= \max\left(\min_{j\in\mathcal{C}_{\mathbf{L},\mathbf{U}}} \mathbf{e}_j\mathbf{Z}\mathbf{r},\ \min_{k\in\mathcal{C}_{\mathbf{L},\mathbf{U}}} \mathbf{e}_k\mathbf{Y}\mathbf{r}\right) \leq E[R] \text{ and} \\ E^{+}_{\mathcal{V}_{\mathbf{L}},\mathcal{V}_{\mathbf{U}}}[R] &= \min\left(\max_{j\in\mathcal{C}_{\mathbf{L},\mathbf{U}}} \mathbf{e}_j\mathbf{Z}\mathbf{r},\ \max_{k\in\mathcal{C}_{\mathbf{L},\mathbf{U}}} \mathbf{e}_k\mathbf{Y}\mathbf{r}\right) \geq E[R] \end{aligned} \tag{3}$$

The theorems show that the tightest possible bounds are computed if only matrix $\mathbf{L}$ ($\mathbf{U}$) is known, because the bound can be reached by some vector from $\mathcal{V}_{\mathbf{L}}$ ($\mathcal{V}_{\mathbf{U}}$) which belongs to a matrix from $\mathcal{P}_{\mathbf{L}}$ ($\mathcal{P}_{\mathbf{U}}$). However, if both matrices $\mathbf{L}$ and $\mathbf{U}$ are known, then the bounds are no longer sharp (i.e., (2) and (3) compute no longer the tightest possible bounds), because there might be no matrix in $\mathcal{P}_{\mathbf{L},\mathbf{U}}$ with a corresponding eigenvector in $\mathcal{V}_{\mathbf{L},\mathbf{U}}$ that reaches the bounds. Therefore we use the notation $\mathbf{p}_{\mathcal{V}_{\mathbf{L}},\mathcal{V}_{\mathbf{U}}}$ ($E_{\mathcal{V}_{\mathbf{L}},\mathcal{V}_{\mathbf{U}}}$) instead of $\mathbf{p}_{\mathcal{V}_{\mathbf{L},\mathbf{U}}}$ ($E_{\mathcal{V}_{\mathbf{L},\mathbf{U}}}$). In the following section we introduce an improved bounding method that computes bounds by considering matrices in $\mathcal{P}_{\mathbf{L},\mathbf{U}}$ and these bounds will be sharp for $\mathbf{p}$, because there is always a matrix in $\mathcal{P}_{\mathbf{L},\mathbf{U}}$ with a corresponding eigenvector in $\mathcal{V}_{\mathbf{L},\mathbf{U}}$ that reaches the computed bound.

Before we introduce the improved bounding method, we extend the basic approach from DTMCs to CTMCs which has also been in done in a similar way in [9]. The transformation is based on randomization of the matrix which transforms the CTMC into a DTMC with the same stationary distribution [14]. Let Y_t be a CTMC with finite state space $\mathcal{S} = \{1, \ldots, n\}$, irreducible generator matrix $\mathbf{Q}$ with stationary distribution $\mathbf{p}$. For any finite $q \geq \max_i(|\mathbf{Q}(i,i)|)$, $\mathbf{P} = \mathbf{Q}/q + \mathbf{I}$ is a stochastic matrix which is guaranteed to be aperiodic if q is chosen larger than the maximum absolute value of a diagonal element. Furthermore, $\mathbf{P}$ is irreducible if and only if $\mathbf{Q}$ is irreducible and $\mathbf{p}$ is the stationary solution of the CTMC and the resulting DTMC. Let $\mathbf{V}$ and $\mathbf{W}$ be two matrices with $\mathbf{V} \leq \mathbf{Q}$ and $\mathbf{V}(i,j) \geq 0.0$ for $i \neq j$ and $\mathbf{W} \geq \mathbf{Q}$ with $\mathbf{W}(i,i) \leq 0$. For any finite $q \geq \max(\max_i(|\mathbf{V}(i,i)|), \max_i(|\mathbf{W}(i,i)|))$, $\mathbf{P} = \mathbf{Q}/q + \mathbf{I}$ is a stochastic matrix, $\mathbf{L} = \mathbf{V}/q + \mathbf{I}$ is a matrix with $\mathbf{0} \leq \mathbf{L} \leq \mathbf{P}$, $\mathbf{L}\mathbf{e}^T \leq \mathbf{e}^T$ and $\mathbf{U} = \mathbf{W}/q + \mathbf{I}$ is a matrix with $\mathbf{U} \geq \mathbf{P}$ and $\mathbf{U}\mathbf{e}^T \geq \mathbf{e}^T$. Furthermore, if $\mathbf{V}$ is irreducible, then $\mathbf{L}$ is irreducible. After these transformations, theorems 2.1 and 2.2 can be applied to compute bounds for the stationary distribution and the expected reward of the CTMC.

Small Example: We will explain the approach by means of a small example. Consider a system with a single server and one buffer place which serves parts that are arriving according a Poisson process with rate λ. During service the server may fail loosing the part in service. After a failure the server has to be repaired. Service requirements, time to failure and repair times are exponentially distributed with rates μ, ω and ν, respectively. The state space can be described by a tuple (x_1, x_2) where x_1 describes the number of parts in service (0 or 1) and x_2 describes the state of the server (0 failed, 1 ok). Thus, the overall state space consists of the states: 1) $(0,1)$, 2) $(1,1)$ and 3) $(0,0)$ and the generator matrix of the CTMC is given by

$$\begin{pmatrix} -\lambda & \lambda & 0 \\ \mu & -(\mu+\omega) & \omega \\ \nu & 0 & -\nu \end{pmatrix}$$

The different rates belong to the following intervals $\lambda \in [0.495, 0.505]$, $\mu \in [0.99, 1.01]$, $\omega \in [9.99\& - 5, 1.01\& - 4]$ and $\nu \in [9.99\& - 4, 1.01\& - 3]$. Thus, all rates are known with a precision of $\pm 1\%$. As result the probability of state 2 should be computed (i.e. $\mathbf{r} = (0, 1, 0)^T$).

With $q = 1.010101$ we obtain the following matrices $\mathbf{L}$ and $\mathbf{U}$.

$$\mathbf{L} = \begin{pmatrix} 5.0005e-1 & 4.9005e-1 & 0.0 \\ 9.8010e-1 & 0.0 & 9.8901e-5 \\ 9.8901e-4 & 0.0 & 9.9900e-1 \end{pmatrix} \quad \mathbf{U} = \begin{pmatrix} 5.0995e-1 & 4.9995e-1 & 0.0 \\ 9.9990e-1 & 1.9801e-1 & 9.9990e-5 \\ 9.9990e-4 & 0.0 & 9.9901e-1 \end{pmatrix}$$

The inverse matrices $\mathbf{N} = (\mathbf{I} - \mathbf{L})^{-1}$ and $\mathbf{M} = (\mathbf{I} - \mathbf{U})^{-1}$ are given by

$$\mathbf{N} = \begin{pmatrix} 51.0098 & 24.974 & 2.4722 \\ 49.9997 & 25.5024 & 2.5222 \\ 50.4487 & 24.7224 & 1002.44 \end{pmatrix} \quad \mathbf{M} = \begin{pmatrix} -50.0013 & -25.5031 & -2.5761 \\ -51.0114 & -24.9981 & -2.5251 \\ -50.5064 & -25.7607 & 1007.5 \end{pmatrix}$$

Since matrix $\mathbf{M}$ does not observe the conditions given in theorem 2.2, it cannot be used for bound computation. Matrix $\mathbf{Z}$ is given by

$$\mathbf{Z} = \begin{pmatrix} 0.65017 & 0.31831 & 0.03151 \\ 0.64082 & 0.32685 & 0.03233 \\ 0.04682 & 0.02294 & 0.93024 \end{pmatrix}$$

such that $E[R] = \mathbf{pr} = \mathbf{pe}_2 \in [0.02294, 0.32685]$. Obviously these bounds are not satisfactory since although the rates differ only by 1%, the bounds differ by more than one oder of magnitude. Thus, it might be worth to consider the problem which yields such wide bounds. Observe that the set $\mathcal{P}_{\mathbf{L}}$ contains all stochastic matrices that are elementwise larger than $\mathbf{L}$. This implies that the set contains also a matrix where the transition rates into state 3) are maximized which means that the difference between minimal and maximal arrival and service rate is added to the last column. The following matrix $\mathbf{Q}^-$ describes this situation.

$$\mathbf{Q}^- = \begin{pmatrix} -0.505 & 0.495 & 0.01 \\ 0.99 & -1.010101 & 2.0101\& - 2 \\ 9.99\& - 4 & 0 & -9.99\& - 4 \end{pmatrix}$$

The stationary solution of this CTMC corresponds to the third row of $\mathbf{Z}$ and describes the lower bound for $\mathbf{p}(2)$.

However, obviously the bounding approach does not exploit all available information. By adding the differences in service and arrival rates to failure rates, probability of a failure is increased drastically and it is not taken into account that the third element in the first row has to be zero and the third element in the second row can be at most $1.001\& - 3$.

3 Improved Stationary Bounds

In the sequel $\mathbf{P}(\bullet j)$ describes column j of matrix $\mathbf{P}$, and $\mathbf{P}(j \bullet)$ describes row j of matrix $\mathbf{P}$. The following theorem shows how to generate a pair of initial bounding matrices $\mathbf{L}^{(0)}$ and $\mathbf{U}^{(0)}$ if bounds for single probabilities have to be computed (i.e, $\mathbf{r} = (\mathbf{e}_i)^T$).

Theorem 3.1 *Let* $\mathbf{L}$ *and* $\mathbf{U}$ *be two matrices with the following properties:*
$\mathbf{L}$ *is irreducible,* $\rho(\mathbf{L}) < 1$, $\rho(\mathbf{U}) > 1$, $\mathbf{0} < \mathbf{L} < \mathbf{U}$. *Let* $i \in \mathcal{S}$.

1. *Define* $\mathbf{L}^{(0)}(j,l) = \mathbf{L}(j,l)$ *if* $l \neq i$ *and* $\mathbf{L}^{(0)}(j,i) = \mathbf{U}(j,i)$ *and* $\mathbf{U}^{(0)}(j,l) = \min\left(\mathbf{U}(j,l), 1.0 - \sum_{m \in \mathcal{S} \setminus \{l\}} \mathbf{L}^{(0)}(j,m)\right)$, *then* $v_i^+ = \max_{\mathbf{v} \in \mathcal{V}_{\mathbf{L}^{(0)},\mathbf{U}^{(0)}}} \mathbf{v}(i) = \max_{\mathbf{v} \in \mathcal{V}_{\mathbf{L},\mathbf{U}}} \mathbf{v}(i)$.

2. *Define* $\mathbf{U}^{(0)}(j,l) = \mathbf{U}(j,l)$ *if* $l \neq i$ *and* $\mathbf{U}^{(0)}(j,i) = \mathbf{L}(j,i)$ *and* $\mathbf{L}^{(0)}(j,l) = \max\left(\mathbf{L}^{(0)}(j,l), 1.0 - \sum_{m\in\mathcal{S}\setminus\{l\}} \mathbf{U}^{(0)}(j,m)\right)$, *then* $v_i^- = \min_{\mathbf{v}\in\mathcal{V}_{\mathbf{L}^{(0)},\mathbf{U}^{(0)}}} \mathbf{v}(i) = \min_{\mathbf{v}\in\mathcal{V}_{\mathbf{L},\mathbf{U}}} \mathbf{v}(i)$.

Proof. We start with proof for 1. and show that there exists a stochastic matrix $\mathbf{P}$ with $\mathbf{P}(\bullet i) = \mathbf{U}(\bullet i)$, $\mathbf{L} \leq \mathbf{P} \leq \mathbf{U}$ which implies $\mathbf{P} \in \mathcal{P}_{\mathbf{L}^{(0)},\mathbf{U}^{(0)}}$ and a normalized left eigenvector $\mathbf{w}$ with $\mathbf{w}(i) = v_i^+$. Each matrix $\mathbf{A} \in \mathcal{P}_{\mathbf{L},\mathbf{U}}$ is of the form $\mathbf{A} = \mathbf{L}+\mathbf{B}+\mathbf{C}$ where $\mathbf{C}\mathbf{e}^T = \mathbf{d}_i = \mathbf{U}(\bullet i) - \mathbf{L}(\bullet i)$ and $\mathbf{B}(\bullet i) = \mathbf{0}$. If $\mathbf{d}_i = \mathbf{0}$, then the result holds obviously since $\mathbf{L} = \mathbf{L}^{(0)}$. Thus we assume $\mathbf{d}_i > \mathbf{0}$. Let $\mathbf{Z} = (diag((\mathbf{I}-\mathbf{L}-\mathbf{B})\mathbf{e}^T)^{-1}(\mathbf{I}-\mathbf{L}-\mathbf{B})^{-1}$. Following [5] $\mathbf{Z}(i,i) \geq \mathbf{Z}(j,i)$ for all $j \neq i$. Furthermore the normalized left eigenvector of $\mathbf{A}$ can be represented as $\mathbf{a}\mathbf{Z}$ with $\mathbf{a} = \mathbf{a}(\mathbf{I}-\mathbf{L}-\mathbf{B})^{-1}\mathbf{C}$ and $\mathbf{a}\mathbf{e}^T = 1.0$ [8]. Since the i-th element of the eigenvector equals $\sum_{j=1}^n \mathbf{a}(j)\mathbf{Z}(j,i)$, vector $\mathbf{a} = \mathbf{e}_i$ maximizes the i-th component of the eigenvector. However, $\mathbf{a} = \mathbf{e}_i$ results from $\mathbf{C} = \mathbf{D}_i = \mathbf{d}_i\mathbf{e}_i$ which completes this part of the proof.

The proof of the minimum 2. is similar. As before we show there exists a stochastic matrix $\mathbf{P}$ with $\mathbf{P}(\bullet i) = \mathbf{L}(\bullet i)$ and a normalized left eigenvector $\mathbf{w}$ with $\mathbf{w}(i) = v_i^-$. Define matrices $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$ and $\mathbf{Z}$ as for the maximum. The elements of vector $\mathbf{a}$ are defined by the columns of matrix $\mathbf{C}$ for fixed matrices $\mathbf{L}$ and $\mathbf{B}$. By choosing $\mathbf{C}(\bullet i) = \mathbf{0}$ $\mathbf{a}(i) = 0$. Since $\mathbf{Z}(i,i) \geq \mathbf{Z}(j,i)$, we can always find an appropriate matrix $\mathbf{C}$ with $\mathbf{C}(\bullet i) = \mathbf{0}$ such that $\mathbf{P} = \mathbf{L}+\mathbf{B}+\mathbf{C}$ and for the corresponding eigenvector $\mathbf{w}(i) = v_i^-$ holds. □

The matrices in the theorem are generated with respect to one state and with respect to the minimum or maximum which should be determined. However, to avoid an overloading of the notation, we do not include the state and the maximum/minimum in our notations. With the previous theorem initial matrices $\mathbf{L}^{(0)}$ and $\mathbf{U}^{(0)}$ are generated which preserve the maximum/minimum of one vector component. For general rewards we assume that $\mathbf{L}^{(0)} = \mathbf{L}$ and $\mathbf{U}^{(0)} = \mathbf{U}$ and still use the notation $\mathbf{L}$ and $\mathbf{U}$ for the initial matrices.

Theorem 3.2 *Let* $\mathbf{P}_1$ *be a stochastic matrix with left eigenvector* $\mathbf{p}_1$, *let* $\mathbf{r}$ *be some reward vector, let* $c^-, c^+ \in \{1,\ldots,n\}$ $(c^- \neq c^+)$ *be two columns and let* $\mathbf{L}$, $\mathbf{U}$ *be two bounding matrices with* $\mathbf{L} < \mathbf{P}_1 < \mathbf{U}$, $\mathbf{L}(\bullet i) = \mathbf{P}_1(\bullet i)$ *for* $i \neq c^-$, $\mathbf{L}(\bullet c^-) = \mathbf{P}_1(\bullet c^-) - \mathbf{d}$, *and* $\mathbf{U}(\bullet i) = \mathbf{P}_1(\bullet i)$ *for* $i \neq c^+$, $\mathbf{U}(\bullet c^+) = \mathbf{P}_1(\bullet c^+) + \mathbf{d}$ *for some vector* $\mathbf{d} < \mathbf{P}_1(\bullet c^-)$.

Define a stochastic matrix $\mathbf{P}_2 = \mathbf{L} + \mathbf{d}(\mathbf{e}_{c^+})^T = \mathbf{P}_1 - \mathbf{d}(\mathbf{e}_{c^-})^T + \mathbf{d}(\mathbf{e}_{c^+})^T$ *with left eigenvector* $\mathbf{p}_2$, *then for all* $\mathbf{p} \in \mathcal{V}_{\mathbf{L},\mathbf{U}}$:

$$\mathbf{p}_1\mathbf{r} \leq \mathbf{p}\mathbf{r} \leq \mathbf{p}_2\mathbf{r} \text{ or } \mathbf{p}_2\mathbf{r} \leq \mathbf{p}\mathbf{r} \leq \mathbf{p}_1\mathbf{r} \ .$$

Proof. Since $\mathcal{C}_{\mathbf{L},\mathbf{U}} = \{c^-, c^+\}$, each $\mathbf{p} \in \mathcal{V}_{\mathbf{L},\mathbf{U}}$ can be represented as $(\lambda\mathbf{e}_{c^-} + (1.0-\lambda)\mathbf{e}_{c^+})\mathbf{Z}$ where $0 \leq \lambda \leq 1.0$ and $\mathbf{Z} = diag((\mathbf{I}-\mathbf{L})^{-1}\mathbf{e}^T)^{-1}(\mathbf{I}-\mathbf{L})^{-1}$.

Furthermore $\mathbf{p}_1 = \mathbf{e}_{c^-}\mathbf{Z}$ and $\mathbf{p}_2 = \mathbf{e}_{c^+}\mathbf{Z}$.

However, for each $\mathbf{p} \in \mathcal{V}_{\mathbf{L},\mathbf{U}}$:
$\min(\mathbf{e}_{c^-}\mathbf{Z}\mathbf{r}, \mathbf{e}_{c^+}\mathbf{Z}\mathbf{r}) = \min(\mathbf{p}_1\mathbf{r}, \mathbf{p}_2\mathbf{r}) \leq \mathbf{p}\mathbf{r} \leq \max(\mathbf{e}_{c^-}\mathbf{Z}\mathbf{r}, \mathbf{e}_{c^+}\mathbf{Z}\mathbf{r}) = \max(\mathbf{p}_1\mathbf{r}, \mathbf{p}_2\mathbf{r})$.
which implies the above relation. □

The previous theorem shows that for a stochastic matrix $\mathbf{P}$ for which lower and upper bounds of some elements are known, one can increase the elements of one column and decrease the elements of another column to generate a stochastic matrix with a left eigenvector where the expected reward is not smaller/larger than the expected reward derived from $\mathbf{P}$. The following definition defines extremal points of the polyhedron $\mathcal{P}_{\mathbf{L},\mathbf{U}}$.

Definition 3.1 *A matrix* $\mathbf{P} \in \mathcal{P}_{\mathbf{L},\mathbf{U}}$ *is an extremal point of the polyhedron, if and only if no matrices* $\mathbf{P}_1, \mathbf{P}_2 \in \mathcal{P}_{\mathbf{L},\mathbf{U}}$ $(\mathbf{P}_1 \neq \mathbf{P}_2)$ *exist such that* $\mathbf{P} = \lambda\mathbf{P}_1 + (1-\lambda)\mathbf{P}_2$ *for* $0 < \lambda < 1$.

The set of extremal points of $\mathcal{P}_{\mathbf{L},\mathbf{U}}$ *is denoted* $\mathcal{E}_{\mathbf{L},\mathbf{U}}$.

Theorem 3.3 $\mathbf{P} \in \mathcal{E}_{\mathbf{L},\mathbf{U}} \Leftrightarrow$
$\forall r \in \{1,\ldots,n\}\ \exists c_r \in \{1,\ldots,n\}$ *such that* $\mathbf{P}(r,i) = \mathbf{L}(r,i)$ *or* $\mathbf{P}(r,i) = \mathbf{U}(r,i)$ *for all* $i \neq c_r$.

Proof. $\Rightarrow$: Assume that two columns c_1, c_2 exist such that
$\mathbf{L}(r,c_1) < \mathbf{P}(r,c_1) < \mathbf{U}(r,c_1)$ and $\mathbf{L}(r,c_2) < \mathbf{P}(r,c_2) < \mathbf{U}(r,c_2)$.
Define $\Delta = \min_{c\in\{c_1,c_2\}}(\mathbf{P}(r,c) - \mathbf{L}(r,c), \mathbf{U}(r,c) - \mathbf{P}(r,c))$.
Define two matrices $\mathbf{P}_1, \mathbf{P}_2$ such that
$\mathbf{P}_1(i,j) = \mathbf{P}_2(i,j) = \mathbf{P}(i,j)$ for $i \neq r$ or $j \neq c_1, c_2$,
$\mathbf{P}_1(r,c_1) = \mathbf{P}(r,c_1) - \Delta$, $\mathbf{P}_1(r,c_2) = \mathbf{P}(r,c_2) + \Delta$,
$\mathbf{P}_2(r,c_1) = \mathbf{P}(r,c_1) + \Delta$ and $\mathbf{P}_2(r,c_2) = \mathbf{P}(r,c_2) - \Delta$.
Since $\mathbf{P}_1$ and $\mathbf{P}_2$ are stochastic matrices and $\mathbf{L} < \mathbf{P}_1, \mathbf{P}_2 < \mathbf{U}$ we have $\mathbf{P}_1, \mathbf{P}_2 \in \mathcal{P}_{\mathbf{L},\mathbf{U}}$. Furthermore $\mathbf{P} = 0.5\mathbf{P}_1 + 0.5\mathbf{P}_2$ such that $\mathbf{P} \in \mathcal{E}_{\mathbf{L},\mathbf{U}}$ cannot hold or matrices $\mathbf{P}_1, \mathbf{P}_2$ cannot exist.

$\Leftarrow$: Since all matrices in $\mathcal{E}_{\mathbf{L},\mathbf{U}}$ are stochastic matrices, all row sums have to be one and the knowledge of $n-1$ elements in a row determines the last element uniquely. A matrix element $\mathbf{P}(i,j)$ which is equal to $\mathbf{L}(i,j)$ or $\mathbf{U}(i,j)$ cannot be represented as a convex linear combination of two different elements since elements cannot become larger or smaller than their bounds. Consequently, $n-1$ elements in each row are fixed such that the whole matrix is fixed and $\mathbf{P}$ cannot be represented as convex linear combination of two matrices from $\mathcal{E}_{\mathbf{L},\mathbf{U}}$. □

Observe that the set $\mathcal{E}_{\mathbf{L},\mathbf{U}}$ is finite. The following theorem shows that maximum or minimum reward can be reached by a left eigenvector of a matrix from $\mathcal{E}_{\mathbf{L},\mathbf{U}}$.

Theorem 3.4 *Let* $\mathbf{P} \in \mathcal{P}_{\mathbf{L},\mathbf{U}}$ *be a matrix from the polyhedron defined by bounding matrices* $\mathbf{L}$ *and* $\mathbf{U}$*, let* $\mathbf{p}$ *be the left eigenvector of* $\mathbf{P}$ *and let* $\mathbf{r}$ *be a reward vector, then there exist matrices* $\mathbf{P}^-, \mathbf{P}^+ \in \mathcal{E}_{\mathbf{L},\mathbf{U}}$ *with eigenvectors* $\mathbf{p}^-$ *and* $\mathbf{p}^+$ *such that* $\mathbf{p}^-\mathbf{r} \leq \mathbf{p}\mathbf{r} \leq \mathbf{p}^+\mathbf{r}$.

Proof. We proof the result by construction of $\mathbf{P}^+$. The construction of $\mathbf{P}^-$ is completely analogous.

Let $r,i,j \in \{1,\ldots,n\}$ $(i < j)$ such that $\mathbf{L}(r,i) < \mathbf{P}(r,i) < \mathbf{U}(r,i)$ and $\mathbf{L}(r,j) < \mathbf{P}(r,j) < \mathbf{U}(r,j)$. If no such elements exist, then $\mathbf{P} \in \mathcal{E}(\mathbf{L},\mathbf{U})$ according to theorem 3.3 and after letting $\mathbf{P} = \mathbf{P}^+ = \mathbf{P}^-$, the proof is done.

Define $\Delta = \min_{k\in\{i,j\}}(\mathbf{P}(r,k) - \mathbf{L}(r,k), \mathbf{U}(r,k) - \mathbf{P}(r,k))$ and matrix $\mathbf{L}_1 = \mathbf{P} - \Delta(\mathbf{e}_r)^T(\mathbf{e}_j + \mathbf{e}_i)$. Since $\mathbf{L}_1$ is an irreducible lower bounding matrix, we can compute $\mathbf{Z}_1$ as the normalized inverse of $(\mathbf{I} - \mathbf{L}_1)$.

We now generate a new matrix $\mathbf{P}_1 \in \mathcal{P}_{\mathbf{L},\mathbf{U}}$ from $\mathbf{P}$ as follows:
If $\mathbf{e}_i\mathbf{Z}_1\mathbf{r} > \mathbf{e}_j\mathbf{Z}_1\mathbf{r}$ let $k = i$ otherwise let $k = j$.
Define $\mathbf{P}_1 = \mathbf{L}_1 + 2\Delta(\mathbf{e}_r)^T\mathbf{e}_k = \mathbf{P} + \Delta((\mathbf{e}_r)^T(\mathbf{e}_k - \mathbf{e}_l)$ where $l = j$ if $k = i$ and $l = i$ if $k = j$. The eigenvector $\mathbf{p}$ and $\mathbf{p}_1$ can be represented as $\mathbf{p} = \lambda\mathbf{e}_i\mathbf{Z}_1 + (1-\lambda)\mathbf{e}_j\mathbf{Z}_1$ for $0 < \lambda < 1$ and $\mathbf{p}_1 = \mathbf{e}_k\mathbf{Z}_1$. For the rewards we have $\mathbf{p}\mathbf{r} = (\lambda\mathbf{e}_i + (1-\lambda)\mathbf{e}_j)\mathbf{Z}_1\mathbf{r} \leq \mathbf{e}_k\mathbf{Z}_1\mathbf{r}$ such that the reward for matrix $\mathbf{P}_1$ larger or equal to the reward of $\mathbf{p}$.

If $\mathbf{P}_1 \in \mathcal{E}_{\mathbf{L},\mathbf{U}}$, then we are done, otherwise the step is repeated with $\mathbf{P}_1$ instead of $\mathbf{P}$. Observe that in each step the reward is increased or if it is not increased, then the element with the larger column index is increased. Thus, the approach cannot produce cycles by generating the same matrices again and the number of elements equal to the upper or lower bound keeps constant or is increased by one. This process eventually generates a matrix from $\mathcal{E}_{\mathbf{L},\mathbf{U}}$. □

Corollary 3.5 *If* $\mathbf{P} \in \mathcal{P}_{\mathbf{L},\mathbf{U}}$ *with left eigenvector* $\mathbf{p}$ *such that* $\mathbf{p}\mathbf{r} \geq \mathbf{p}_1\mathbf{r}$ *for all* $\mathbf{p}_1 \in \mathcal{V}_{\mathbf{L},\mathbf{U}}$*, then exists some matrix* $\mathbf{P}_2 \in \mathcal{E}_{\mathbf{L},\mathbf{U}}$ *with eigenvector* $\mathbf{p}_2$ *and* $\mathbf{p}\mathbf{r} = \mathbf{p}_2\mathbf{r}$*. If* $\mathbf{p}\mathbf{r} \leq \mathbf{p}_1\mathbf{r}$ *for all* $\mathbf{p}_1 \in \mathcal{V}_{\mathbf{L},\mathbf{U}}$*, then exists some matrix* $\mathbf{P}_3 \in \mathcal{E}_{\mathbf{L},\mathbf{U}}$ *with eigenvector* $\mathbf{p}_3$ *and* $\mathbf{p}\mathbf{r} = \mathbf{p}_3\mathbf{r}$.

The corollary shows that the finite set $\mathcal{E}_{\mathbf{L},\mathbf{U}}$ contains a matrix with an eigenvector maximizing/minimizing the reward. Unfortunately, the number of possible orderings which have to be considered when generating the matrix grows exponentially in n and it is not clear whether the optimum has been reached or not before testing all matrices in the set. At least the latter problem can be solved using the following results.

Definition 3.2 *Let $\mathbf{P} \in \mathcal{P}_{\mathbf{L},\mathbf{U}}$ and let i, j $(i \neq j)$ such that $\mathbf{d}_{\mathbf{P}}^{i,j} > \mathbf{0}$ where $\mathbf{d}_{\mathbf{P}}^{i,j}(k) = \min(\mathbf{P}(i,k) - \mathbf{L}(i,k), \mathbf{U}(j,k) - \mathbf{P}(j,k))$ for all $k \in \{1, \ldots, n\}$. Define for $k > 1$*

$$\begin{aligned}
&\mathcal{N}^{(1)}(\mathbf{P}) = \{\mathbf{P}' | \exists i, j : \mathbf{P}' = \mathbf{P} + \mathbf{d}_{\mathbf{P}}^{i,j}(\mathbf{e}_j - \mathbf{e}_i)\} \ , \\
&\mathcal{N}^{(k)}(\mathbf{P}) = \cup_{\mathbf{P}' \in \mathcal{N}^{(1)}(\mathbf{P})} \mathcal{N}^{(k-1)}(\mathbf{P}') \ \textit{and} \\
&\mathcal{M}^{(1)}(\mathbf{P}) = \{\mathbf{P}' | \exists \mathbf{0} < \mathbf{c}^{i,j} \leq \mathbf{d}_{\mathbf{P}}^{i,j} : \mathbf{P}' = \mathbf{P} + \mathbf{c}^{i,j}(\mathbf{e}_j - \mathbf{e}_i)\} \ , \\
&\mathcal{M}^{(k)}(\mathbf{P}) = \cup_{\mathbf{P}' \in \mathcal{M}^{(1)}(\mathbf{P})} \mathcal{M}^{(k-1)}(\mathbf{P}')
\end{aligned}$$

The sets $\mathcal{N}^{(k)}(\mathbf{P})$ define an in k increasing neighborhood of matrix $\mathbf{P}$. Obviously, $\mathcal{N}^{(k)}(\mathbf{P}) \subseteq \mathcal{P}_{\mathbf{L},\mathbf{U}}$ for $\mathbf{P} \in \mathcal{P}_{\mathbf{L},\mathbf{U}}$. Observe that $\mathcal{N}^{(k)}$ is finite, whereas $\mathcal{M}^{(k)}(\mathbf{P})$ is infinite for every $k \geq 1$ whenever $\mathcal{P}_{\mathbf{L},\mathbf{U}}$ contains more than one matrix. In the sequel we use the notation $\mathcal{V}(\mathcal{P})$ for the set of all eigenvectors $\mathbf{p}'$ of matrices $\mathbf{P}' \in \mathcal{P}$.

Theorem 3.6 *Let $\mathbf{P} \in \mathcal{P}_{\mathbf{L},\mathbf{U}}$ and $\mathbf{p}$ be the normalized left eigenvector. If $\mathbf{pr} \geq \mathbf{p}'\mathbf{r}$ for all $\mathbf{p}' \in \mathcal{V}(\mathcal{N}^{(1)}(\mathbf{P}))$, then $\mathbf{pr} \geq \mathbf{p}''\mathbf{r}$ for all $\mathbf{p}'' \in \mathcal{V}(\mathcal{M}^{(1)}(\mathbf{P}))$.*

Proof. Define a matrix $\mathbf{L}'$ such that $\mathbf{L}'(i\bullet) = \mathbf{P}(i\bullet) - \mathbf{d}_{\mathbf{P}}^{i,j}$ and $\mathbf{L}'(k\bullet) = \mathbf{P}(k\bullet)$ for $k \neq i$. Let $\mathbf{N} = (\mathbf{I} - \mathbf{L}')^{-1}$ and $\mathbf{Z} = diag(\mathbf{N}\mathbf{e}^T)^{-1}\mathbf{N}$. Furthermore choose $\mathbf{P}' = \mathbf{P} + \mathbf{d}_{\mathbf{P}}^{i,j}(\mathbf{e}_j - \mathbf{e}_i)$ and $\mathbf{P}'' = \mathbf{P} + \mathbf{c}^{i,j}(\mathbf{e}_j - \mathbf{e}_i)$ where $\mathbf{c}^{i,j} < \mathbf{d}_{\mathbf{P}}^{i,j}$, then we have $\mathbf{pr} = \mathbf{e}_i\mathbf{Zr} \geq \mathbf{p}'\mathbf{r} = \mathbf{e}_j\mathbf{Zr}$ and $\mathbf{p}''\mathbf{r} = (\lambda\mathbf{e}_i + (1-\lambda)\mathbf{e}_j)\mathbf{Zr}$ which implies $\mathbf{pr} \geq \mathbf{p}''\mathbf{r}$. □

The following theorem shows that a matrix $\mathbf{P}$ yielding a local optimum of the reward vector according to its neighborhood is also a global optimum. This is a fundamental observation which is exploited in the bounding algorithm developed in the following subsection.

Theorem 3.7 *If for some matrix $\mathbf{P} \in \mathcal{P}_{\mathbf{L},\mathbf{U}}$ with eigenvector $\mathbf{p}$: $\mathbf{pr} \geq \mathbf{p}'\mathbf{r}$ for all $\mathbf{p}' \in \mathcal{V}(\mathcal{N}^{(1)}(\mathbf{P}))$, then $\mathbf{pr} \geq \mathbf{p}'\mathbf{r}$ for all $\mathbf{p}' \in \mathcal{V}(\mathcal{P}_{\mathbf{L},\mathbf{U}})$.*
If for some matrix $\mathbf{P} \in \mathcal{P}_{\mathbf{L},\mathbf{U}}$ with eigenvector $\mathbf{p}$: $\mathbf{pr} \leq \mathbf{p}'\mathbf{r}$ for all $\mathbf{p}' \in \mathcal{V}(\mathcal{N}^{(1)}(\mathbf{P}))$, then $\mathbf{pr} \leq \mathbf{p}'\mathbf{r}$ for all $\mathbf{p}' \in \mathcal{V}(\mathcal{P}_{\mathbf{L},\mathbf{U}})$.

Proof. The proof can be found in the appendix. □

The theorem defines a maximum and minimum for the reward value. However, since rewards are assumed to be non negative, each minimization problem can be transformed into an equivalent maximization problem with negative reward vector $-\mathbf{r}$. Therefore we consider only the computation of the maximum in the following section.

4 A New Bounding Algorithm

An algorithm to compute bounds has to be based on theorem 3.7 to check for a given matrix $\mathbf{P} \in \mathcal{P}_{\mathbf{L},\mathbf{U}}$ with eigenvector $\mathbf{p}$ whether for all $\mathbf{P}' \in \mathcal{N}^{(1)}(\mathbf{P})$ with eigenvectors $\mathbf{p}'$ the relation $\mathbf{pr} \geq \mathbf{p}'\mathbf{r}$ holds. If this is not the case, then some matrix $\mathbf{P}' \in \mathcal{N}^{(1)}(\mathbf{P})$ improves the reward and this matrix can be used as a base for further iterative improvements until the maximum has been reached.

For an algorithmic description of the approach define for some matrix $\mathbf{P} \in \mathcal{P}_{\mathbf{L},\mathbf{U}}$ and some column index $i \in \{1,\ldots,n\}$ with $\mathbf{L}(\bullet i) < \mathbf{P}(\bullet i)$ the matrix

$$\begin{pmatrix} \mathbf{D} & \mathbf{d} \\ \mathbf{e}_i & 0 \end{pmatrix}$$

where $\mathbf{P} = \mathbf{D} + \mathbf{d}\mathbf{e}_i$ and $\mathbf{d} = \mathbf{P}(\bullet i) - \mathbf{L}(\bullet i)$. Let $\mathbf{N} = (\mathbf{I} - \mathbf{D})^{-1}$ and $\mathbf{Z} = (diag(\mathbf{N}\mathbf{e}^T))^{-1}\mathbf{N}$. By assumption the inverse matrix exists. The stationary vector and the expected reward of the Markov process described by $\mathbf{P}$ can be expressed as $\mathbf{e}_i\mathbf{Z}$ and $\mathbf{e}_i\mathbf{Z}\mathbf{r}$, respectively. Define two sets

$$\begin{array}{l} \mathcal{C}^+_{\mathbf{D},i} = \{j | j \in \{1,\ldots,n\} \wedge j \neq i \wedge (\mathbf{U}(\bullet j) - \mathbf{D}(\bullet j))^T\mathbf{d} > 0\} \quad \text{and} \\ \mathcal{C}^-_{\mathbf{D},i} = \{j | j \in \{1,\ldots,n\} \wedge j \neq i \wedge \mathbf{P}(\bullet j) > \mathbf{L}(\bullet j)\} \ . \end{array} \tag{4}$$

$\mathcal{C}^+_{\mathbf{D},i}$ contains all columns j into which probability mass can be shifted from column i. If probability mass is shifted from column i to j, then the expected reward resulting from the modified matrix can be expressed as
$(\lambda\mathbf{e}_i + (1-\lambda)\mathbf{e}_j)\mathbf{Z}\mathbf{r}$ for $0 \leq \lambda < 1$.
The modified matrix yields a larger reward, if $\mathbf{e}_j\mathbf{Z}\mathbf{r} > \mathbf{e}_i\mathbf{Z}\mathbf{r}$. Consequently, if some $j \in \mathcal{C}^+_{\mathbf{D},i}$ with $\mathbf{e}_j\mathbf{Z}\mathbf{r} > \mathbf{e}_i\mathbf{Z}\mathbf{r}$ exists, then a new matrix $\mathbf{P}' = \mathbf{P} - (\mathbf{e}_i - \mathbf{e}_j)\mathbf{c}$ exists with $\mathbf{c}(k) = \min(\mathbf{d}(k), \mathbf{U}(k,j) - \mathbf{P}(k,j))$. By definition of the set $\mathcal{C}^+_{\mathbf{D},i}$, $\mathbf{c} > \mathbf{0}$. To continue with the new matrix $\mathbf{P}'$, a representation similar to matrix $\mathbf{D}$ has to be defined. Let

$$\mathbf{D}' = \mathbf{D} + (\mathbf{d} - \mathbf{c})\mathbf{e}_i - (\mathbf{P}(\bullet j) - \mathbf{L}(\bullet j))\mathbf{e}_j \quad \text{and} \quad \mathbf{d}' = \mathbf{c} + \mathbf{P}(\bullet j) - \mathbf{L}(\bullet j) \tag{5}$$

and substitute $\mathbf{e}_i$ by $\mathbf{e}_j$ such that $\mathbf{D}'$, $\mathbf{d}'$ and $\mathbf{e}_j$ represent the new Markov chain. To continue with matrix $\mathbf{P}'$, the inverse matrix $\mathbf{N}' = (\mathbf{I} - \mathbf{D}')^{-1}$ has to be known. Instead of computing the inverse from scratch, one can compute $\mathbf{N}'$ more efficiently from $\mathbf{N}$ using the Sherman-Morrison-Woodbury formula [7, 11]. Adopted to our specific case, we have to compute
$(\mathbf{I} - \mathbf{D} - (\mathbf{d} - \mathbf{c})\mathbf{e}_i + (\mathbf{P}(\bullet j) - \mathbf{L}(\bullet j))\mathbf{e}_j)^{-1}$ from $\mathbf{N} = (\mathbf{I} - \mathbf{D})^{-1}$. The computation is done in two steps computing first the inverse of $(\mathbf{I} - \mathbf{D} - (\mathbf{P}(\bullet j) - \mathbf{L}(\bullet j))\mathbf{e}_j$ which is given by

$$\mathbf{N}^* = \mathbf{N} + \mathbf{N}(\mathbf{P}(\bullet j) - \mathbf{L}(\bullet j))\mathbf{e}_j\mathbf{N}/(1 - \mathbf{e}_j\mathbf{N}(\mathbf{P}(\bullet j) - \mathbf{L}(\bullet j))) \tag{6}$$

and a second step yielding

$$\mathbf{N}' = \mathbf{N}^* + \mathbf{N}^*(\mathbf{d} - \mathbf{c})\mathbf{e}_i\mathbf{N}^*/(1 + \mathbf{e}_i\mathbf{N}^*(\mathbf{d} - \mathbf{c})) \ . \tag{7}$$

$\mathbf{Z}'$ can be easily derived from $\mathbf{N}'$ after computation of the row sums. Since (6) is computed before (7), the intermediate matrix $\mathbf{N}^*$ exists. Observe that (6) and (7) both require an effort in $O(n^2)$ instead of $O(n^3)$ which would be necessary to compute the inverse from the new matrix. If the vectors $\mathbf{P}(\bullet j) - \mathbf{L}(\bullet j)$ and $\mathbf{d} - \mathbf{c}$ are sparse, which is often the case, then the effort is further reduced. The computation using (6) and (7) is usually sufficiently accurate. However, if the values in $\mathbf{c}$ become small, then an alternative computation exists which requires slightly more effort, but is numerically more stable (see [11] for further details).

With the introduced steps it is possible to increase the reward by shifting probability from one distinguished column to another column. The approach can be iterated until $\mathcal{C}^+_{\mathbf{D},i}$ contains no column index yielding an improved reward. However, there might be other columns in $\mathcal{C}^-_{\mathbf{D},i}$ from which probability can be shifted away to improve the reward. Thus, if from the distinguished column i the reward cannot be improved, i is marked as *checked* and another column $j \in \mathcal{C}^-_{\mathbf{D},i}$ which has not been checked is chosen as new distinguished column. For this modification the following operations are performed

$$\mathbf{D}' = \mathbf{D} - (\mathbf{P}(\bullet j) - \mathbf{L}(\bullet j))\mathbf{e}_j + \mathbf{d}\mathbf{e}_i \ , \ \mathbf{d}' = \mathbf{P}(\bullet j) - \mathbf{L}(\bullet j)$$

and j becomes the new distinguished state. The new inverse matrix is computed from (6) and (7) where in (7) $\mathbf{c}$ is set to $\mathbf{0}$. The updates have to be performed in the given order because otherwise the intermediate inverse matrix does not exist. Observe that the transformation does not modify matrix $\mathbf{P}$, it only modifies its representation.

With the new distinguished state, one can continue and try to improve the reward. Whenever the reward is improved and matrix $\mathbf{P}$ is modified, no more states are assume to be checked, because the matrix check has been done according to a different matrix. After checking all states from $\mathcal{C}^-_{\mathbf{D},i}$ without modifying the matrix $\mathbf{P}$, no improvement is possible and the optimum is reached, since no matrix in the neighborhood $\mathcal{N}^{(1)}(\mathbf{P})$ yields a better reward.

The outlined algorithm is finite, since in every step, the reward is improved by shifting as much as possible of the probability mass between two states or a state is marked as checked. Eventually these steps end with a matrix yielding a maximum reward. The following algorithm computes the upper bound for the reward and a matrix $\mathbf{P}$ yielding the upper bound.

```
Initialize some P ∈ P_{L,U} and i ∈ {1,...,n} which define D and d ;
Compute N = (I − D)^{-1}, Z = (diag(Ne^T))^{-1}N, C^+_{D,i} and C^-_{D,i} (via (4));
Initialize checked = ∅ ;
while ((S \ checked) ∩ (C^-_{D,i} ∪ {i}) != ∅) do
  if (∃j ∈ C^+_{D,i} with e_j Zr > e_i Zr) then
    compute D', d' and j according to (5) ;
    checked = ∅ ;
  else
    checked = checked ∪ {i} ;
    if (∃j ∈ C^-_{D,i} \ checked) then
      compute D', d' and j according to (5) using c = 0 ;
    endif
  endif
  if (a new matrix D' has been generated) then
    compute N' according to (6) and (7) and Z' = (diag(N'e^T))^{-1}N' ;
    set N = N', D = D', Z = Z', d = d' and i = j ;
    recompute C^+_{D,i} and C^-_{D,i} using (4) ;
  endif
endwhile
```

The algorithm leaves open which initial matrix is chosen and, if several indices exist that can be chosen from the sets $\mathcal{C}^+_{\mathbf{D},i}$ and $\mathcal{C}^-_{\mathbf{D},i}$, which index to choose. Like for the simplex algorithm in linear programming, no optimal strategy can be defined. In our current implementation, always the smallest possible index is used and the initial matrix is generated by increasing the elements in the rows of $\mathbf{L}$ consecutively starting with the first row until the matrix becomes stochastic. Of course, a greedy strategy increasing or choosing always columns yielding the highest improvement might yield better results, but this has not been tested yet. The worst case runtime of the algorithm is exponential in the number of states since the number of matrices in $\mathcal{E}_{\mathbf{L},\mathbf{U}}$ can be exponential in n. Our observations indicate that the number of iterations in the while loop is fairly small, often in $O(n)$ which means that the overall runtime is often in $O(n^3)$. Thus, the behavior seems to be similar to the behavior of the simplex algorithm, but many more experiments are necessary to validate this claim.

Small Example (continued): The improved approach is applied to the small example which has been presented in detail in Sect. 2. We begin with the computation of the lower bound. Starting from matrix $\mathbf{Z} = (\mathbf{I} - \mathbf{L})^{-1}$ the value of i is set to 3 since $\mathbf{Z}(3\bullet)\mathbf{r}$ is minimal. Thus, vector $\mathbf{d}$ becomes $\mathbf{U}(\bullet 3) - \mathbf{L}(\bullet 3) = (0.0, 1.089e-6, 1.089e-5)^T$. Since $\mathbf{L} + \mathbf{d}\mathbf{e}_3$ is a substochastic matrix, the elements in the first two rows of $\mathbf{L}$ have to be increased to generate matrix $\mathbf{D}$. In the current implementation elements are increased columnwise until the upper bound is reached or the row sum becomes 1.0. In this way we obtain

$$(\mathbf{D}|\mathbf{d}) = \left(\begin{array}{ccc|c} 5.0995e-1 & 4.9005e-1 & 0.0 & 0.0 \\ 9.9990e-1 & 0.0 & 9.8901e-5 & 1.0890e-6 \\ 9.8901e-4 & 0.0 & 9.9900e-1 & 1.0890e-5 \end{array}\right)$$

$$\mathbf{Z} = \begin{pmatrix} 6.49975e-1 & 3.18520e-1 & 3.15051e-1 \\ 6.49976e-1 & 3.18521e-1 & 3.15052e-1 \\ 6.56674e-1 & 3.21803e-1 & 3.18298e-1 \end{pmatrix}$$

The current reward equals 0.31852. Since $\mathbf{D}(\bullet 1) < \mathbf{U}(\bullet 1)$ and $\mathbf{D}(\bullet 2) < \mathbf{U}(\bullet 2)$ probability mass may be shifted from column 3 to 1 or 2. In both cases the reward would be reduced. Consequently, we exchange 3 and 1 yielding

$$(\mathbf{D}|\mathbf{d}) = \left(\begin{array}{ccc|c} 5.0005e-1 & 4.9005e-1 & 0.0 & 9.9000e-1 \\ 9.8010e-1 & 0.0 & 9.9990e-5 & 1.9800e-2 \\ 9.8901e-4 & 0.0 & 9.9901e-1 & 0.0 \end{array}\right)$$

$$\mathbf{Z} = \begin{pmatrix} 6.49522e-1 & 3.18298e-1 & 3.21803e-2 \\ 6.53298e-1 & 3.20149e-1 & 3.23674e-2 \\ 4.68156e-2 & 2.29420e-2 & 2.31946e-3 \end{pmatrix}$$

In this case, a shift of probability from 1 to 3 would reduce the reward, but since $\mathbf{D}(\bullet 3) = \mathbf{U}(\bullet 3)$, such a modification is not possible. Shifting probability from column 1 to 2 would increase the reward and is therefore not possible. Thus, we cannot improve the bound by shifting probability away from column 1. Since $\mathbf{D}(\bullet 2) = \mathbf{L}(\bullet 2)$ we can also not shift probability away from column 2. Thus, i has to be set again to 3 to check whether probability can be shifted away from column 3. The results of this check is negative such that the above matrix describes the final result, namely the lower bound 0.318298 of the reward. The corresponding generator matrix equals

$$\mathbf{Q}^- = \begin{pmatrix} -4.95e-1 & 4.95e-1 & 0.0 \\ 1.01 & -1.0101 & 1.01e-4 \\ 9.99e-4 & 0.0 & -9.99e-4 \end{pmatrix}$$

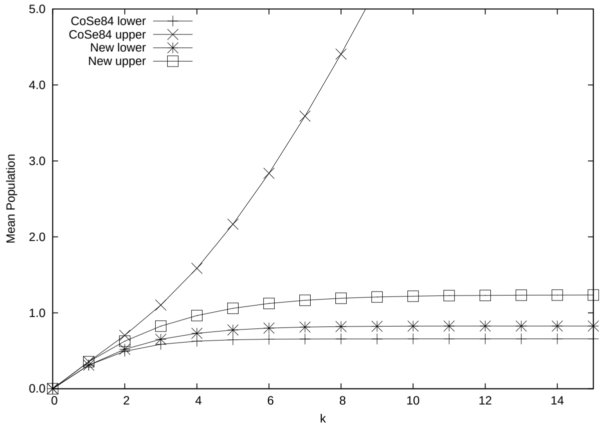
In a similar way, the upper bound is computed. In this case, we start with $i = 1$ and shift probability from 1 to 0 and subsequently from 0 to 2 yielding at the end the matrix

$$\mathbf{Q}^+ = \begin{pmatrix} -5.05e-1 & 5.05e-1 & 0.0 \\ 9.90e-1 & -9.9001e-1 & 9.99e-5 \\ 1.01e-3 & 0.0 & -1.01e-3 \end{pmatrix}$$

with an upper bound of 0.32685. Observe that the lower bound is improved from 0.02294 to 0.318298 and the upper bound remains nearly the same after using the improved bound computation.

5 Some Examples

We introduce four different examples to show the quality of the generated bounds. The first example is an M/M/1/k system for which optimal bounds have been known in the past, the remaining examples are more complex and improved bounds have not been known for these examples.



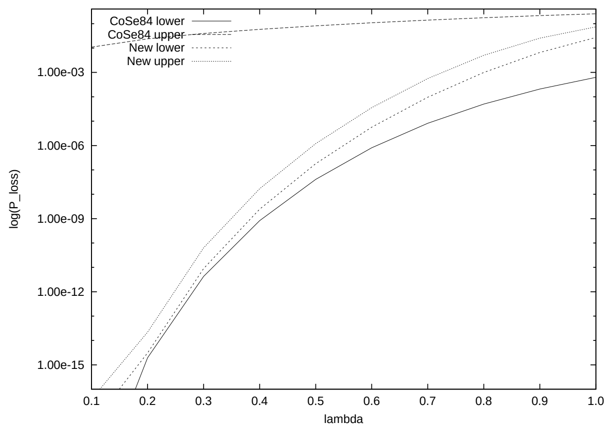


Figure 1: Bounds for the population and the loss rate of a M/M/1/20 system.

5.1 A Simple M/M/1/k model

We start with a very simple model, namely a M/M/1/k system. Arrival and service rate are known with a precision of $\epsilon = 0.05$ such that the arrival rate is in the interval $[(1-\epsilon)\cdot\lambda, (1+\epsilon)\cdot\lambda]$ and the service rate is in the interval $[(1-\epsilon)\cdot\mu, (1+\epsilon)\cdot\mu]$. As rewards we consider the mean population and the loss rate of the system. If states are numbered consecutively according to the number of customers in the system, then we obtain a birth-death process with birth rate λ_i^* and death rate μ_i^* $(i = 0, \ldots, k)$. Both rewards are non-decreasing in the state numbers, i.e., $\mathbf{r}(i) \leq \mathbf{r}(j)$ for $i < j$. It is known [10] that for this process the reward is minimized if λ_i^* is set to the minimal value and μ_i^* is set to the maximal value. Similarly, the reward is maximized by setting λ_i^* to the maximal and μ_i^* to the minimal value. Of course, these are exactly the processes generated by the algorithm for bound optimization.

Using the basic bounding approach [4], the lower and upper bounds result from a matrix where the elements of the vector $(\mathbf{I} - \mathbf{L})\mathbf{e}^T$ are located in the first and last column, respectively. This obviously yields a much looser bound because at a system level this implies that instead of changing the arrival or service rate, a new transition is introduced which empties or fills the system in a single step. The rate of this new transition results from the difference between minimal and maximal arrival and service rate. Of course, this modified model is the best bounding model based on the information given by $\mathbf{L}$ or $\mathbf{U}$ alone.

The difference between both bounds can be seen in Figure 1 where the upper and lower bounds for the mean population in a system with $\mu = 1$, $\lambda = 0.5$ and $\epsilon = 0.05$ are shown on the left side for $k = 1, \ldots, 15$. Obviously, the new bounds are much tighter than the original bounds from [4] which additionally become looser with an increasing number of states. The second result we consider for the simple M/M/1/k system is the loss rate for a system with a fixed k equal to 20 and service rate $\mu = 1.0$ for an increasing arrival rate λ which is assumed to be known with an error of $\pm 5\%$. Thus the true arrival rate is from the interval $[0.95\cdot\lambda, 1.05\cdot\lambda]$. On the right side of figure 1 the logarithm of the bounds for the loss rate is printed. As for the population, the basic bounds resulting from the lower and upper bound matrix are very loose. Especially for small arrival rates the upper bound is much too large, whereas the improved bounds are tight for all arrival rates.

5.2 A Performability Model

As a second example we consider a simple performability model consisting a of a M/M/2/20 system where servers are subject to failures and repairs. All parameters are known with a precision of 1%. Arrival and service rate are from the intervals $[0.792, 0.808]$ and $[0.99, 1.01]$, respectively. The failure and repair rate are chosen from the intervals $[0.99 \cdot 10^{-x-1}, 1.01 \cdot 10^{-x-1}]$ and $[0.99 \cdot 10^{-x}, 1.01 \cdot 10^{-x}]$. We assume that failure and repair times are exponentially distributed, that only active servers fail and that a single repair station exists. As performance measure we consider the mean population in the queue for x ranging from 1 through 7.

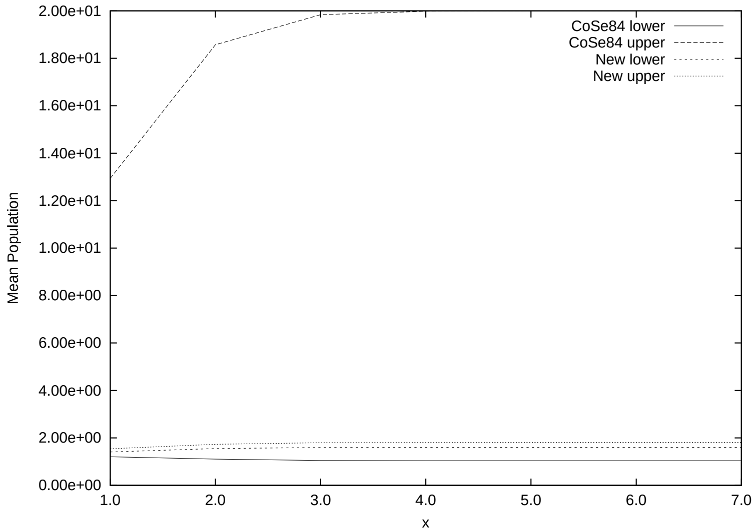


Figure 2: Population bounds for the performability model.

The model results in a Markov chain with 64 states. Figure 2 shows the bounds for the population using the improved bounds and the basic bounds. As for the M/M/1 system, the improved bounds have a spread of about 10% whereas the basic bounds almost useless since the upper bound is much larger than necessary. The reason for this behavior is that from matrix **L** or **U** alone, it is not visible that failure and repair rates differ only by 1%. Thus, the worst case occurs if the difference in the arrival and service rate is added to the failure rate such that the failure rate becomes much larger than the repair rate. Without using upper and lower bounds on the elements of the matrix, it is not possible to compute tight bounds for the model.

5.3 A Nearly Lumpable Central Server

Lumpability [8, 1] has been used in several modeling approaches as a means to reduce the size of CTMCs or DTMCs by exact aggregation. However, often models are not completely lumpable instead they are nearly or quasi lumpable [1, 6] which means that rates differ slightly such that the conditions of lumpability are not observed. A typical example are central server systems where

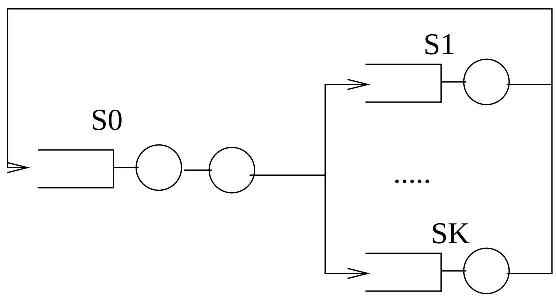


Figure 3: Central server system.

K	N	Orig. states	Agg. states	Throughput Bounds [4]	Throughput New Bounds	Population Bounds [4]	Population New Bounds
		$\epsilon = 0.1$					
4	6	336	45	$[1.801, 3.395]$	$[2.509, 2.730]$	$[0.278, 0.954]$	$[0.431, 0.496]$
4	8	825	91	$[1.825, 3.928]$	$[2.784, 3.028]$	$[0.292, 1.530]$	$[0.536, 0.631]$
4	10	1716	165	$[1.830, 4.302]$	$[2.973, 3.239]$	$[0.296, 2.233]$	$[0.626, 0.754]$
6	8	4719	108	$[1.977, 4.350]$	$[3.365, 3.624]$	$[0.340, 1.807]$	$[0.762, 0.897]$
6	10	13013	215	$[1.980, 4.689]$	$[3.675, 3.948]$	$[0.348, 2.637]$	$[0.984, 1.191]$
8	10	68068	232	$[2.056, 4.847]$	$[4.087, 4.327]$	$[0.379, 2.855]$	$[1.282, 1.535]$
		$\epsilon = 0.01$					
4	6	336	45	$[2.394, 2.619]$	$[2.509, 2.532]$	$[0.405, 0.491]$	$[0.431, 0.437]$
4	8	825	91	$[2.596, 2.943]$	$[2.780, 2.806]$	$[0.486, 0.665]$	$[0.536, 0.545]$
4	10	1716	165	$[2.718, 3.188]$	$[2.971, 2.998]$	$[0.547, 0.857]$	$[0.627, 0.639]$
6	8	4719	108	$[3.069, 3.516]$	$[3.365, 3.392]$	$[0.666, 0.908]$	$[0.762, 0.775]$
6	10	13013	215	$[3.251, 3.863]$	$[3.675, 3.704]$	$[0.807, 1.251]$	$[0.985, 1.004]$
8	10	68068	232	$[3.553, 4.236]$	$[4.087, 4.113]$	$[1.013, 1.550]$	$[1.282, 1.307]$

Figure 4: Bounds for the central server system.

the service rates of the parallel stations are not completely identical. We consider as an example a central server system where the central station $S0$ has an Erlang-2 service time distribution and the service times of the remaining stations $S1$ through SK is exponentially distributed (see Fig. 3). Customers leaving the central station enter with probability k^{-1} one of the stations $S1$ - SK. If the service rates of all stations $S1 - SK$ are identical, then a lumped Markov chain can be generated by counting the number of stations with a fixed population instead of using the detailed population at each station (see [6] for further details). This modification reduces the size of the state space significantly. If the service rates differ, then exact lumping cannot be applied. However, if the difference in the service rates is only small, one can still build the lumped model and generate upper and lower bounding models using the minimum and maximum of the service rates. Observe that the lumped model can be generated from the model description without first computing the complete Markov chain or state space (e.g., [3, 12]). The resulting lumped Markov chains are lower and upper bounds for a reduced Markov chain resulting from exact aggregation. The approach of computing aggregated bounding CTMCs for quasi lumpable partitions has been proposed in [6] where the method from [4] is used to compute the bounds. Here we use the improved bounding approach to compute bounds from the aggregated Markov chains.

In our examples we assume a mean service time of 0.2 at $S0$ and service rates between 1.0 and $1.0 + \epsilon$ at the remaining stations. Figure 4 includes the sizes of the state spaces of the unaggregated and aggregated system and the bounds on the population and throughput at station $S0$ for different populations N in the system and different numbers of stations K. The value of ϵ equals 0.1 and 0.01. Also for the this example the improved bounds are much tighter than the basic bounds using the lower and upper bounds matrix in isolation. The spread of the improved bounds is in the range of ϵ whereas the basic bounds are much wider.

5.4 Optimization of a System with Switch-Over Times

For the last example we apply the bounding method as an optimization method to find an optimal strategy to switch a server between two queues. We consider two buffers of size 1 and a single server. Packets arrive to buffer i according to a Poison process with rate λ_i. Service time is exponentially distributed with rate $\mu = 1.0$. The server can switch between the buffers, but switching takes an exponentially distributed time with rate 1.0. We assume that the servers may stay an exponentially distributed time serving customers from one buffer. Let $\omega_i(n_1, n_2)$ be the rate of sojourn time distribution of the server at queue i $(i = 1, 2)$ when buffer 1 contains n_1 packets and buffer 2 contains n_2 packets. We assume that the values for $\omega_i(n_1, n_2)$ have to be chosen from the interval $[0.01, 100]$. The goal of the optimization is to find a state dependent strategy to switch the server between the queues to minimize the overall occupation of the queues.

		$\omega_1(n_1, n_2)$				$\omega_2(n_1, n_2)$				
λ_1	λ_2	(0,0)	(0,1)	(1,0)	(1,1)	(0,0)	(0,1)	(1,0)	(1,1)	Reward
0.9	0.1	0.01	0.01	0.01	0.01	100	100	0.01	0.01	0.375
0.6	0.4	0.01	0.01	100	0.01	0.01	100	0.01	0.01	0.450
0.5	0.5	0.01	0.01	100	0.01	0.01	100	0.01	0.01	0.454

Table 1: Optimal switching strategy for the simple two buffer system

The optimal strategy can be derived from the matrix generated for the lower bound of the reward. The lower bound matrix results from the Markov chain with $\omega_i(n_1, n_2) = 0.01$ for all states, whereas the upper bound results from model with $\omega_i(n_1, n_2) = 100$ for all states. The reward of a state equals $n_1 + n_2$. The improved bounding algorithm applied to this system computes the minimal reward and generates a matrix $\mathbf{P}$ for the minimum. From this matrix, the optimal strategy can be derived. Table 1 contains for some pairs of arrival rates, the optimal strategies and the resulting reward values. The columns 3 through 10 contain the rates $\omega_i(n_1, n_2)$. Of course, for the optimal strategy the optimal rate is either 0.01 or 100 in a given state. The strategy depends on the arrival rates and the service rates.

6 Conclusions and Future Research

In this paper we present an improved bounding method for stationary reward measures in finite Markov processes. The approach extends the method of Courtois and Semal [4] by considering lower and upper bound matrices in one step instead of computing two sets of bounds. The bounds computed with the approach cannot be further improved since the set of allowed matrices $\mathcal{P}_{\mathbf{L},\mathbf{U}}$ contains a matrix $\mathbf{P}$ that yields the bound. It has been shown that the resulting bounds are usually much tighter than the bounds resulting from the upper and lower bound matrix alone. In particular, the bounds are independent of the dimension of the matrix, which is usually not the case for the bounds of [4] which often become looser if the dimension of the matrix increases. However, the price for the tight bounds is an additional effort to generate a matrix yielding the bound. This step has to be performed for the upper and lower bound separately and has to be repeated for every reward vector. For specific matrix structures the computation can be reduced significantly. A typical example are the matrices presented in [10] where the bounding matrix can be generated without any additional computation.

