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# AN ERROR ESTIMATION FOR MOMENT CLOSURE APPROXIMATION OF CHEMICAL REACTION SYSTEMS

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ABSTRACT. The moment closure method is an approximation method to compute the moments for stochastic models of chemical reaction systems. In this paper, we develop an analytic estimation of errors generated from the approximation of an infinite system of differential equations into a finite system truncated by the moment closure method. As an example, we apply the result to an essential bimolecular reaction system, the dimerization model.

## 1. INTRODUCTION

When a chemical reaction system has small number of molecular species, researchers often use the stochastic models to capture intrinsic fluctuations [1, 2, 3]. The governing equation for the stochastic model with $s$ species and $n$ reactions is described by the chemical master equation in the form of

$$\frac{\partial}{\partial t}p(\mathbf{x},t) = \sum_{k=1}^{n} [r_k(\mathbf{x}-V_k)p(\mathbf{x}-V_k,t) - r_k(\mathbf{x})p(\mathbf{x},t)], \tag{1.1}$$

where $p(\mathbf{x},t)$ is the probability that there are $\mathbf{x} = (x_1,\ldots,x_s)$ molecules in the given system at time $t$, each $r_k, i = 1,...,n$, is the propensity which is the probability of an occurrence of the $k$-th reaction per unit time, and $V_k$ is the $k$-th column vector of the stoichiometric matrix $V$ [4]. Moreover, one can write the equation (1.1) as a form of the linear system

$$\frac{d\mathbf{p}(t)}{dt} = A\mathbf{p}(t), \tag{1.2}$$

where $A$ is the matrix of transition probability rates between the states and **p** is the vector of probabilities of the states [5].

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Finding the exact solution of (1.1) or (1.2) is mostly difficult or impossible, since the stochastic models of most reaction systems have a large or infinite number of the states except for relatively simple systems [5]. Alternatively, Monte Carlo type algorithms such as Gillespie's stochastic simulation algorithm are used for finding the numerical solutions [3, 6]. However, if there are fast reactions or a certain number of molecules in the system, computations by the stochastic simulation algorithm are very inefficient and for this case, one has to rely on approximation methods to replace the SSA such as tau-leaping method, probability generating function method, reduction method on slow time scale, and moment closure approximation [7, 8, 9, 10, 11, 12, 13]. