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# Approximations for the Moments of Nonstationary and State Dependent Birth-Death Queues

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Closure approximations are useful methods for approximating the moments of complex Markovian stochastic systems. However, it has been typically very difficult to prove rigorous error bounds that show that the closure approximation is close to the stochastic model being approximated. In this paper, we propose a new methodology for approximating the transient moment dynamics of Markovian birth-death processes by expanding the transition probabilities of the Markov process in terms of Poisson-Charlier polynomials. We specifically rely on the novel construction of new weighted discrete Sobolev spaces, which we use to derive error bounds for the transition probabilities. We also leverage our transition probability approximations to construct new weak a priori estimates for approximating the moments of the Markov processs using a truncated form of the expansion. As a result, we are the first to provide explicit error bounds and estimates on the performance of a *moment closure approximation*. Finally, we demonstrate through several numerical examples from the queueing and epidemic literature that our approximations are quite accurate with a small number of terms.

*Key words*: Multi-Server Queues, Spectral-Galerkin method, Discrete approximation, Unbounded domain, Abandonment, Time-Varying Rates, Birth-Death Processes, Poisson-Charlier Polynomials.

**1. Introduction** Markovian birth-death processes are very important modeling tools in engineering, operations research, mathematics, physics, and a variety of other fields. The development of Markovian stochastic models has made a profound impact on the way we understand complex dynamics in these fields of study. One particular way to explore the dynamics of these processes that transcends a particular application setting is to study the behavior of the transition probabilities and the state probabilities, which provide the entire distribution of the process for all time points of interest. However, an explicit study of the transition probabilities or state probabilities has often eluded researchers since the transition or state probabilities do not have explicit solutions in general with some exceptions in some very special cases. Moreover, when analyzing large models such as large scale service systems or moderately sized queueing networks a full understanding of the transition or state probabilities in their explicit form is rather intractable in both a mathematical and numerical sense.

Thus, many researchers have spent considerable effort in trying to develop ways of understanding the moments of Markovian birth-death processes. Moments like the mean and variance can provide considerable insight into understanding the "typical" stochastic behavior of the system. However, a full understanding of the moments also is quite difficult to obtain. One major difficulty that is often encountered in Markovian systems is that the system of differential equations describing the moments of the birth-death process might not be *closed*. This means that it is necessary that one know the true distribution of the Markov process or at least its higher moments in order to compute the lower moments of the stochastic process.

One common approach to circumvent the lack of closure is to apply asymptotic methods such as heavy traffic limit theorems. Such results scale or speed up the rates of the stochastic process in order to simplify the stochastic analysis of the Markov process, see for example Massey [17] and Mandelbaum et al. [16]. However, these methods are asymptotic and therefore only apply when the stochastic processes rates are infinite or very large. They do not apply directly to a process that has moderately sized rates. Moreover, currently, there are no methods to determine how close our nonstationary approximations are to the true stochastic process for a particular finite rate.

An alternative method for computing the moments of the Markov process is to apply what are known as *closure approximations* to the stochastic process under consideration. Closure approximations attempt to intelligently approximate the distribution of the Markov process and use this approximate distribution to estimate the moments of the stochastic process. By using the closure approximation, it should be simple to calculate the moment dynamics and perhaps more importantly, the moment dynamics should be close to the true dynamics of the original process. See for example Krishnarajah et al. [14, 15] in the epidemic process setting and Rothkopf and Oren [27], Clark [3], and Taaffe and Ong [28] in the queueing process setting.

A more recent method developed by Massey and Pender [18, 19], Pender and Massey [25] is to use Hermite polynomial expansions to approximate the distribution of the queue length process. Taking two or three terms of the expansion works quite well. Since the Hermite polynomials are orthogonal to the Gaussian distribution, which has support on the entire real line, these Hermite polynomial chaos expansions do not take into account the discreteness of the queueing process and the fact that the queueing process is non-negative. Work by J. Pender [26] uses Laguerre polynomials, which are orthogonal with respect to the gamma distribution on the positive real line, but also ignores the discrete nature of the queueing process. Lastly, Pender [23] provides a Poisson-Charlier expansion for the *queue length* process, however, this work does not prove error bounds for the method and nor does it expand the transition or state probabilities, which we will show is much easier to do. For the continuous distributions like the Hermite and Laguerre it is also quite difficult to prove error bounds on these approximations due to the discrete nature of the queueing process. Therefore, in the context of queueing theory, it is still an open problem to develop closure methods using a *discrete* reference distribution with provable error bounds for the truncation error.

We also find it important to mention recent work in approximating queueing networks with Gaussian distributions. Recent work by Gurvich et al. [9], Huang and Gurvich [10], Dai and Shi [4], Braverman et al. [1] uses excursions and Stein's method to provide explicit error bounds for Gaussian approximations and steady state queue length proceses. With an exception of a small section in Huang and Gurvich [10] that covers transient systems, all of the work is in steady state and assumes some type of scaling for the queue length processes. Our approach is complementary to these approaches, yet is quite different in three major ways. First, we do not use Gaussian distributions to derive our approximations. Second, we do not assume any type of scaling for the queue length processes, which we argue is unnatural for finite sized systems. Finally, our approximations are discrete and not continuous, which is also more natural for discrete queueing systems.

In this paper, we study one dimensional birth-death models that have nonstationary as well as non-trivial state dependent rates. To develop approximations for the moments and the state probabilities, we use the Poisson-Charlier polynomials to expand the state probabilities of the Markov process in terms of a Poisson reference distribution. This Poisson representation of the transition probabilities is quite natural since a linear birth-death process such as an infinite server queue, has a Poisson distribution when initialized at zero or with a Poisson distribution. Therefore, the terms that serve to correct the true distribution from the Poisson reference distribution can be written explicitly in terms of integrals with respect to the Poisson distribution, which is quite simple. In addition, we should expect that processes that are close to an infinite server queue, should also be approximated quite well with a small number of terms. Moreover, the Poisson reference distribution also allows us to derive explicit approximations for many important stochastic models in the operations research literature such as the nonstationary Erlang-A model, nonstationary Erlang loss model, and even some quadratic birth-death models that are relevant in the applied probability literature. This is because we are able to explicit calculate the rate functions that appear in the functional forward equations using the discrete representation of the incomplete gamma function.

Our approach, which is similar to the spectral Galerkin method of Wulkow [29, 30], later developed by Deuflhard et al. [5], and independently by S. Engblom [8], not only exploits the properties of the Poisson distribution, but also allows us to derive explicit bounds for the transition probabilties and weak *a priori* estimates for estimating the moments of our approximation method. These bounds and estimates help us understand how many terms we might need to approximate the moments of our birth-death process with good accuracy. Moreover, we can show that as we add more terms to the expansion, the approximate transition probabilities and the moments of the birth-death model converge to the true transition probabilties and moments of the underlying Markov process. However, unlike their continuous counterparts, discrete orthogonal polynomials such as the Poisson-Charlier and their properties are much less studied. This forces us to define new weighted Sobolev spaces to analyze the convergence of our discrete closure approximation. These Sobolev spaces allow us to prove spectral convergence of the method, with error estimates decaying faster than any inverse power of the expansion order $N$, and also allow us to prove that the moments converge by adding more terms to the approximation of the transition probabilities.

**Contributions to Literature** In this work we make the following contributions:

- We expand the state probabilities of one-dimensional birth-death Markov processes in terms of Poisson-Charlier polynomials.
- We prove the convergence of the state probabilities and the moments of one-dimensional birth-death Markov processes as we add more terms to the Poisson-Charlier expansion by constructing the appropriate Sobolev sequence spaces. We also prove explicit error bounds for the transition probabilities and moments when we truncate the expansion to a finite number of terms. Thus, we provide the first moment closure with provable error bounds.
- We show numerically that our approximatons are quite accurate at describing the moment dynamics of the underlying Markov process with only a small number of terms.

**Organization of Paper** The rest of the paper is organized as follows. In Section 2, we introduce the nonstationary and state dependent birth death model that we consider for the remainder of the paper. In Section 3, we introduce the Poisson-Charlier expansion method that we use in the paper and describe the new sequence spaces that are needed to prove convergence of our method. In Section 4, we derive our error bounds for the transition probabilities and the moments for a general birth-death process. In Section 5, we provide extensive numerical results illustrating the power of our method. Finally, in Section 6, we conclude with future work.

## 2. Nonstationary Birth-Death Model

In this section, we give a description of the birth-death model that is under consideration. Birth-death processes are very important processes in the stochastic community. They arise in variety of applications from queueing theory, chemical reaction networks, neuroscience, and healthcare modelling. Thus, it is important to have a good understanding of the dynamics of these models. In addition, in all of these applications, it is also very important to understand the nonstationary and state dependent aspects of these models. Nonstationary and state dependent dynamics are prevalent in our society, especially in a queueing context, where arrivals of customers is almost never stationary and often depend substantially on the size of the queue.

We consider a continuous time one-dimensional nonhomogeneous birth-death process (BDP) $Q(t)$, $t \geq 0$ on the state space $\mathbf{Z}_+ = \{0, 1, 2, \ldots\}$ with time dependent and state dependent rate functions. The rate function for the birth process is denoted by $\lambda_x(t)$ and the rate functions for the death process are denoted by $\mu_x(t)$, $t \geq 0$, $x \in \mathbf{Z}_+$. Moreover, we have that

$$\mathbb{P}(Q(t+h) = j | Q(t) = i) = \begin{cases} \lambda_i(t) \cdot h + o(h) & \text{if } j = i+1, \\ \mu_i(t) \cdot h + o(h) & \text{if } j = i-1, \\ 1 - \lambda_i(t) \cdot h - \mu_i(t) \cdot h + o(h) & \text{if } j = i, \\ o(h) & \text{if } |i-j| > 1. \end{cases} \tag{1}$$

It is assumed that the time interval $h > 0$ is sufficiently small to eliminate the possibility of multiple events occurring in the same interval. We also denote $o(h) = o_i(t, h)$, $i \in \mathbf{Z}_+$ such that

$$\lim_{h \to 0} \frac{\sup_i \; o_i(t,h)}{h} = 0. \tag{2}$$

Thus, we define the transition probabilities and the state probabilities respectively as

$$p_{ij}(s,t) = \mathbb{P}(Q(t) = j | Q(s) = i), \tag{3}$$

and

$$p_i(t) = \mathbb{P}(Q(t) = i | Q(0) = 0). \tag{4}$$

If we let $\mathbf{p(t)} \equiv \{p_0(t), p_1(t), \ldots. p_\infty(t)\}$ and we let $\mathcal{A}(t)$ be the matrix induced by (1), then we have that

$$\overset{\bullet}{\mathbf{p}}(t) = \mathcal{A}(t)\mathbf{p}. \tag{5}$$

We assume that the rates of birth and death are given by the transition probabilities of a Markov chain. Mathematically, this means that the changes in the system in a small time interval are determined by the following transition probabilities

$$\begin{aligned} \mathbb{P}\{\Delta Q(t+\Delta t) = 1\} &\equiv \psi_\alpha(t, Q(t)) \cdot \Delta t \\ \mathbb{P}\{\Delta Q(t+\Delta t) = -1\} &\equiv \psi_\delta(t, Q(t)) \cdot \Delta t \end{aligned}$$

Brémaud [2, §8.4.3] gives verifiable conditions for non-explosion of the birth and death generator. Typically in the physical or chemical literature the functions $\psi_\alpha$ and $\psi_\delta$ are polynomials functions of the state $Q(t)$. Although they may be non-linear, they are smooth functions of the state process. However, in fields such as queueing theory, these functions can be nonlinear and non-smooth with respect to the state variable $Q(t)$. In fact, these rate functions are sometimes even discontinuous.

From now on for ease of notation, we will suppress the time dependence of the stochastic process $Q(t)$ and the rate functions. Using the above functional form of the transition probabilities, we can state the Kolmogorov forward equations of the Markov process. Implicit conditions for the validity of the forward equations are found in [2, §8.3.2], while general explicit conditions can be found in Meyn and Tweedie [20]. Compare also the discussion in Engblom [6] targeting applications in chemical kinetics. In the present case and for the purposes herein, the conditions in Engblom [6] simplify considerably.

Proposition 1 **(see Theorem 4.5 in Englblom [6])**. *Suppose the birth and death rates satisfy for $x, y \in \mathbf{Z}_+$,*

$$\psi_\alpha(x) + \psi_\delta(x) \leq C(1+x), \tag{6}$$

*and suppose further that $f : \mathbf{Z}_+ \to \mathbf{R}$ is bounded by some finite pth order moment, $|f(x)| \leq C_p(1 + x^p)$. Then the Markovian birth-death process satisfies the following set of functional Kolmogorov forward equations:*

$$\begin{aligned} \overset{\bullet}{E}[f(Q(t))] &\equiv \overset{\bullet}{E}[f(Q(t)) \mid Q(0) = 0\ ] \\ &= E[\psi_\alpha(t,Q) \cdot (f(Q+1) - f(Q))] + E[\psi_\delta(t,Q) \cdot (f(Q-1) - f(Q))]. \end{aligned}$$

Proposition 2. *Suppose that $\psi_\alpha(t,Q)$ and $\psi_\delta(t,Q)$ satisfy the sufficient conditions given in Proposition 1, then we have that the $m^{th}$ moment of the birth-death process satisfies the following differential equation*

$$\overset{\bullet}{E}[Q^m(t)] = \sum_{k=0}^{m-1} \binom{m}{k} \cdot \left( E[Q^k \cdot \psi_\alpha(t,Q)] + (-1)^{m-k} \cdot E[Q^k \cdot \psi_\delta(t,Q)] \right) \tag{7}$$

***Proof:*** *Using the binomial theorem, we have that*

$$\begin{aligned} \overset{\bullet}{E}[Q^m(t)] &= E[\psi_\alpha(t,Q) \cdot ((Q+1)^m - Q^m)] + E[\psi_\delta(t,Q) \cdot ((Q-1)^m - Q^m)] \\ &= E\left[\psi_\alpha(t,Q) \cdot \left( \sum_{k=0}^{m} \binom{m}{k} \cdot Q^k - Q^m \right)\right] \\ &+ E\left[\psi_\delta(t,Q) \cdot \left( \sum_{k=0}^{m} \binom{m}{k} \cdot (-1)^{m-k} \cdot Q^k - Q^m \right)\right] \\ &= \sum_{k=0}^{m-1} \binom{m}{k} \cdot E[Q^k \cdot \psi_\alpha(t,Q)] + \sum_{k=0}^{m-1} \binom{m}{k} \cdot (-1)^{m-k} \cdot E[Q^k \cdot \psi_\delta(t,Q)] \\ &= \sum_{k=0}^{m-1} \binom{m}{k} \cdot \left( E[Q^k \cdot \psi_\alpha(t,Q)] + (-1)^{m-k} \cdot E[Q^k \cdot \psi_\delta(t,Q)] \right) \end{aligned}$$

■

Corollary 1. *Using Proposition 2 the time derivatives of the first four cumulant moments satisfy the following equations*

$$\begin{aligned} \overset{\bullet}{E}[Q(t)] &= E[\psi_\alpha(t,Q)] - E[\psi_\delta(t,Q)] \\ \overset{\bullet}{\mathrm{Var}}[Q(t)] &= E[\psi_\alpha t, Q)] + E[\psi_\beta(t,Q)] + 2 \cdot \mathrm{Cov}[Q, \psi_\alpha(t,Q)] - 2 \cdot \mathrm{Cov}[Q, \psi_\beta(t,Q)] \\ \overset{\bullet}{C}^{(3)}[Q(t)] &= E[\psi_\alpha(t,Q)] - E[\psi_\beta(t,Q)] + 3 \cdot \mathrm{Cov}[Q, \psi_\alpha(t,Q)] + 3 \cdot \mathrm{Cov}[Q, \psi_\beta(t,Q)] \\ &\quad +3 \cdot \mathrm{Cov}\left[\overline{Q}^2, \psi_\alpha(t,Q)\right] - 3 \cdot \mathrm{Cov}\left[\overline{Q}^2, \psi_\beta(t,Q)\right] \\ \overset{\bullet}{C}^{(4)}[Q(t)] &= E[\psi_\alpha(t,Q)] + E[\psi_\beta(t,Q)] + 4 \cdot \mathrm{Cov}[Q, \psi_\alpha(t,Q)] - 4 \cdot \mathrm{Cov}[Q, \psi_\beta(t,Q)] \\ &\quad +6 \cdot \mathrm{Cov}\left[\overline{Q}^2, \psi_\alpha(t,Q)\right] + 6 \cdot \mathrm{Cov}\left[\overline{Q}^2, \psi_\beta(t,Q)\right] \\ &\quad +4 \cdot \mathrm{Cov}[\overline{Q}^3, \psi_\alpha(t,Q)] - 4 \cdot \mathrm{Cov}[\overline{Q}^3, \psi_\beta(t,Q)] \\ &\quad +12 \cdot \mathrm{Var}[Q] \cdot (\mathrm{Cov}[Q, \psi_\alpha(t,Q)] + \mathrm{Cov}[Q, \psi_\beta(t,Q)]) \end{aligned}$$

*where* $\overline{Q} = Q - E[Q]$ *and* $\mathrm{Cov}[f(Q), g(Q)] = E[f(Q) \cdot g(Q)] - E[f(Q)] \cdot E[g(Q)]$.

Thus, using the functional forward equations, it appears at first sight that we might be able to calculate the moments of the birth-death process directly. However, this is quite complicated unless the rate functions $\psi_\alpha(t,Q)$ and $\psi_\beta(t,Q)$ are constant, linear, or some other very special case. One way to see this complication is to make $\psi_\beta(t,Q)$ quadratic. Thus, it is easily seen that the differential equation for the mean of the birth death process depends on the second moment of the process, which is unknown. When the moments of lower order either depend on higher order moments or functions of higher order moment, this system of equations is said to be *not closed*. Thus, closure approximations were developed to address this complication by approximating the higher order moment terms with functions of the lower order moments. However, one complication is that typically closure approximations have no theoretical guarantees for performance and are quite heuristic. In the next section, we describe a new closure method based on Poisson-Charlier polynomials and Sobolev space estimates that not only has theoretical guareentees for approximating the distribution and its moments, but also has good numerical performance.

**3. Poisson-Charlier Expansions** In this section we describe our method for approximating the dynamics of one-dimensional Markovian birth-death processes. We first give an outline and motivation for the method and how it is extremely useful in our context.

**3.1. Motivation** Our method expands the state probabilities of the birth-death Markov process in terms of Poisson-Charlier polynomials and the Poisson reference distribution. This means that we project the actual state probabilities onto a finite set of Poisson-Charlier polynomials. We then use this approximation to derive estimates for the moment of the Markov process, by using the functional forward equations. One important result is that we can exploit various properties of the Poisson distribution to derive *explicit* and *closed-form* approximations for various Markovian birth-death processes with explicit and rigorous error bounds on the expansion or truncation error. We know from the theory of Hilbert spaces and the fact that probabilities are bounded that the transition probabilities of our queueing process can be written in terms of an infinite Poisson-Charlier polynomial expansion,

$$\mathbb{P}(Q(t)=x)=\omega(x)\sum_{j=0}^{\infty}c_j(t)\cdot C_j^a(x), \tag{8}$$

where the $C_j(a,x)$ are the Poisson-Charlier polynomials with parameter $a$ and $\omega(x)$ is the Poisson distribution weight function. Now if one truncates the distribution at a finite number of terms, then one has the following approximation for the value of the state probabilities of the Markovian birth-death process as

$$\mathbb{P}^{(N)}(Q(t)=x)=\omega(x)\sum_{j=0}^{N}c_j(t)\cdot C_j^a(x). \tag{9}$$

This introduces the following error for the state probabilities when approximated by a truncated expansion

$$\text{Error} \equiv E_x^{(N)}=\mathbb{P}^{(N)}(Q(t)=x)-\mathbb{P}(Q(t)=x)=\omega(x)\sum_{j=N+1}^{\infty}c_j(t)\cdot C_j^a(x). \tag{10}$$

It is obvious that as we add more terms that $\lim_{N\to\infty}E_x^{(N)}=0$ for each value of $x\in\mathbf{Z}_+$, however, the details of this convergence are not trivial.

In addition to the state probabilities, it is also possible to derive approximations for the moments of the stochastic process. Using the state probabilities, we have the following expression for the $m^{th}$ moment of the birth-death process in terms of Poisson-Charlier polynomials

$$E[Q^m(t)] = \sum_{x=0}^{\infty} x^m \cdot \omega(x) \sum_{j=0}^{\infty} c_j(t) \cdot C_j^a(x). \tag{11}$$

Moreover, by truncating the Poisson-Charlier expansion at N terms, we have the following approximation for the $m^{th}$ moment of the birth-death process as

$$E^{(N)}[Q^m(t)] = \sum_{x=0}^{\infty} x^m \cdot \omega(x) \sum_{j=0}^{N} c_j(t) \cdot C_j^a(x). \tag{12}$$

Thus, like in the state probability case, we can substract the two and get the error induced by truncating the two expressions.

**3.2. A Review of Poisson Charlier Polynomials and Properties** In this section, we describe how to use Poisson-Charlier polynomials in conjuction with the functional forward equations in order to construct approximations for our nonstationary queueing processes. The Poisson-Charlier polynomials are an orthogonal polynomial sequence with respect to the Poisson distribution with rate $a$ i.e

$$\omega(x) = e^{-a} \frac{a^x}{x!} \qquad x = 0, 1, 2, ..... \tag{13}$$

As a result, the Poisson-Charlier polynomials solve the following recurrence relation

$$\tilde{C}_{n+1}^a(x) = (x - n - a) \cdot \tilde{C}_n^a(x) - n \cdot \alpha \cdot \tilde{C}_{n-1}^a(x). \tag{14}$$

The first four unnormalized Poisson-Charlier polynomials are defined as

$$\tilde{C}_0^a(x) = 1 \tag{15}$$
$$\tilde{C}_1^a(x) = x - a \tag{16}$$
$$\tilde{C}_2^a(x) = x^2 - 2 \cdot x \cdot a + a^2 - x \tag{17}$$
$$\tilde{C}_3^a(x) = x^3 - 3 \cdot (a+1) \cdot x^2 + (3 \cdot a^2 + 3 \cdot a + 2) \cdot x - a^3 \tag{18}$$

and the first few orthonormal Poisson-Charlier polynomials can be generated according to

$$\begin{aligned} C_0^a(x) &\equiv 1, \\ C_1^a(x) &\equiv \frac{a-x}{\sqrt{a}}, \\ C_{n+1}^a(x) &= \frac{n+a-x}{\sqrt{a(n+1)}} C_n^a(x) - \sqrt{\frac{n}{n+1}} C_{n-1}^a(x). \end{aligned} \tag{19}$$

Moreover, the Poisson-Charlier polynomials satisfy the following Sturm-Liouville equation

$$\mathcal{S}p \equiv -\omega^{-1}(x) \cdot [\nabla (\omega(x) \cdot \triangle C_n^a(x))] = \frac{n}{a} C_n^a(x) \tag{20}$$

where $\nabla$ and $\triangle$ are defined as the backward and forward difference operators respectively and where $\mathcal{S}$ is the following Sturm-Liouville operator

$$\mathcal{S}p \equiv \frac{x}{a} \triangle p - \nabla p. \tag{21}$$

Although not as well studied as the convergence properties of the Hermite polynomials or the Laguerre polynomials, the convergence properties of the Poisson-Charlier projection (34)–(35) has been investigated in S. Engblom [7]. Now suppose that we have a function $f(x)$, which is defined on the integers and satifies the inequality

$$\sum_{x=0}^{\infty} f^2(x)\cdot\omega(a,x) < \infty, \quad \text{for some } a>0. \tag{22}$$

Then we have the following expansion in terms of Poisson-Charlier polynomials in the Hilbert space $l^2(\mathbb{N},\omega(a,x))$.

Proposition 3. *Any function f(x) $\in l^2(\mathbb{N},\omega(a,x))$ can be expanded into a Poisson-Charlier series i.e.*

$$f(x) = \sum_{x=0}^{\infty} c_j \cdot C_j^a(x) \tag{23}$$

*where* $c_j = \sum_{x=0}^{\infty} f(x) C_j^a(x)\omega(a,x)$.

Proof: See Ogura [21]. ■

Remark 1. This expansion can also be extended to the case where the independent variable of the function $f(k)$ is a stochastic process and also depends on time itself.

Lemma 1.

$$\sum_{x=0}^{\infty} \omega(a,x)\cdot C_j^a(x) = E[C_j^a(x)] = 0 \quad \text{for all } j\geq 1. \tag{24}$$

Proof: This follows from the orthogonality of the Poisson-Charlier polynomials with constants, which is the zeroth order term. ■

It is important to know how close our distribution is to the Poisson distribution. The Chen Stein method can help in our understanding of how close our queueing process is to the Poisson distribution.

Theorem 1 **(Chen-Stein)**. *Let Q be a random variable with values in $\mathbb{N}$. Then, Q has the Poisson distribution with mean rate q if and only if, for every bounded function $f:\mathbb{N}\to\mathbb{N}$,*

$$\mathbb{E}[Q\cdot f(Q)] = q\cdot\mathbb{E}[f(Q+1)] \tag{25}$$

Proof: See Peccati and Taqqu [22]. ■

**3.3. Weighted Sobolev sequence spaces** In this section we put forward a theory for convergence of orthogonal expansions in terms of Charlier polynomials and associated Poisson functions. Due to the discreteness of the underlying Poisson measure the theory requires a special hierarchy of discrtete Sobolev spaces which is devloped in §3.3. Another important reason that the Sobolev spaces are needed is that polynomials or (moments) are not integrable on unbounded domains without a sufficiently fast decaying measure. Moreover, the type of convergence we are interested in is detailed in §4 and forms the basis for our later developments. The material in here draws on some earlier accounts S. Engblom [7, 8], but several salient and novel extensions are proposed to deal with our new problems.

First, since in the current work we aim for a consistent moment closure rather than a convergent spectral method for the probability density itself, the correct Hilbert spaces to work with are not the same as S. Engblom [7, 8]. More specifically, the targeted densities have to belong to a certain more restrictive class of weighted Hilbert spaces than what is required for spectral approximations to the densities themselves. Secondly, we present a general weak error bound of our method which predicts the weak convergence of arbitrary functionals in a certain class. This convergence is extremely relevant for approximating the moments of the Markov process since we want to be confident that our method also converges for moments based on our transition probability approximations.

For real-valued functions over the non-negative integers $\mathbf{Z}_+ = \{0, 1, 2, \ldots\}$ we associate the usual discrete Euclidean inner product,

$$(p, q) \equiv \sum_{x \geq 0} p(x) q(x), \tag{26}$$

and we define the $l^2(\mathbf{Z}_+)$-sequence space accordingly,

$$\|q\|^2_{l^2(\mathbf{Z}_+)} \equiv (q, q), \tag{27}$$
$$l^2(\mathbf{Z}_+) = \left\{ q : \mathbf{Z}_+ \to \mathbf{R};\ \|q\|_{l^2(\mathbf{Z}_+)} < \infty \right\}. \tag{28}$$

Now we introduce the important class of discrete Sobolev sequence spaces that are necessary for our analysis

$$h^m(\mathbf{Z}_+) = \left\{ q : \mathbf{Z}_+ \to \mathbf{R};\ \sqrt{x^{\underline{k}}} \cdot q(x) \in l^2(\mathbf{Z}_+) \text{ for } 0 \leq k \leq m \right\}, \tag{29}$$
$$\|q\|^2_{h^m(\mathbf{Z}_+)} \equiv \sum_{k=0}^{m} a^{-k} \|\sqrt{x^{\underline{k}}} \cdot q(x)\|^2_{l^2(\mathbf{Z}_+)}, \tag{30}$$

where the falling factorial power is defiend by $x^{\underline{m}} = x!/(x-m)! = \prod_{i=0}^{m-1}(x-i)$ and where the free parameter $a \in \mathbf{R}_+$.