The paper presents a first algorithm to compute the bounds by repeated rank one modifications of a stochastic matrix from the set $\mathcal{P}_{\mathbf{L},\mathbf{U}}$ which is defined by the bounding matrices $\mathbf{L}$ and $\mathbf{U}$. The algorithm is based on the fundamental results of theorem 3.7 which shows that an optimal reward is reached if the reward cannot be improved by exchanging probability between two columns of the matrix. This result, which is proved in the appendix, shows that a locally optimal matrix is also globally optimal. The resulting algorithm is somehow related to the simplex algorithm in linear programming and it is also related to policy iteration in Markov decision processes. However, this relation has to be further investigated.

In this paper the bounding method is presented in the context where transition rates or probabilities are only approximately known. Of course, the improved bounds can also be used in the context of decomposition and aggregation of large Markov chains [4]. Additionally, the improvements for the basic approach given in [9] can also be combined with the improved bounds.

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A APPENDIX: Proof of theorem 3.7

Proof. We prove the theorem for the maximum, i.e., we show $\mathbf{pr} \geq \mathbf{p'r}$ for all $\mathbf{p'} \in \mathcal{V}(\mathcal{N}^{(1)}(\mathbf{P}))$ implies that the maximum has been reached. The proof for the minimum is completely analogous.

The idea of the proof can be seen schematically in Fig. 5. We show that if for a matrix $\mathbf{P}$ no matrix $\mathbf{P}_1 \in \mathcal{M}^{(1)}(\mathbf{P})$ exists that yields a larger reward, then $\mathcal{M}^{(1)}$ contains for each matrix $\mathbf{P}_2 \in \mathcal{M}^{(2)}(\mathbf{P}) \setminus \{\mathbf{P}\}$ some matrix $\mathbf{P}'_1$ such that the reward resulting from $\mathbf{P}'_1$ is at least as large than the reward from $\mathbf{P}_2$. If this has been shown, an inductive argument can be applied. For $\mathbf{P}_2 \in \mathcal{M}^{(2)}(\mathbf{P})$, a matrix $\mathbf{P}_1 \in \mathcal{M}^{(1)}(\mathbf{P}) \cap \mathcal{M}^{(1)}(\mathbf{P}_2)$ exists such that the reward resulting from $\mathbf{P}_1$ is not smaller than the reward resulting from any $\mathbf{P}_3 \in \mathcal{M}^{(1)}(\mathbf{P}_1) \setminus \{\mathbf{P}\}$. Now the argument can be applied inductively setting $\mathbf{P} = \mathbf{P}_1$. Due to theorem 3.6 it is sufficient to prove that the reward

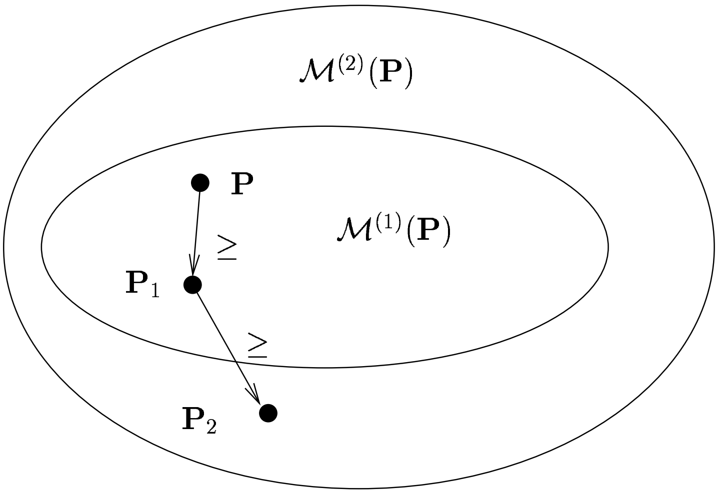

Figure 5: Schematic presentation of the idea of the proof.

resulting from $\mathbf{P}$ is larger than the reward resulting from any $\mathbf{P}_1 \in \mathcal{N}^{(1)}(\mathbf{P})$ since this implies that the reward is also larger than the reward resulting from any $\mathbf{P}'_1 \in \mathcal{M}^{(1)}(\mathbf{P})$.

Let $\mathbf{P}$ be a matrix observing the conditions of the theorem. The proof will be done by induction. We prove that if for each $\mathbf{P}_1 \in \mathcal{M}^{(k)}(\mathbf{P})$ exists some $\mathbf{P}_0 \in \mathcal{M}^{(k-1)}(\mathbf{P})$ such that $\mathbf{P}_1 \in \mathcal{M}^{(1)}(\mathbf{P}_0)$ and $\mathbf{p}_0\mathbf{r} \geq \mathbf{p}_1\mathbf{r}$, then this implies that for each $\mathbf{P}_3 \in \mathcal{M}^{(k+1)}(\mathbf{P}) \setminus \{\mathbf{P}_1\}$ exists some $\mathbf{P}_2 \in \mathcal{M}^{(k)}(\mathbf{P})$ such that $\mathbf{P}_3 \in \mathcal{M}^{(1)}(\mathbf{P}_2)$ and $\mathbf{p}_2\mathbf{r} \geq \mathbf{p}_3\mathbf{r}$. If this holds for all $k > 0$, then $\mathbf{pr} \geq \mathbf{p}'\mathbf{r}$ for $\mathbf{p}' \in \mathcal{V}(\mathcal{M}^{(k)}(\mathbf{P}))$ and $k > 0$. Obviously, this result implies $\mathbf{pr} \geq \mathbf{p}'\mathbf{r}$ for all $\mathbf{p}' \in \mathcal{V}(\mathcal{P}_{\mathbf{L},\mathbf{U}})$.

Assume that the precondition holds for each $\mathbf{P}_1 \in \mathcal{M}^{(k)}$. For $k = 1$ it holds by the assumption of the theorem together with theorem 3.6. Now we prove the result for $k+1$ and choose some arbitrary matrix $\mathbf{P}_3 \in \mathcal{M}^{(k+1)}(\mathbf{P}) \setminus \{\mathbf{P}_1\}$. A matrix $\mathbf{P}_1 \in \mathcal{M}^{(k)}(\mathbf{P})$ with $\mathbf{P}_3 \in \mathcal{M}^{(1)}(\mathbf{P}_1)$ exists. Furthermore matrix $\mathbf{P}_0 \in \mathcal{M}^{(k-1)}(\mathbf{P})$ with $\mathbf{P}_1 \in \mathcal{M}^{(1)}(\mathbf{P}_0)$ and $\mathbf{p}_0\mathbf{r} \geq \mathbf{p}_1\mathbf{r}$ exists by assumption. Let

$$\mathbf{P}_1 = \mathbf{P}_0 - \mathbf{c}^{r,s}(\mathbf{e}_s - \mathbf{e}_r) \ , \mathbf{P}_2 = \mathbf{P}_0 - \mathbf{c}^{x,y}(\mathbf{e}_x - \mathbf{e}_y) \text{ and } \mathbf{P}_3 = \mathbf{P}_0 - \mathbf{c}^{r,s}(\mathbf{e}_s - \mathbf{e}_r) - \mathbf{c}^{x,y}(\mathbf{e}_x - \mathbf{e}_y)$$

for appropriate vectors $\mathbf{c}^{r,s}$ and $\mathbf{c}^{x,y}$. Obviously $r \neq s$ and $x \neq y$ has to hold. For the moment we assume $s \neq r \neq x \neq y$ and handle the remaining cases separately below.

Under these restrictions matrix $\mathbf{P}_2 \in \mathcal{M}^{(k)}(\mathbf{P}) \cap \mathcal{M}^{(1)}(\mathbf{P}_0)$. If $\mathbf{p}_2\mathbf{r} > \mathbf{p}_0\mathbf{r}$, we set $\mathbf{P}_1 = \mathbf{P}_2$ and use a new $\mathbf{P}_0$ such that $\mathbf{P}_1 \in \mathcal{M}^{(1)}(\mathbf{P}_0)$ and $\mathbf{p}_0\mathbf{r} \geq \mathbf{p}_1\mathbf{r}$. By assumption such a $\mathbf{P}_0$ has to exist. For these matrices $\mathbf{P}_0$ and $\mathbf{P}_1$ a new $\mathbf{P}_2$ is defined and $\mathbf{p}_0\mathbf{r} \geq \mathbf{p}_2\mathbf{r}$ is checked. If the relation does not hold, then the approach is iterated. In the end matrices $\mathbf{P}_0$, $\mathbf{P}_1$ and $\mathbf{P}_2$ have been found such that $\mathbf{P}_0 \in \mathcal{M}^{(k-1)}(\mathbf{P})$, $\mathbf{P}_1, \mathbf{P}_2 \in \mathcal{M}^{(1)}(\mathbf{P}_0)$, $\mathbf{P}_3 \in \mathcal{M}^{(1)}(\mathbf{P}_1) \cap \mathcal{M}^{(1)}(\mathbf{P}_2)$ and $\mathbf{p}_0\mathbf{r} \geq \max(\mathbf{p}_1\mathbf{r}, \mathbf{p}_2\mathbf{r})$. We have to prove that

$$\mathbf{p}_0\mathbf{r} \geq \mathbf{p}_1\mathbf{r} \wedge \mathbf{p}_0\mathbf{r} \geq \mathbf{p}_2\mathbf{r} \ \Rightarrow \ \mathbf{p}_1\mathbf{r} \geq \mathbf{p}_3\mathbf{r} \vee \mathbf{p}_2\mathbf{r} \geq \mathbf{p}_3\mathbf{r} \ . \tag{8}$$

To prove the relation let $\mathbf{L}' = \mathbf{P}_0 - \mathbf{c}^{r,s}\mathbf{e}_r - \mathbf{c}^{x,y}\mathbf{e}_x$ by assumption the inverse $\mathbf{N} = (\mathbf{I} - \mathbf{L}')^{-1}$ and the normalized inverse $\mathbf{Z} = (diag(\mathbf{N}\mathbf{e}^T))^{-1}\mathbf{N}$ exist. From the results of [4] it is clear that vector $\mathbf{p}_m$ $(m = 0, \ldots, 3\}$ can be represented as

$$\begin{array}{ll} \mathbf{p}_0 = \lambda_0\mathbf{e}_r\mathbf{Z} + (1-\lambda_0)\mathbf{e}_x\mathbf{Z} \ , & \mathbf{p}_1 = \lambda_1\mathbf{e}_s\mathbf{Z} + (1-\lambda_1)\mathbf{e}_x\mathbf{Z} \ , \\ \mathbf{p}_2 = \lambda_2\mathbf{e}_r\mathbf{Z} + (1-\lambda_2)\mathbf{e}_y\mathbf{Z} \ , & \mathbf{p}_3 = \lambda_3\mathbf{e}_s\mathbf{Z} + (1-\lambda_3)\mathbf{e}_y\mathbf{Z} \ . \end{array}$$

Since vector $\mathbf{a}$ is the solution of $\mathbf{aZC} = \mathbf{0}$ where $\mathbf{C} = \mathbf{c}^{r,s}\mathbf{e}_r + \mathbf{c}^{x,y}\mathbf{e}_x$ for the computation of λ_0, the value of λ_0 is the solution of $\lambda_0 = \lambda_0 \cdot (\mathbf{N}(r\bullet) \cdot \mathbf{c}^{r,s}) + (1-\lambda_0) \cdot (\mathbf{N}(x\bullet) \cdot \mathbf{c}^{r,s})$. Similarly, the remaining values of λ_i are computed resulting in

$$\begin{aligned}\lambda_0 &= \frac{\mathbf{N}(x\bullet)\cdot\mathbf{c}^{r,s}}{1-\mathbf{N}(r\bullet)\cdot\mathbf{c}^{r,s}+\mathbf{N}(x\bullet)\cdot\mathbf{c}^{r,s}}\ , & \lambda_1 &= \frac{\mathbf{N}(x\bullet)\cdot\mathbf{c}^{r,s}}{1-\mathbf{N}(s\bullet)\cdot\mathbf{c}^{r,s}+\mathbf{N}(x\bullet)\cdot\mathbf{c}^{r,s}}\ , \\ \lambda_2 &= \frac{\mathbf{N}(y\bullet)\cdot\mathbf{c}^{r,s}}{1-\mathbf{N}(r\bullet)\cdot\mathbf{c}^{r,s}+\mathbf{N}(y\bullet)\cdot\mathbf{c}^{r,s}}\ , & \lambda_3 &= \frac{\mathbf{N}(y\bullet)\cdot\mathbf{c}^{r,s}}{1-\mathbf{N}(s\bullet)\cdot\mathbf{c}^{r,s}+\mathbf{N}(y\bullet)\cdot\mathbf{c}^{r,s}}\ .\end{aligned} \tag{9}$$

Since the rewards are given by

$$\begin{aligned}&\lambda_0\,(\mathbf{e}_r\mathbf{Zr}) + (1-\lambda_0)\,(\mathbf{e}_x\mathbf{Zr})\ ,\quad \lambda_1\,(\mathbf{e}_s\mathbf{Zr}) + (1-\lambda_1)\,(\mathbf{e}_x\mathbf{Zr})\ ,\\ &\lambda_2\,(\mathbf{e}_r\mathbf{Zr}) + (1-\lambda_2)\,(\mathbf{e}_y\mathbf{Zr})\ ,\quad \lambda_3\,(\mathbf{e}_s\mathbf{Zr}) + (1-\lambda_3)\,(\mathbf{e}_y\mathbf{Zr})\ ,\end{aligned} \tag{10}$$

we have to prove (8) using (9) and (10). For the proof use the following abbreviations

$$\begin{array}{llll} a = (\mathbf{e}_x\mathbf{Zr}) & b = (\mathbf{e}_r\mathbf{Zr}) & c = (\mathbf{e}_y\mathbf{Zr}) & d = (\mathbf{e}_s\mathbf{Zr}) \\ \alpha = \mathbf{N}(x\bullet)\cdot\mathbf{c}^{r,s} & \beta = 1-\mathbf{N}(r\bullet)\cdot\mathbf{c}^{r,s} & \gamma = \mathbf{N}(y\bullet)\cdot\mathbf{c}^{r,s} & \delta = 1-\mathbf{N}(s\bullet)\cdot\mathbf{c}^{r,s}\end{array}$$

Such that a, b, c, d are non negative and $0 < \alpha, \beta, \gamma, \delta < 1$. With these notations (8) becomes

$$\begin{gathered}\tfrac{1}{\alpha+\beta}(\alpha\cdot a+\beta\cdot b) \geq \tfrac{1}{\alpha+\delta}(\alpha\cdot a+\delta\cdot d) \wedge \tfrac{1}{\alpha+\beta}(\alpha\cdot a+\beta\cdot b) \geq \tfrac{1}{\gamma+\beta}(\gamma\cdot c+\beta\cdot b)\\ \Rightarrow \\ \tfrac{1}{\alpha+\delta}(\alpha\cdot a+\delta\cdot d) \geq \tfrac{1}{\gamma+\delta}(\gamma\cdot c+\delta\cdot d) \vee \tfrac{1}{\gamma+\beta}(\gamma\cdot c+\beta\cdot b) \geq \tfrac{1}{\gamma+\delta}(\gamma\cdot c+\delta\cdot d)\end{gathered} \tag{11}$$

which has to be proved now. Without loss of generality we assume that

$$\frac{1}{\alpha+\delta}(\alpha\cdot a+\delta\cdot d) \geq \frac{1}{\gamma+\beta}(\gamma\cdot c+\beta\cdot b)\ .$$

which can be always assured by renaming row and column indices. Now assume that (11) does not hold, then the following system of inequalities has to hold.

$$\begin{aligned}&\tfrac{1}{\alpha+\beta}(\alpha\cdot a+\beta\cdot b) \geq \tfrac{1}{\alpha+\delta}(\alpha\cdot a+\delta\cdot d)\ ,\quad \tfrac{1}{\alpha+\beta}(\alpha\cdot a+\beta\cdot b) \geq \tfrac{1}{\gamma+\beta}(\gamma\cdot c+\beta\cdot b)\ ,\\ &\tfrac{1}{\alpha+\delta}(\alpha\cdot a+\delta\cdot d) \geq \tfrac{1}{\gamma+\beta}(\gamma\cdot c+\beta\cdot b)\ ,\quad \tfrac{1}{\gamma+\delta}(\gamma\cdot c+\delta\cdot d) > \tfrac{1}{\alpha+\delta}(\alpha\cdot a+\delta\cdot d)\end{aligned}$$

which can be equivalently represented as

$$\begin{array}{ll} i) & \alpha\beta(b-a)+\alpha\delta(a-d)+\beta\delta(b-d) \geq 0 \\ ii) & \alpha\beta(a-b)+\alpha\gamma(a-c)+\beta\gamma(b-c) \geq 0 \\ iii) & \alpha\beta(a-b)+\alpha\gamma(a-c)+\beta\delta(d-b)+\gamma\delta(d-c) \geq 0 \\ iv) & \alpha\gamma(c-a)+\alpha\delta(d-a)+\gamma\delta(c-d) > 0 \end{array} \tag{12}$$

since all variables are non negative. We show by contradiction that (12) cannot hold.

From $iii)$ we obtain $\alpha\beta(a-b)+\alpha\gamma(a-c)+\beta\delta(d-b) \geq \gamma\delta(c-d)$.

The left side is substituted for $\gamma\delta(c-d)$ in $iv)$ yielding $iv')$ $\alpha\beta(a-b)+\alpha\delta(d-a)+\beta\delta(d-b) > 0$.

From $i)$ we obtain $\alpha\delta(a-d)+\beta\delta(b-d) \geq \alpha\beta(a-b)$ such that the left hand side can be substituted for $\alpha\beta(a-b)$ in $iv')$ resulting in $0 > 0$ which is a contradiction such that the assumption cannot hold and (11) is true.

It remains to prove the remaining cases where the indices are not all different.

Case $r = x$ and $s = y$ **:**
In this case $\mathbf{P}_3 \in \mathcal{M}(\mathbf{P}_1)$ since $\mathbf{P}_3 = \mathbf{P}_1 - (\mathbf{c}^{r,s} + \mathbf{c}^{x,y})(\mathbf{e}_r - \mathbf{e}_s)$. Then $\mathbf{p}_1\mathbf{r} \geq \mathbf{p}_3\mathbf{r}$ holds by assumption.

Case $r = y$ and $s = x$ **:**
Define two vectors $\mathbf{f}^{r,s}$ and $\mathbf{f}^{s,r}$ such that

$$\mathbf{f}^{r,s}(k) = \max(0, \mathbf{c}^{r,s}(k) - \mathbf{c}^{s,r}(k)) \text{ and } \mathbf{f}^{s,r}(k) = \max(0, \mathbf{c}^{s,r}(k) - \mathbf{c}^{r,s}(k))\ .$$

Then $\mathbf{P}_1 = \mathbf{P}_0 - \mathbf{f}^{r,s}(\mathbf{e}_r - \mathbf{e}_s)$, $\mathbf{P}_2 = \mathbf{P}_0 - \mathbf{f}^{s,r}(\mathbf{e}_s - \mathbf{e}_r)$, $\mathbf{P}_3 = \mathbf{P}_0 - \mathbf{f}^{r,s}(\mathbf{e}_r - \mathbf{e}_s) - \mathbf{f}^{s,r}(\mathbf{e}_s - \mathbf{e}_r)$ and the proof for the general case where all indices are different can be applied.

Case $r = x$ and $s \neq y$ **:**
Define $\mathbf{L}' = \mathbf{P}_0 - (\mathbf{c}^{r,s} + \mathbf{c}^{r,y})\mathbf{e}_r$ and $\mathbf{Z}$ using $\mathbf{L}'$ as usual. We have

$$\mathbf{p}_0\mathbf{r} = \mathbf{e}_r\mathbf{Z}\mathbf{r} \geq \mathbf{p}_1\mathbf{r} = (\lambda_1\mathbf{e}_r + (1-\lambda_1)\mathbf{e}_s)\mathbf{Z}\mathbf{r} \text{ and } \mathbf{p}_0\mathbf{r} = \mathbf{e}_r\mathbf{Z}\mathbf{r} \geq \mathbf{p}_2\mathbf{r} = (\lambda_1\mathbf{e}_s + (1-\lambda_1)\mathbf{e}_y)\mathbf{Z}\mathbf{r}$$

for $1 > \lambda_1, \lambda_2 > 0$ which implies $\mathbf{e}_r\mathbf{Z}\mathbf{r} \geq \mathbf{e}_s\mathbf{Z}\mathbf{r}$ and $\mathbf{e}_r\mathbf{Z}\mathbf{r} \geq \mathbf{e}_y\mathbf{Z}\mathbf{r}$ and since $\mathbf{p}_3\mathbf{Z}\mathbf{r} = (\lambda_3\mathbf{e}_s + (1-\lambda_3)\mathbf{e}_y)\mathbf{Z}\mathbf{r}$ either $\mathbf{p}_1\mathbf{r} \geq \mathbf{p}_3\mathbf{r}$ or $\mathbf{p}_2\mathbf{r} \geq \mathbf{p}_3\mathbf{r}$ has to hold.

Case $s = y$ and $r \neq x$**:**
Define $\mathbf{L}' = \mathbf{P}_0 - (\mathbf{c}^{r,s}\mathbf{e}_r + \mathbf{c}^{x,s}\mathbf{e}_x)$ and $\mathbf{Z}$ using $\mathbf{L}'$ as usual. We have

$$\begin{aligned}\mathbf{p}_0\mathbf{r} &= (\lambda_0\mathbf{e}_r + (1-\lambda_0)\mathbf{e}_x)\mathbf{Z}\mathbf{r} \geq \mathbf{p}_1\mathbf{r} = (\lambda_1\mathbf{e}_s + (1-\lambda_1)\mathbf{e}_x)\mathbf{Z}\mathbf{r} \text{ and}\\ \mathbf{p}_0\mathbf{r} &= (\lambda_0\mathbf{e}_r + (1-\lambda_0)\mathbf{e}_x)\mathbf{Z}\mathbf{r} \geq \mathbf{p}_2\mathbf{r} = (\lambda_2\mathbf{e}_r + (1-\lambda_1)\mathbf{e}_s)\mathbf{Z}\mathbf{r}\end{aligned}$$

and $\mathbf{p}_3\mathbf{Z}\mathbf{r} = \mathbf{e}_s\mathbf{Z}\mathbf{r}$. For the first two inequalities to hold, $\max(\mathbf{e}_r\mathbf{Z}\mathbf{r}, \mathbf{e}_x\mathbf{Z}\mathbf{r}) \geq \mathbf{e}_s\mathbf{Z}\mathbf{r}$ has to hold. This implies that $\mathbf{p}_1\mathbf{r} \geq \mathbf{p}_3\mathbf{r}$ or $\mathbf{p}_2\mathbf{r} \geq \mathbf{p}_3\mathbf{r}$.

Case $r \neq y$ and $s = x$ **:**
In this case $\mathbf{P}_2 = \mathbf{P}_0 - \mathbf{c}^{x,y}(\mathbf{e}_x - \mathbf{e}_y) = \mathbf{P}_0 - \mathbf{c}^{s,y}(\mathbf{e}_s - \mathbf{e}_y)$ might not be in $\mathcal{M}^{(1)}(\mathbf{P}_0)$ since $\mathbf{P}_2(s,k) < \mathbf{L}(s,k)$ can hold for some k. Define three vector $\mathbf{f}^{r,s}, \mathbf{f}^{r,y}(k), \mathbf{f}^{s,y}$ such that

$$\mathbf{f}^{r,s}(k) = \max(0, \mathbf{c}^{r,s}(k) - \mathbf{c}^{s,y}(k))\ ,\ \mathbf{f}^{r,y}(k) = \min(\mathbf{c}^{r,s}(k), \mathbf{c}^{s,y}(k)) \text{ and } \mathbf{f}^{s,y}(k) = \max(0, \mathbf{c}^{s,y}(k) - \mathbf{c}^{r,s}(k))$$

for all $k \in \{1, \ldots, n\}$. Obviously

$$\mathbf{P}_3 = \mathbf{P}_0 - \mathbf{c}^{r,s}(\mathbf{e}_r - \mathbf{e}_s) - \mathbf{c}^{s,y}(\mathbf{e}_s - \mathbf{e}_y) = \mathbf{P}_0 - \mathbf{f}^{r,s}(\mathbf{e}_r - \mathbf{e}_s) - \mathbf{f}^{r,y}(\mathbf{e}_r - \mathbf{e}_y) - \mathbf{f}^{s,y}(\mathbf{e}_s - \mathbf{e}_y)$$

holds and all possible intermediate matrices of the form $\mathbf{P}_0 - \mathbf{f}^{v_1,w_1}(\mathbf{e}_v - \mathbf{e}_w)$ and $\mathbf{P}_0 - \mathbf{f}^{v_1,w_1}(\mathbf{e}_{v_1} - \mathbf{e}_{w_1}) - \mathbf{f}^{v_2,w_2}(\mathbf{e}_{v_2} - \mathbf{e}_{w_2})$ with appropriate indices $v_i, w_i \in \{r, s, y\}$ belong to $\mathcal{P}_{\mathbf{L},\mathbf{U}}$.

Define matrix $\mathbf{L}' = \mathbf{P}_0 - \mathbf{c}^{r,s}\mathbf{e}_r - \mathbf{f}^{s,y}\mathbf{e}_s$ and let $\mathbf{Z}$ be the normalized inverse of $\mathbf{L}'$. Stationary vectors of the matrices $\mathbf{P}_0$, $\mathbf{P}_1$ and $\mathbf{P}_3$ can be represented as

$$\mathbf{p}_0 = \lambda_0\mathbf{e}_r\mathbf{Z} + (1-\lambda_0)\mathbf{e}_s\mathbf{Z}\ ,\ \mathbf{p}_1 = \mathbf{e}_s\mathbf{Z}\ ,\ \mathbf{p}_3 = \lambda_3\mathbf{e}_s\mathbf{Z} + (1-\lambda_3)\mathbf{e}_y\mathbf{Z}\ .$$

Since $\mathbf{p}_0\mathbf{r} \geq \mathbf{p}_1\mathbf{r} \Rightarrow \mathbf{e}_r\mathbf{Z}\mathbf{r} \geq \mathbf{e}_s\mathbf{Z}\mathbf{r}$. If $\mathbf{e}_s\mathbf{Z}\mathbf{r} \geq \mathbf{e}_y\mathbf{Z}\mathbf{r}$, then $\mathbf{p}_0\mathbf{r} \geq \mathbf{p}_1\mathbf{r} \geq \mathbf{p}_3\mathbf{r}$ and since $\mathbf{P}_3 \in \mathcal{M}^{(1)}(\mathbf{P}_1)$ and $\mathbf{P}_1 \in \mathcal{M}^{(1)}(\mathbf{P}_0)$ the proof is complete.