Define as usual the Poisson weight function by

$$w(x) = \frac{a^x}{x!} \cdot e^{-a}. \tag{31}$$

We need to consider two related *weighted* inner products. Define $(p, q)_w := (p, qw)$ and similarly $(p, q)_{w^{-1}} := (p, qw^{-1})$, where in the latter case clearly some regularity of $p$ and $q$ is understood. A useful observation is that by the Cauchy-Schwartz inequality we have that,

$$(p, q) = (pw^{1/2}, qw^{-1/2}) \tag{32}$$
$$\leq \|p\|_{l^2(w;\, \mathbf{Z}_+)} \|q\|_{l^2(w^{-1};\, \mathbf{Z}_+)}, \tag{33}$$

again provided that $p$ and $q$ are measurable in the respective weighted $l^2$-spaces which we denote by $l^2(w;\, \mathbf{Z}_+)$ and $l^2(w^{-1};\, \mathbf{Z}_+)$, respectively.

From these weighted $l^2$-spaces we readily define two hierarchies of weighted Sobolev sequence spaces $h^m(w;\, \mathbf{Z}_+)$ and $h^m(w^{-1};\, \mathbf{Z}_+)$ by simply following the prescription in (29)–(30). The following is a consequence of these definitions and is an important property of the Sobolev spaces $h^m(w;\, \mathbf{Z}_+)$ and $h^m(w^{-1};\, \mathbf{Z}_+)$ that will be used throughout the rest of the paper.

PROPOSITION 4. *The map $p \mapsto wp$ is an isometry between $h^m(w;\, \mathbf{Z}_+)$ and $h^m(w^{-1};\, \mathbf{Z}_+)$.*

Proof: For an arbitrary $p \in h^m(w;\, \mathbf{Z}_+)$, put $q = wp$. Then by (30),

$$\begin{aligned}
\|q\|^2_{h^m(w^{-1};\, \mathbf{Z}_+)} &= \sum_{k=0}^{m} a^{-k} \sum_{x=0}^{\infty} x^{\underline{k}} \cdot q(x)^2 w(x)^{-1} \\
&= \sum_{k=0}^{m} a^{-k} \sum_{x=0}^{\infty} x^{\underline{k}} \cdot p(x)^2 w(x) \\
&= \|p\|^2_{h^m(w;\, \mathbf{Z}_+)}
\end{aligned}$$

as claimed. ■

**4. Main Results** For a given Poisson parameter $a>0$, and keeping in mind that different normalizations are sometimes used, we will let $C_n^a(x)$ denote the *normalized* $n$th degree Poisson-Charlier polynomial Koekoek and Swarttouw [13]. These polynomials are orthonormal with respect to the $l_w^2$-product and hence we may define $\pi_N$ as the orthogonal projection onto the space of polynomials $P_N$ of degree $\leq N$;

$$\pi_N p(x) \equiv \sum_{n=0}^{N} c_n C_n^a(x), \tag{34}$$

$$c_n = (p(x), C_n^a(x))_w. \tag{35}$$

THEOREM 2. *For any nonnegative integers $k$ and $m$, $k \leq m$, there exists a positive constant $C$ depending only on $m$ and $a$ such that, for any function $p \in h^m(w; \mathbf{Z}_+)$, the following estimate holds*

$$\|\pi_{N-1}p - p\|_{h^k(w;\mathbf{Z}_+)} \leq C(a/N)^{m/2}(1 \vee N/a)^{k/2}\|p\|_{h^m(w;\mathbf{Z}_+)}. \tag{36}$$

*If $a \geq 1$ is assumed, then $C$ depends only on $m$.*

Proof: We will prove this result in two steps. The first step is to make the observation that it is enough to prove our result for the uniformly equivalent norm $\|\cdot\|_{h^k(w,\triangle;\mathbf{Z}_+)}$. The second step is to prove the subsequent result using induction. Thus, we will show the result for the value $k=0$ and then make the inductive step. Now we show the result for $k=0$ and for even integers. A similar argument can be made for odd integers.

We know that for any integrable function $p \in l^2(w; \mathbf{Z}_+)$

$$\|\pi_{N-1}p - p\|^2_{l^2(w;\mathbf{Z}_+)} = \sum_{n \geq N}^{\infty} \bar{p}_n^2. \tag{37}$$

Moreover, we know that

$$\bar{p}_n = (p, C_n^a)_\omega \tag{38}$$

$$= \left(\frac{a}{n}\right)^{m/2} \cdot \left(\mathcal{S}^{m/2}p, C_n^a\right)_\omega. \tag{39}$$

Thus, combining our results, we have that

$$\|\pi_{N-1}p - p\|^2_{l^2(w;\mathbf{Z}_+)} = \sum_{n \geq N}^{\infty} \bar{p}_n^2 \tag{40}$$

$$\leq \sum_{n \geq N}^{\infty} \left(\frac{a}{n}\right)^m \cdot \left(\mathcal{S}^{m/2}p, C_n^a\right)_\omega^2 \tag{41}$$

$$\leq \left(\frac{a}{N}\right)^m \cdot \sum_{n \geq N}^{\infty} \left(\mathcal{S}^{m/2}p, C_n^a\right)_\omega^2 \tag{42}$$

$$\leq \left(\frac{a}{N}\right)^m \cdot \|\mathcal{S}^{m/2}p\|^2_{l^2(w;\mathbf{Z}_+)} \tag{43}$$

Thus, we have shown the result for the case $k=0$. We will finish the proof by using induction. First we assume that the result given in Equation 36 holds for the case of $k$, thus we must show the result for $k+1$. Using this assumption the decomposition of the discrete Sobolev spaces, we can then bound the error in terms of the following useful partition

$$\|\pi_{N-1}p - p\|_{h^{k+1}(w,\triangle;\mathbf{Z}_+)} \leq \|\pi_{N-1}p - p\|_{l^2(w;\mathbf{Z}_+)} + \|\pi_{N-1}\triangle p - \triangle \pi_{N-1}p\|_{h^k(w,\triangle;\mathbf{Z}_+)} + \|\pi_{N-1}\triangle p - \triangle p\|_{h^k(w,\triangle;\mathbf{Z}_+)}. \tag{44}$$

Using the case where $k=0$, we have that

$$\|\pi_{N-1}p-p\|_{h^{k+1}(w,\triangle;\mathbf{Z}_+)} \leq C\left(\frac{a}{N}\right)^{m/2}\|p\|_{h^m(w,\triangle;\mathbf{Z}_+)} + \|\pi_{N-1}\triangle p-\triangle\pi_{N-1}p\|_{h^k(w,\triangle;\mathbf{Z}_+)} \quad (45)$$
$$+\|\pi_{N-1}\triangle p-\triangle p\|_{h^k(w,\triangle;\mathbf{Z}_+)}. \quad (46)$$

Moreover, using the equivalence of norms, we also have that

$$\|\triangle p\|_{h^{m-1}(w,\triangle;\mathbf{Z}_+)} \leq \|p\|_{h^m(w,\triangle;\mathbf{Z}_+)}, \quad (47)$$

which implies that

$$\|\pi_{N-1}p-p\|_{h^{k+1}(w,\triangle;\mathbf{Z}_+)} \leq C\left(\frac{a}{N}\right)^{m/2}\|p\|_{h^m(w,\triangle;\mathbf{Z}_+)} + \|\pi_{N-1}\triangle p-\triangle\pi_{N-1}p\|_{h^k(w,\triangle;\mathbf{Z}_+)} \quad (48)$$
$$+C\left(\frac{a}{N}\right)^{(m-1)/2-k/2}\|\triangle p\|_{h^{m-1}(w,\triangle;\mathbf{Z}_+)}. \quad (49)$$

Now that we have two terms bounded in terms of the correct norm given in Equation 36, it now remains to bound the middle term to complete the proof. Thus, we must show that

$$\|\pi_{N-1}\triangle p-\triangle\pi_{N-1}p\|_{h^k(w,\triangle;\mathbf{Z}_+)} \leq C\left(\frac{a}{N}\right)^{m/2}\cdot\max\left(1,\frac{N}{a}\right)^{(k+1)/2}\cdot\|\triangle p\|_{h^{m-1}(w,\triangle;\mathbf{Z}_+)}. \quad (50)$$

To this end, exploit the Poisson-Charlier expansion for the function $p$, we make the following two observations that $\pi_{N-1}\triangle p \equiv \sum_{n=0}^{N}\bar{p}_n\triangle C_n^a$ and $\triangle\pi_{N-1}p\equiv\sum_{n=0}^{N-1}\bar{p}_n\triangle C_n^a$.