Thus, we have to consider the case $\mathbf{e}_y\mathbf{Z}\mathbf{r} > \mathbf{e}_s\mathbf{Z}\mathbf{r}$. Since matrix $\mathbf{P}_4 = \mathbf{P}_0 - \mathbf{f}^{s,y}(\mathbf{e}_s - \mathbf{e}_y) \in \mathcal{M}^{(1)}(\mathbf{P}_0)$ we have $\mathbf{p}_0\mathbf{r} \geq \mathbf{p}_4\mathbf{r}$ and $\mathbf{p}_4 = \lambda_4\mathbf{e}_r\mathbf{Z} + (1-\lambda_4)\mathbf{e}_y\mathbf{Z}$ the relation $\mathbf{e}_r\mathbf{Z}\mathbf{r} \geq \mathbf{e}_y\mathbf{Z}\mathbf{r}$ has to hold. Thus, it remains to prove the case where $\mathbf{e}_r\mathbf{Z}\mathbf{r} \geq \mathbf{e}_y\mathbf{Z}\mathbf{r} > \mathbf{e}_s\mathbf{Z}\mathbf{r}$.

We first show that $\mathbf{p}_0\mathbf{r} \geq \mathbf{p}_3\mathbf{r}$ by showing that $\mathbf{p}_3\mathbf{r} > \mathbf{p}_4\mathbf{r}$ cannot hold such that $\mathbf{p}_0\mathbf{r} \geq \mathbf{p}_4\mathbf{r} \geq \mathbf{p}_3\mathbf{r}$ holds. Relation $\mathbf{p}_3\mathbf{r} > \mathbf{p}_4\mathbf{r}$ implies $\lambda_3\mathbf{e}_s\mathbf{Z}\mathbf{r} + (1-\lambda_3)\mathbf{e}_y\mathbf{Z}\mathbf{r} > \lambda_4\mathbf{e}_r\mathbf{Z}\mathbf{r} + (1-\lambda_4)\mathbf{e}_y\mathbf{Z}\mathbf{r}$ for $0 \leq \lambda_i \leq 1$ ($i = 3, 4$). Since $\mathbf{e}_r\mathbf{Z}\mathbf{r} \geq \mathbf{e}_s\mathbf{Z}\mathbf{r}$ this implies $(1-\lambda_3) > (1-\lambda_4) \Rightarrow \lambda_4 > \lambda_3$. However, then the relation $\lambda_4\mathbf{e}_r\mathbf{Z}\mathbf{r} + (1-\lambda_4)\mathbf{e}_y\mathbf{Z}\mathbf{r} \geq \lambda_3\mathbf{e}_r\mathbf{Z}\mathbf{r} + (1-\lambda_3)\mathbf{e}_y\mathbf{Z}\mathbf{r} > \lambda_3\mathbf{e}_s\mathbf{Z}\mathbf{r} + (1-\lambda_3)\mathbf{e}_y\mathbf{Z}\mathbf{r}$ holds which implies $\mathbf{p}_0\mathbf{r} \geq \mathbf{p}_3\mathbf{r}$.

It remains to find some matrix $\mathbf{P}_5$ such that $\mathbf{P}_3 \in \mathcal{M}^{(1)}(\mathbf{P}_5)$ and $\mathbf{p}_5\mathbf{r} \geq \mathbf{p}_3\mathbf{r}$.
Let $\mathbf{P}_5 = \mathbf{P}_0 - \mathbf{f}^{r,y}(\mathbf{e}_r - \mathbf{e}_y) - \mathbf{f}^{s,y}(\mathbf{e}_s - \mathbf{e}_y) = \mathbf{P}_3 - \mathbf{f}^{r,s}(\mathbf{e}_r - \mathbf{e}_s)$ with $\mathbf{p}_5 = \lambda_5\mathbf{e}_r\mathbf{Z} + (1-\lambda_5)\mathbf{e}_y\mathbf{Z}$ such that $\mathbf{p}_5\mathbf{r} = \lambda_5\mathbf{e}_r\mathbf{Z}\mathbf{r} + (1-\lambda_5)\mathbf{e}_y\mathbf{Z}\mathbf{r} \geq \mathbf{e}_y\mathbf{Z}\mathbf{r} \geq \lambda_3\mathbf{e}_s\mathbf{Z}\mathbf{r} + (1-\lambda_3)\mathbf{e}_y\mathbf{Z}\mathbf{r} = \mathbf{p}_3\mathbf{r}$.

Case $r = y$ **and** $s \neq x$ **:**
Matrix $\mathbf{P}_2$ needs not to be in $\mathcal{P}_{\mathbf{L},\mathbf{U}}$ since $\mathbf{P}_2(r,k) > \mathbf{U}(r,k)$ might hold for some k. For the proof define the following vectors elementwise

$$\begin{aligned}\mathbf{f}^{x,s}(k) &= \min(\mathbf{c}^{r,s}(k), \mathbf{c}^{x,r}(k)) \ , \\ \mathbf{f}^{r,s}(k) &= \max(0, \mathbf{c}^{r,s}(k) - \mathbf{c}^{x,r}(k)) \text{ and} \\ \mathbf{f}^{x,r}(k) &= \max(0, \mathbf{c}^{x,r}(k) - \mathbf{c}^{r,s}(k))\end{aligned}$$

for $k \in \{1, \ldots, n\}$. We have

$$\mathbf{P}_3 = \mathbf{P}_0 - \mathbf{f}^{x,s}(\mathbf{e}_x - \mathbf{e}_s) - \mathbf{f}^{r,s}(\mathbf{e}_r - \mathbf{e}_s) - \mathbf{f}^{x,r}(\mathbf{e}_x - \mathbf{e}_r) \ .$$

Let $\mathbf{L}' = \mathbf{P}_0 - \mathbf{f}^{r,s}\mathbf{e}_r - \mathbf{c}^{x,r}\mathbf{e}_x$ and define $\mathbf{N}$ and $\mathbf{Z}$ as usual using $\mathbf{L}'$.The following matrices are all in $\mathcal{M}^{(1)}(\mathbf{P}_0)$:

$$\begin{aligned}\mathbf{P}_4 &= \mathbf{P}_0 - \mathbf{f}^{x,s}(\mathbf{e}_x - \mathbf{e}_s) \ , \\ \mathbf{P}_5 &= \mathbf{P}_0 - \mathbf{f}^{r,s}(\mathbf{e}_r - \mathbf{e}_s) \text{ and} \\ \mathbf{P}_6 &= \mathbf{P}_0 - \mathbf{f}^{x,r}(\mathbf{e}_x - \mathbf{e}_r) \ .\end{aligned}$$

By assumption $\mathbf{p}_0\mathbf{r} \geq \max(\mathbf{p}_4\mathbf{r}, \mathbf{p}_5\mathbf{r}, \mathbf{p}_6\mathbf{r})$. Furthermore, the following matrices are in $\mathcal{M}^{(2)}(\mathbf{P}_0)$:

$$\begin{aligned}\mathbf{P}_7 &= \mathbf{P}_0 - \mathbf{f}^{x,s}(\mathbf{e}_x - \mathbf{e}_s) - \mathbf{f}^{r,s}(\mathbf{e}_r - \mathbf{e}_s) \text{ and} \\ \mathbf{P}_8 &= \mathbf{P}_0 - \mathbf{f}^{x,s}(\mathbf{e}_x - \mathbf{e}_s) - \mathbf{f}^{x,r}(\mathbf{e}_x - \mathbf{e}_r) \ .\end{aligned}$$

Using the cases $(x \neq r \wedge y = s)$ and $(x = r \wedge s \neq y)$ it follows that $\mathbf{p}_0\mathbf{r} \geq \max(\mathbf{p}_4\mathbf{r}, \mathbf{p}_5\mathbf{r}) \geq \mathbf{p}_7\mathbf{r}$ and $\mathbf{p}_0\mathbf{r} \geq \max(\mathbf{p}_4\mathbf{r}, \mathbf{p}_6\mathbf{r}) \geq \mathbf{p}_8\mathbf{r}$ and $\mathbf{P}_3 \in \mathcal{M}^{(1)}(\mathbf{P}_7) \cap \mathcal{M}^{(1)}(\mathbf{P}_8)$. The different stationary vectors can be represented by means of $\mathbf{Z}$ as

$$\begin{aligned}\mathbf{p}_0 &= \lambda_0\mathbf{e}_r\mathbf{Z} + (1-\lambda_0)\mathbf{e}_x\mathbf{Z} \ , & \mathbf{p}_3 &= \lambda_3\mathbf{e}_r\mathbf{Z} + (1-\lambda_3)\mathbf{e}_s\mathbf{Z} \ , \\ \mathbf{p}_5 &= \lambda_5\mathbf{e}_s\mathbf{Z} + (1-\lambda_5)\mathbf{e}_x\mathbf{Z} \ , & \mathbf{p}_6 &= \lambda_6\mathbf{e}_r\mathbf{Z} + (1-\lambda_6)\mathbf{e}_x\mathbf{Z} \ , \\ \mathbf{p}_7 &= \lambda_7\mathbf{e}_s\mathbf{Z} + (1-\lambda_7)\mathbf{e}_x\mathbf{Z} \text{ and} & \mathbf{p}_8 &= \lambda_8\mathbf{e}_r\mathbf{Z} + (1-\lambda_8)\mathbf{e}_s\mathbf{Z} \ .\end{aligned}$$

Matrix $\mathbf{P}_6$ results from $\mathbf{P}_0$ by shifting probability mass from column x to column r. This implies $\lambda_6 \geq \lambda_0$ which can be formally proved by noticing the representations

$$\lambda_0 = \lambda_0\mathbf{N}(r\bullet)\mathbf{f}^{r,s} + (1-\lambda_0)\mathbf{N}(x\bullet)\mathbf{f}^{r,s} \text{ and } \lambda_6 = \lambda_6\mathbf{N}(r\bullet)(\mathbf{f}^{r,s} + \mathbf{f}^{x,r}) + (1-\lambda_0)\mathbf{N}(x\bullet)(\mathbf{f}^{r,s} + \mathbf{f}^{x,r})$$

for $0 \leq \mathbf{N}(r\bullet)\mathbf{f}^{r,s} \leq \mathbf{N}(r\bullet)(\mathbf{f}^{r,s} + \mathbf{f}^{x,r}) \leq 1$ and $0 \leq \mathbf{N}(x\bullet)\mathbf{f}^{r,s} \leq \mathbf{N}(x\bullet)(\mathbf{f}^{r,s} + \mathbf{f}^{x,r}) \leq 1$ the relation $\lambda_6 \geq \lambda_0$ follows. Since $\mathbf{p}_0\mathbf{r} \geq \mathbf{p}_6\mathbf{r}$ this implies $\mathbf{e}_x\mathbf{Z}\mathbf{r} \geq \mathbf{e}_r\mathbf{Z}\mathbf{r}$. This relation together with $\mathbf{p}_0\mathbf{r} \geq \mathbf{p}_5\mathbf{r}$ implies $\mathbf{e}_x\mathbf{Z}\mathbf{r} \geq \mathbf{e}_s\mathbf{Z}\mathbf{r}$.

We have no relation between $\mathbf{e}_s\mathbf{Z}\mathbf{r}$ and $\mathbf{e}_r\mathbf{Z}\mathbf{r}$. Assume that $\mathbf{e}_s\mathbf{Z}\mathbf{r} \geq \mathbf{e}_r\mathbf{Z}\mathbf{r}$, then $\mathbf{p}_7\mathbf{r} \geq \mathbf{p}_3\mathbf{r}$ and the proof is complete. If $\mathbf{e}_r\mathbf{Z}\mathbf{r} > \mathbf{e}_s\mathbf{Z}\mathbf{r}$, then we first notice that $\lambda_8 \geq \lambda_3$ because $\mathbf{P}_3$ results from $\mathbf{P}_8$ by shifting probability mass from column r to column s and we can use the same proof that had been used to show $\lambda_6 \geq \lambda_0$. However, $\lambda_8 \geq \lambda_3$ together with $\mathbf{e}_r\mathbf{Z}\mathbf{r} > \mathbf{e}_s\mathbf{Z}\mathbf{r}$ implies $\mathbf{p}_8\mathbf{r} \geq \mathbf{p}_3\mathbf{r}$ which completes the proof. $\square$