Thus, the difference between the two expressions can be bounded by

$$\|\pi_{N-1}\triangle p-\triangle\pi_{N-1}p\|_{h^k(w,\triangle;\mathbf{Z}_+)} = \|\sum_{n=0}^{N}\bar{p}_n\triangle C_n^a - \sum_{n=0}^{N-1}\bar{p}_n\triangle C_n^a\|_{h^k(w,\triangle;\mathbf{Z}_+)} \quad (51)$$
$$=\|\bar{p}_N\triangle C_N^a\|_{h^k(w,\triangle;\mathbf{Z}_+)} \quad (52)$$
$$\leq |\bar{p}_N|\|\triangle C_N^a\|_{h^k(w,\triangle;\mathbf{Z}_+)} \quad (53)$$
$$\leq C\cdot|(p,C_N^a)_\omega|\cdot\|\triangle C_N^a\|_{h^k(w,\triangle;\mathbf{Z}_+)}. \quad (54)$$

Finally, by using standard Sobolev bounds for the Poisson-Charlier polynomials, the Sturm-Liouville representation of the Poisson-Charlier polynomials and the Cauchy-Bunyakovsky-Schwartz inequality, we have that

$$\|\pi_{N-1}\triangle p-\triangle\pi_{N-1}p\|_{h^k(w,\triangle;\mathbf{Z}_+)} \leq C\left(\frac{a}{N}\right)^{m/2}\cdot\max\left(1,\frac{N}{a}\right)^{(k+1)/2}\cdot\|\triangle p\|_{h^{m-1}(w,\triangle;\mathbf{Z}_+)}. \quad (55)$$

Thus, we complete our proof by combining all of the estimates and bounds together. ■

In addition to our approximations in terms of Poisson-Charlier polynomials, we also need to consider the corresponding approximation results in terms of *Poisson-Charlier functions*. These are defined for $n=0,1,\dots$ by $\tilde{C}_n(a,x)\equiv C_n^a(x)\cdot w(x)$ and spans the space $\tilde{P}_N\equiv\{p(x)=q(x)\cdot w(x);\, q\in P_N\}$. Using orthonormality under the inner product $(\cdot,\cdot)_{w^{-1}}$ we define $\tilde{\pi}_N$ to denote the orthogonal projection on $\tilde{P}_N$. Thus, we have the following relation between the two projection operators of which $\tilde{\pi}_N p$ will be the most important for our approximations since it is related to the Poisson-Charlier functions.

Proposition 5.

$$\tilde{\pi}_N p = w(x)\pi_N\left[w(x)^{-1}\cdot p(x)\right]. \quad (56)$$

Proof: For $p \in l^2(w^{-1}; \mathbf{Z}_+)$ by orthonormality we have the Fourier series

$$\tilde{\pi}_N p = \sum_{n=0}^{N-1} (p, \tilde{C}_n^a)_{w^{-1}} \tilde{C}_n^a.$$

Expanding we get

$$\begin{aligned}\tilde{\pi}_N p &= w(x) \sum_{n=0}^{N-1} (w^{-1}p, C_n^a)_w C_n^a \\ &= w(x)\pi_N \left[w(x)^{-1} \cdot p(x)\right]\end{aligned}$$

by inspection. ■

The natural setting for measuring convergence is now the hierarchy of inversely weighted Sobolev-spaces $h^m(w^{-1}; \mathbf{Z}_+)$. Theorem 2 governs the case of convergence in the weighted $l^2$-space. For sufficiently regular functions we may use the representation in Proposition 5 and the isometry in Proposition 4 to arrive at the following result which is crucial to the approach taken in this paper.

Theorem 3 (***Poisson-Charlier expansion***). *For any nonnegative integers $k$ and $m$, $k \leq m$, there exists a positive constant $C$ depending only on $m$ and $a$ such that, for any function $p \in h^m(w^{-1}; \mathbf{Z}_+)$, the following estimate holds*

$$\|\tilde{\pi}_{N-1} p - p\|_{h^k(w^{-1}; \mathbf{Z}_+)} \leq C(a/N)^{m/2}(1 \vee N/a)^{k/2} \|p\|_{h^m(w^{-1}; \mathbf{Z}_+)}. \tag{57}$$

*Again, if $a \geq 1$ is assumed, then $C$ depends only on $m$.*

Proof: By Proposition 4, we know that $p \mapsto w^{-1}p$ is an isometry between the Sobolev spaces $h^k(w^{-1}; \mathbf{Z}_+)$ and $h^k(w; \mathbf{Z}_+)$. Thus, we can move back and forth between the spaces keeping in mind the different weighting functions. For some $p \in h^m(w^{-1}; \mathbf{Z}_+)$, put $q = w^{-1}p$. Then

$$\begin{aligned}\|\tilde{\pi}_{N-1} p - p\|^2_{h^k(w^{-1}; \mathbf{Z}_+)} &= \|w\pi_N \left[w^{-1} \cdot p\right] - p\|^2_{h^k(w^{-1}; \mathbf{Z}_+)} \\ &= \|\pi_N \left[w^{-1} \cdot p\right] - w^{-1}p\|^2_{h^k(w; \mathbf{Z}_+)} \\ &= \|\pi_N q - q\|^2_{h^k(w; \mathbf{Z}_+)},\end{aligned}$$

where Theorem 2 clearly applies and yields (57) expressed in terms of the $h^m(w^{-1}; \mathbf{Z}_+)$-norm of $q$. Using the isometry in Proposition 4 again finalizes the proof. ■

Example 1. Consider a Poisson distribution $p(x) = \exp(-\lambda)\lambda^x/x!$ for some constant $\lambda > 0$. Write $p_N = \tilde{\pi}_{N-1}p$ for $a \neq \lambda$. We compute explicitly

$$\begin{aligned}\|p\|^2_{h^m(w^{-1}; \mathbf{Z}_+)} &= \sum_{k=0}^m a^{-k} \sum_{x \geq 0} x^{\underline{k}} \cdot p(x)^2 w(x)^{-1} \\ &= \sum_{k=0}^m a^{-k} \sum_{x \geq 0} \frac{x!}{(x-k)!} \exp(-2\lambda) \frac{\lambda^{2x}}{(x!)^2} \cdot \exp(a) \frac{x!}{a^x} \\ &= \sum_{k=0}^m a^{-k} \sum_{x \geq 0} \frac{1}{(x-k)!} \exp(-2\lambda) \cdot \lambda^{2x} \cdot \exp(a) \frac{1}{a^x} \\ &= \sum_{k=0}^m a^{-k} \sum_{x \geq 0} \frac{1}{x!} \cdot \exp(a - 2\lambda) \cdot \left(\frac{\lambda^2}{a}\right)^{x+k} \\ &= \sum_{k=0}^m \left(\frac{\lambda}{a}\right)^{2k} \exp((a-\lambda)^2/a) \\ &= \frac{1 - (\lambda/a)^{2(m+1)}}{1 - (\lambda/a)^2} \exp((a-\lambda)^2/a).\end{aligned}$$

Inspired by this evaluation let us make the abstract assumption that

$$\|p\|_{h^m(w^{-1};\mathbf{Z}_+)} \le C_a \theta_a^m, \tag{58}$$

for some positive constants $(C_a, \theta_a)$ possibly depending on $a$, and refer to this class of distributions as being "highly regular". We see that for $p$ in this class and for a fix $k$ we obtain from Theorem 3 that for $N$ large enough,

$$\|\tilde{\pi}_{N-1}p - p\|_{h^k(w^{-1};\mathbf{Z}_+)} \le C_a (a/N)^{(m-k)/2} \theta_a^m.$$

By selecting $N$ large enough we may now let $m \to \infty$ and get an error estimate that decreases faster than any inverse power of $N$. Hence in fact, for $p$ sufficiently regular in the sense of (58),

$$\|\tilde{\pi}_{N-1}p - p\|_{h^k(w^{-1};\mathbf{Z}_+)} \le \exp(-cN),$$

for some $c > 0$ and any fixed value of $k$.

Let us write $p_N = \tilde{\pi}_{N-1}p$ for $p$ some unknown but sufficiently regular probability distribution. Assume that $X \sim p$ and let $X_N \sim p_N$ be considered an approximation to $X$. What can then be said about weak errors of the form $Ef(X_N) - Ef(X)$? Firstly, note that $p_N$ is not guaranteed to be a probability distribution; it need not hold true that $p_N(x) \ge 0$ for all $x \in \mathbf{Z}_+$. However, $(1, p_N) = (\tilde{C}_0^a, p_N)_{w^{-1}} = (\tilde{C}_0^a, p)_{w^{-1}} = (1, p)$, and hence the normalization is the correct one. In a practical setting we can therefore adopt

$$Ef(X_N) = \sum_{x \ge 0} f(x) p_N(x) = (f, p_N) \tag{59}$$

as a *definition* of the numerical expectation value. With these considerations in mind we get the following result.

Theorem 4 ***(A Priori Weak Error)***. *Let $p \in h^k(w^{-1}; \mathbf{Z}_+)$, $f \in l^2(w; \mathbf{Z}_+)$ and put $p_N = \tilde{\pi}_{N-1}p$. Then*

$$|Ef(X_N) - Ef(X)| \le C(a/N)^{m/2} \|f\|_{l^2(w;\mathbf{Z}_+)} \|p\|_{h^m(w^{-1};\mathbf{Z}_+)}. \tag{60}$$

Proof: Using the projection as our surrogate distribution for the transition probabilities, we know that the difference between our approximation and the true expected value of the functional $f(x)$ is

$$\begin{aligned} Ef(X_N) - Ef(X) &= (f, p_N - p) \\ &= (f \cdot w^{1/2}, (p_N - p) \cdot w^{-1/2}) \\ &\le \|f\|_{l^2(w;\mathbf{Z}_+)} \|p_N - p\|_{l^2(w^{-1};\mathbf{Z}_+)} \\ &\le C(a/N)^{m/2} \|f\|_{l^2(w;\mathbf{Z}_+)} \|p\|_{h^m(w^{-1};\mathbf{Z}_+)} \end{aligned}$$

after invoking Theorem 3 with $k = 1$. ■

Example 2. Continuing with $p$ as in Example 1, put $f(x) = x^k$. Then the error in the $k$th mean can be estimated as

$$\left| EX_N^k - EX^k \right| \le C(a/N)^{m/2} \left( M_a^{2k} \right)^{1/2} \left( \frac{1 - (\lambda/a)^{2(m+1)}}{1 - (\lambda/a)^2} \right)^{1/2} \exp((a-\lambda)^2/(2a)),$$

where $M_a^{2k}$ is the $2k$th moment of a Poisson distribution of parameter $a$. Reasoning as in Example 1 we find that for sufficiently regular target distrbutions $p$, and for a fix order of the moment $k$,

$$\left| EX_N^k - EX^k \right| \le \exp(-cN),$$

as $N$ tends to infinity.

Therefore we have shown in this section that we can approximate our Markov process with projections onto the Poisson-Charlier functions. Moreover, when we use the projection estimates for the transition probabilities, we can also extrapolate these approximations for the moments of the Markov process and bound the truncation error. These estimates are the basis for our explicit approximations in the next section, which are based on the projections onto the Poisson-Charlier functions. We will show that a small number of terms of the expansion are all that is needed to capture much of the dynamics of several Markov processes.

**5. Numerical Results** In this section, we demonstrate the performance and accuracy of our approximation methods using several orders of the approximation. Errors were measured in a time averaged relative sense,

$$\text{Error} \equiv \int_0^T \frac{|u-u^*|}{|u^*|}\frac{dt}{T},$$

with $u$ an approximation to $u^*$. For the cases where the initial data at $t=0$ caused difficulties with division by zero the lower limit of integration was simply replaced with 1 and the measure of integration renormalized accordingly. In practice, the integral was approximated using discrete points spaced 0.001 units apart. For the exact solution we used a numerical solution of order at least twice as high the order of the approximation to be judged. Lastly, in all examples we set the time interval [0,T] to [0,50].

**5.1. Erlang-A Model** Here we provide some tables for the relative errors of the several orders of the approximation for the mean, variance, skewness, and kurtosis of the Erlang-A queueing model. We see in Tables 1 - 5 that the spectral method is performing quite well at approximating the dynamics of the queueing process. We see that unlike the fluid and diffusion limits, the performance of the method is independent of the scaling of the queueing process since the method works just as well in Table 1 as it does for Table 5.

| $N$ | Mean | Variance | Skewness | Kurtosis |
|---|---|---|---|---|
| 1 | $2.53\cdot10^{-3}$ | $2.71\cdot10^{-1}$ | $6.04\cdot10^{-1}$ | $4.67\cdot10^{-2}$ |
| 2 | $5.18\cdot10^{-4}$ | $1.60\cdot10^{-2}$ | $4.90\cdot10^{-1}$ | $1.03\cdot10^{-1}$ |
| 3 | $2.80\cdot10^{-4}$ | $3.10\cdot10^{-3}$ | $6.23\cdot10^{-2}$ | $8.92\cdot10^{-2}$ |
| 4 | $1.67\cdot10^{-4}$ | $2.44\cdot10^{-3}$ | $1.25\cdot10^{-2}$ | $6.57\cdot10^{-3}$ |
| 5 | $1.57\cdot10^{-4}$ | $2.04\cdot10^{-3}$ | $1.10\cdot10^{-2}$ | $3.43\cdot10^{-3}$ |
| 6 | $1.11\cdot10^{-4}$ | $1.72\cdot10^{-3}$ | $1.33\cdot10^{-2}$ | $2.33\cdot10^{-3}$ |
| 7 | $7.59\cdot10^{-5}$ | $1.24\cdot10^{-3}$ | $9.04\cdot10^{-3}$ | $1.37\cdot10^{-3}$ |

TABLE 1. Relative error in the first four moments for increasing order $N$. $\lambda(t)=100+20\sin(t)$, $\mu=1$, $\beta=0.5$, $c=100$. $\psi_\alpha=\lambda(t)$, $\psi_\delta=\mu\cdot(Q\wedge c)+\beta\cdot(Q-c)^+$.

**5.2. Quadratic Rate or SIS Epidemic Model** Here we provide some tables for the relative errors of the several orders of the approximation for the mean, variance, skewness, and kurtosis for a quadratic rate birth death model, which is also known as the SIS epidemic model in the mathematical biology literature. We see in Tables 6 - 10 that the spectral method performs quite well at approximating the dynamics of the quadratic rate birth-death process. Like in the queueing model before, the performance of the method is independent of the scaling of the queueing process since the method works just as well in Table 6 as it does for Table 10. Thus, we have confidence that the spectral method is approximating the nonstationary and state dependent dynamics of the stochastic model quite well.

| $N$ | Mean | Variance | Skewness | Kurtosis |
|---|---|---|---|---|
| 1 | $1.05 \cdot 10^{-6}$ | $1.05 \cdot 10^{-6}$ | $5.23 \cdot 10^{-7}$ | $3.91 \cdot 10^{-9}$ |
| 2 | $1.05 \cdot 10^{-7}$ | $8.41 \cdot 10^{-8}$ | $8.31 \cdot 10^{-8}$ | $8.01 \cdot 10^{-10}$ |
| 3 | $1.05 \cdot 10^{-8}$ | $8.49 \cdot 10^{-9}$ | $7.30 \cdot 10^{-9}$ | $5.39 \cdot 10^{-11}$ |
| 4 | $1.14 \cdot 10^{-9}$ | $9.28 \cdot 10^{-10}$ | $7.90 \cdot 10^{-10}$ | $2.99 \cdot 10^{-9}$ |
| 5 | $2.48 \cdot 10^{-10}$ | $2.24 \cdot 10^{-10}$ | $1.35 \cdot 10^{-10}$ | $1.74 \cdot 10^{-11}$ |
| 6 | $1.51 \cdot 10^{-10}$ | $1.53 \cdot 10^{-10}$ | $7.30 \cdot 10^{-11}$ | $8.44 \cdot 10^{-13}$ |
| 7 | $3.06 \cdot 10^{-10}$ | $3.07 \cdot 10^{-10}$ | $1.52 \cdot 10^{-10}$ | $1.03 \cdot 10^{-12}$ |

Table 2. Relative error in the first four moments for increasing order $N$. $\lambda(t) = 100 + 20\sin(t)$, $\mu = 1$, $\beta = 1.0$, $c = 100$. $\psi_\alpha = \lambda(t)$, $\psi_\delta = \mu \cdot (Q \wedge c) + \beta \cdot (Q - c)^+$.

| $N$ | Mean | Variance | Skewness | Kurtosis |
|---|---|---|---|---|
| 1 | $3.05 \cdot 10^{-3}$ | $3.31 \cdot 10^{-1}$ | $9.27 \cdot 10^{0}$ | $4.24 \cdot 10^{-2}$ |
| 2 | $1.06 \cdot 10^{-3}$ | $3.14 \cdot 10^{-2}$ | $7.29 \cdot 10^{0}$ | $2.49 \cdot 10^{-1}$ |
| 3 | $6.60 \cdot 10^{-4}$ | $1.05 \cdot 10^{-2}$ | $2.33 \cdot 10^{0}$ | $1.90 \cdot 10^{-1}$ |
| 4 | $6.12 \cdot 10^{-4}$ | $1.29 \cdot 10^{-2}$ | $1.51 \cdot 10^{0}$ | $2.16 \cdot 10^{-2}$ |
| 5 | $3.51 \cdot 10^{-4}$ | $7.42 \cdot 10^{-3}$ | $9.65 \cdot 10^{-1}$ | $8.70 \cdot 10^{-3}$ |
| 6 | $3.13 \cdot 10^{-4}$ | $6.68 \cdot 10^{-3}$ | $8.87 \cdot 10^{-1}$ | $8.64 \cdot 10^{-3}$ |
| 7 | $3.95 \cdot 10^{-4}$ | $7.86 \cdot 10^{-3}$ | $3.78 \cdot 10^{-1}$ | $9.01 \cdot 10^{-3}$ |

Table 3. Relative error in the first four moments for increasing order $N$. $\lambda(t) = 100 + 20\sin(t)$, $\mu = 1$, $\beta = 2.0$, $c = 100$. $\psi_\alpha = \lambda(t)$, $\psi_\delta = \mu \cdot (Q \wedge c) + \beta \cdot (Q - c)^+$.

| $N$ | Mean | Variance | Skewness | Kurtosis |
|---|---|---|---|---|
| 1 | $7.92 \cdot 10^{-3}$ | $2.75 \cdot 10^{-1}$ | $5.07 \cdot 10^{-1}$ | $4.55 \cdot 10^{-2}$ |
| 2 | $1.24 \cdot 10^{-3}$ | $1.03 \cdot 10^{-2}$ | $3.61 \cdot 10^{-1}$ | $1.00 \cdot 10^{-1}$ |
| 3 | $1.05 \cdot 10^{-3}$ | $6.84 \cdot 10^{-3}$ | $3.90 \cdot 10^{-2}$ | $6.27 \cdot 10^{-2}$ |
| 4 | $9.38 \cdot 10^{-4}$ | $4.89 \cdot 10^{-3}$ | $2.25 \cdot 10^{-2}$ | $8.18 \cdot 10^{-3}$ |
| 5 | $8.99 \cdot 10^{-4}$ | $3.16 \cdot 10^{-3}$ | $1.68 \cdot 10^{-2}$ | $4.85 \cdot 10^{-3}$ |
| 6 | $5.82 \cdot 10^{-4}$ | $2.92 \cdot 10^{-3}$ | $1.41 \cdot 10^{-2}$ | $3.95 \cdot 10^{-3}$ |
| 7 | $3.52 \cdot 10^{-4}$ | $1.71 \cdot 10^{-3}$ | $8.04 \cdot 10^{-3}$ | $2.10 \cdot 10^{-3}$ |

Table 4. Relative error in the first four moments for increasing order $N$. $\lambda(t) = 25 + 5\sin(t)$, $\mu = 1$, $\beta = 0.5$, $c = 25$. $\psi_\alpha = \lambda(t)$, $\psi_\delta = \mu \cdot (Q \wedge c) + \beta \cdot (Q - c)^+$.

| $N$ | Mean | Variance | Skewness | Kurtosis |
|---|---|---|---|---|
| 1 | $1.34 \cdot 10^{-2}$ | $2.67 \cdot 10^{-1}$ | $3.94 \cdot 10^{-1}$ | $4.93 \cdot 10^{-2}$ |
| 2 | $2.24 \cdot 10^{-3}$ | $6.11 \cdot 10^{-3}$ | $2.17 \cdot 10^{-1}$ | $8.67 \cdot 10^{-2}$ |
| 3 | $2.50 \cdot 10^{-3}$ | $4.10 \cdot 10^{-3}$ | $3.91 \cdot 10^{-2}$ | $4.26 \cdot 10^{-2}$ |
| 4 | $2.23 \cdot 10^{-3}$ | $5.74 \cdot 10^{-3}$ | $2.08 \cdot 10^{-2}$ | $5.27 \cdot 10^{-3}$ |
| 5 | $1.22 \cdot 10^{-3}$ | $2.15 \cdot 10^{-3}$ | $1.32 \cdot 10^{-2}$ | $2.76 \cdot 10^{-3}$ |
| 6 | $1.15 \cdot 10^{-3}$ | $2.30 \cdot 10^{-3}$ | $1.31 \cdot 10^{-2}$ | $3.25 \cdot 10^{-3}$ |
| 7 | $1.10 \cdot 10^{-3}$ | $3.63 \cdot 10^{-3}$ | $9.57 \cdot 10^{-3}$ | $3.61 \cdot 10^{-3}$ |

Table 5. Relative error in the first four moments for increasing order $N$. $\lambda(t) = 10 + 2\sin(t)$, $\mu = 1$, $\beta = 0.5$, $c = 10$. $\psi_\alpha = \lambda(t)$, $\psi_\delta = \mu \cdot (Q \wedge c) + \beta \cdot (Q - c)^+$.

**6. Conclusion and Final Remarks** In this paper, we have demonstrated that we can approximate a variety of Markovian birth death processes with nonstationary and state dependent rates. We have used a spectral approach that expands the transition probabilities with the Poisson-Charlier polynomials, which are orthgonal to the Poisson distribution. We have also proven

| $N$ | Mean | Variance | Skewness | Kurtosis |
|---|---|---|---|---|
| 1 | $1.85 \cdot 10^{-2}$ | $2.80 \cdot 10^{0}$ | $1.51 \cdot 10^{0}$ | $2.56 \cdot 10^{-2}$ |
| 2 | $5.57 \cdot 10^{-4}$ | $8.75 \cdot 10^{-2}$ | $2.84 \cdot 10^{0}$ | $6.97 \cdot 10^{0}$ |
| 3 | $1.01 \cdot 10^{-3}$ | $1.56 \cdot 10^{-1}$ | $7.69 \cdot 10^{0}$ | $1.16 \cdot 10^{1}$ |
| 4 | $1.11 \cdot 10^{-4}$ | $1.74 \cdot 10^{-2}$ | $6.72 \cdot 10^{-1}$ | $9.34 \cdot 10^{-1}$ |
| 5 | $8.66 \cdot 10^{-5}$ | $1.34 \cdot 10^{-2}$ | $4.88 \cdot 10^{-1}$ | $6.56 \cdot 10^{-1}$ |
| 6 | $2.13 \cdot 10^{-5}$ | $3.33 \cdot 10^{-3}$ | $1.24 \cdot 10^{-1}$ | $1.69 \cdot 10^{-1}$ |
| 7 | $9.04 \cdot 10^{-6}$ | $1.39 \cdot 10^{-3}$ | $5.20 \cdot 10^{-2}$ | $7.02 \cdot 10^{-2}$ |

Table 6. Relative error in the first four moments for increasing order $N$. $\lambda(t) = 0.1 + 0.02\sin(t)$, $\tilde{Q} = 50$, $\beta = 1$, $Q(0) = 20$, $\psi_\alpha = \lambda(t) \cdot Q(\tilde{Q} - Q)$, $\psi_\delta = \beta \cdot Q$.

| $N$ | Mean | Variance | Skewness | Kurtosis |
|---|---|---|---|---|
| 1 | $8.60 \cdot 10^{-3}$ | $3.61 \cdot 10^{-1}$ | $1.82 \cdot 10^{0}$ | $2.72 \cdot 10^{-2}$ |
| 2 | $1.24 \cdot 10^{-3}$ | $4.63 \cdot 10^{-2}$ | $1.15 \cdot 10^{0}$ | $3.02 \cdot 10^{-1}$ |
| 3 | $6.47 \cdot 10^{-4}$ | $2.60 \cdot 10^{-2}$ | $6.45 \cdot 10^{-1}$ | $3.38 \cdot 10^{-1}$ |
| 4 | $2.66 \cdot 10^{-5}$ | $1.16 \cdot 10^{-3}$ | $2.53 \cdot 10^{-2}$ | $1.21 \cdot 10^{-2}$ |
| 5 | $3.39 \cdot 10^{-5}$ | $1.57 \cdot 10^{-3}$ | $3.93 \cdot 10^{-2}$ | $2.06 \cdot 10^{-2}$ |
| 6 | $2.31 \cdot 10^{-5}$ | $9.80 \cdot 10^{-4}$ | $1.88 \cdot 10^{-2}$ | $9.96 \cdot 10^{-3}$ |
| 7 | $1.52 \cdot 10^{-5}$ | $6.54 \cdot 10^{-4}$ | $1.39 \cdot 10^{-2}$ | $7.58 \cdot 10^{-3}$ |

Table 7. Relative error in the first four moments for increasing order $N$. $\lambda(t) = 0.05 + 0.01\sin(t)$, $\tilde{Q} = 50$, $\beta = 1$, $Q(0) = 20$, $\psi_\alpha = \lambda(t) \cdot Q(\tilde{Q} - Q)$, $\psi_\delta = \beta \cdot Q$.

| $N$ | Mean | Variance | Skewness | Kurtosis |
|---|---|---|---|---|
| 1 | $3.08 \cdot 10^{-1}$ | $6.74 \cdot 10^{-1}$ | $9.25 \cdot 10^{0}$ | $3.87 \cdot 10^{-1}$ |
| 2 | $1.98 \cdot 10^{-1}$ | $3.49 \cdot 10^{-1}$ | $1.30 \cdot 10^{1}$ | $1.57 \cdot 10^{-1}$ |
| 3 | $1.96 \cdot 10^{-1}$ | $3.35 \cdot 10^{-1}$ | $9.19 \cdot 10^{0}$ | $1.43 \cdot 10^{-1}$ |
| 4 | $1.57 \cdot 10^{-1}$ | $2.54 \cdot 10^{-1}$ | $4.42 \cdot 10^{0}$ | $1.22 \cdot 10^{-1}$ |
| 5 | $1.44 \cdot 10^{-1}$ | $2.25 \cdot 10^{-1}$ | $3.79 \cdot 10^{0}$ | $1.17 \cdot 10^{-1}$ |
| 6 | $1.16 \cdot 10^{-1}$ | $1.74 \cdot 10^{-1}$ | $3.60 \cdot 10^{0}$ | $1.03 \cdot 10^{-1}$ |
| 7 | $9.51 \cdot 10^{-2}$ | $1.37 \cdot 10^{-1}$ | $3.26 \cdot 10^{0}$ | $8.55 \cdot 10^{-2}$ |

Table 8. Relative error in the first four moments for increasing order $N$. $\lambda(t) = 0.03 + 0.01\sin(t)$, $\tilde{Q} = 50$, $\beta = 1$, $Q(0) = 20$, $\psi_\alpha = \lambda(t) \cdot Q(\tilde{Q} - Q)$, $\psi_\delta = \beta \cdot Q$.

| $N$ | Mean | Variance | Skewness | Kurtosis |
|---|---|---|---|---|
| 1 | $9.79 \cdot 10^{-3}$ | $7.94 \cdot 10^{0}$ | $1.36 \cdot 10^{0}$ | $2.88 \cdot 10^{-2}$ |
| 2 | $1.81 \cdot 10^{-4}$ | $1.51 \cdot 10^{-1}$ | $1.04 \cdot 10^{1}$ | $5.07 \cdot 10^{1}$ |
| 3 | $2.83 \cdot 10^{-4}$ | $2.33 \cdot 10^{-1}$ | $3.49 \cdot 10^{1}$ | $1.55 \cdot 10^{2}$ |
| 4 | $1.82 \cdot 10^{-5}$ | $1.52 \cdot 10^{-2}$ | $1.38 \cdot 10^{0}$ | $4.93 \cdot 10^{0}$ |
| 5 | $1.30 \cdot 10^{-5}$ | $1.08 \cdot 10^{-2}$ | $9.35 \cdot 10^{-1}$ | $3.24 \cdot 10^{0}$ |
| 6 | $1.82 \cdot 10^{-6}$ | $1.52 \cdot 10^{-3}$ | $1.35 \cdot 10^{-1}$ | $4.74 \cdot 10^{-1}$ |
| 7 | $7.76 \cdot 10^{-7}$ | $6.41 \cdot 10^{-4}$ | $5.69 \cdot 10^{-2}$ | $1.99 \cdot 10^{-1}$ |

Table 9. Relative error in the first four moments for increasing order $N$. $\lambda(t) = 0.1 + 0.05\sin(t)$, $\tilde{Q} = 100$, $\beta = 1$, $Q(0) = 40$, $\psi_\alpha = \lambda(t) \cdot Q(\tilde{Q} - Q)$, $\psi_\delta = \beta \cdot Q$.

that as we add more terms to the truncated expansion, our approximations converge to the true stochastic process. We gave explicit error bounds on the convergence rate not only for the transition probabilities, but also for the moments of the birth-death process.

| $N$ | Mean | Variance | Skewness | Kurtosis |
|---|---|---|---|---|
| 1 | $9.86 \cdot 10^{-3}$ | $7.85 \cdot 10^{0}$ | $1.34 \cdot 10^{0}$ | $2.87 \cdot 10^{-2}$ |
| 2 | $1.86 \cdot 10^{-4}$ | $1.50 \cdot 10^{-1}$ | $1.06 \cdot 10^{1}$ | $4.62 \cdot 10^{1}$ |
| 3 | $2.86 \cdot 10^{-4}$ | $2.30 \cdot 10^{-1}$ | $3.07 \cdot 10^{1}$ | $1.08 \cdot 10^{2}$ |
| 4 | $1.87 \cdot 10^{-5}$ | $1.51 \cdot 10^{-2}$ | $1.36 \cdot 10^{0}$ | $4.13 \cdot 10^{0}$ |
| 5 | $1.32 \cdot 10^{-5}$ | $1.07 \cdot 10^{-2}$ | $9.22 \cdot 10^{-1}$ | $2.77 \cdot 10^{0}$ |
| 6 | $1.88 \cdot 10^{-6}$ | $1.51 \cdot 10^{-3}$ | $1.33 \cdot 10^{-1}$ | $4.01 \cdot 10^{-1}$ |
| 7 | $7.88 \cdot 10^{-7}$ | $6.34 \cdot 10^{-4}$ | $5.59 \cdot 10^{-2}$ | $1.69 \cdot 10^{-1}$ |

TABLE 10. Relative error in the first four moments for increasing order $N$. $\lambda(t) = 0.1 + 0.02\sin(t)$, $\tilde{Q} = 100$, $\beta = 1$, $Q(0) = 40$, $\psi_\alpha = \lambda(t) \cdot Q(\tilde{Q} - Q)$, $\psi_\delta = \beta \cdot Q$.

There are many new problems that emerge from our work. One obvious, but non-trivial extension to our results that we intend to pursue is the multidimensional setting, where many individual birth-death processes interact with one another in a more complex network. This would involve the multi-dimensional analogue of the Poisson-Charlier polynomials. In the context of operations research and queueing theory problems, this extension would not only provide new approximations for Jackson networks, but also it would allow us to approximate some non-Markovian queueing networks that can be modeled with phase type distributions Pender and Ko [24], Ko and Pender [12, 11]. Moreover, if we were also able to prove error bounds for our approximations, it would give insight into how close some non-Markovian systems are to the Poisson reference distribution and what parameters affect this closeness.

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## References

[1] Anton Braverman, JG Dai, et al. Stein's method for steady-state diffusion approximations of M/Ph/n+M systems. *The Annals of Applied Probability*, 27(1):550–581, 2017.

[2] P. Brémaud. *Markov Chains: Gibbs Fields, Monte Carlo Simulation, and Queues.* Number 31 in Texts in Applied Mathematics. Springer, New York, 1999.

[3] Gordon M Clark. Use of Polya distributions in approximate solutions to nonstationary M/M/s queues. *Communications of the ACM*, 24(4):206–217, 1981.

[4] Jim Dai and Pengyi Shi. Stein's method for steady-state approximations: Error bounds and engineering solutions. 2016.

[5] Peter Deuflhard, Wilhelm Huisinga, T Jahnke, and Michael Wulkow. Adaptive discrete galerkin methods applied to the chemical master equation. *SIAM Journal on Scientific Computing*, 30(6):2990–3011, 2008.

[6] Stefan Engblom. On the stability of stochastic jump kinetics. *Applied Mathematics*, 5:3217–3239, 2014.

[7] S. Engblom. Spectral approximation of solutions to the chemical master equation. *J. Comput. Appl. Math.*, 229(1):208–221, 2009. doi:10.1016/j.cam.2008.10.029.

[8] S. Engblom. Galerkin spectral method applied to the chemical master equation. *Commun. Comput. Phys.*, 5(5):871–896, 2009.

[9] Itai Gurvich, Junfei Huang, and Avishai Mandelbaum. Excursion-based universal approximations for the erlang-a queue in steady-state. *Mathematics of Operations Research*, 39(2):325–373, 2013.

[10] Junfei Huang and Itai Gurvich. Beyond heavy-traffic regimes: Universal bounds and controls for the single-server queue. 2016.

[11] Young Myoung Ko and Jamol Pender. Strong approximations for time-varying infinite-server queues with non-renewal arrival and service processes. *Cornell University, Ithaca, NY*, 2016.

[12] Young Myoung Ko and Jamol Pender. Diffusion limits for the (mapt/pht/) n queueing network. *Operations Research Letters*, 45(3):248–253, 2017.

[13] R. Koekoek and R. F. Swarttouw. The Askey-scheme of hypergeometric orthogonal polynomials and its $q$-analogue. Technical Report 98-17, Delft University of Technology, Faculty of Information Technology and Systems, Department of Technical Mathematics and Informatics, 1998. Available at http://aw.twi.tudelft.nl/∼koekoek/askey.html.

[14] Isthrinayagy Krishnarajah, Alex Cook, Glenn Marion, and Gavin Gibson. Novel moment closure approximations in stochastic epidemics. *Bulletin of mathematical biology*, 67(4):855–873, 2005.

[15] Isthrinayagy Krishnarajah, Glenn Marion, and Gavin Gibson. Novel bivariate moment-closure approximations. *Mathematical biosciences*, 208(2):621–643, 2007.

[16] Avi Mandelbaum, William A Massey, and Martin I Reiman. Strong approximations for Markovian service networks. *Queueing Systems*, 30(1-2):149–201, 1998.

[17] W.A. Massey. Asymptotic Analysis of the Time Dependent M/M/1 Queue. *Mathematics of Operations Research*, 10(10):305–327, 1985.

[18] W.A. Massey and J. Pender. Skewness Variance Approximation for Dynamic Rate Multi-server Queues with Abandonment. *Performance Evaluation Review*, 39:74–74, 2011.

[19] W.A. Massey and J. Pender. Gaussian skewness approximation for dynamic rate multi-server queues with abandonment. *Queueing Systems*, 75(2):243–277, 2013.

[20] Sean P. Meyn and R. L. Tweedie. Stability of Markovian processes iii: Foster-Lyapunov criteria for continuous-time processes. *Adv. in Appl. Probab.*, 25(3):518–548, 1993.

[21] Hisanao Ogura. Orthogonal functionals of the Poisson process. *IEEE Transactions on Information Theory*, 18(4):473–481, 1972.

[22] Giovanni Peccati and Murad S Taqqu. *Wiener Chaos: Moments, Cumulants and Diagrams: A Survey with Computer Implementation*, volume 1. Springer, 2011.

[23] Jamol Pender. A Poisson-Charlier approximation for nonstationary queues. *Operations Research Letters*, 42(4):293–298, 2014.

[24] Jamol Pender and Young Myoung Ko. Approximations for the queue length distributions of time-varying many-server queues. *INFORMS Journal on Computing*, 29(4):688–704, 2017.

[25] Jamol Pender and William A Massey. Approximating and stabilizing dynamic rate jackson networks with abandonment. *Probability in the Engineering and Informational Sciences*, 31(1):1–42, 2017.

[26] J. Pender. Laguerre Polynomial Expansions for Time Varying Multiserver Queues with Abandonment. Available at http://www.columbia.edu/∼jp3404/LSA.html, 2014.

[27] Michael H Rothkopf and Shmuel S Oren. A Closure approximation for the Nonstationary M/M/s queue. *Management Science*, 25(6):522–534, 1979.

[28] Michael R Taaffe and Kim L Ong. Approximating Nonstationary Ph(t)/M(t)/s/c queueing systems. *Annals of Operations Research*, 8(1):103–116, 1987.

[29] M. Wulkow. Adaptive treatment of polyreactions in weighted sequence spaces. *IMPACT Comput. Sci. Eng.*, 4(2):153–193, 1992. doi:10.1016/0899-8248(92)90020-9.

[30] M. Wulkow. The simulation of molecular weight distributions in polyreaction kinetics by discrete Galerkin methods. *Macromol. Theory. Simul.*, 5(3):393–416, 1996. doi:10.1002/mats.1996.040050303.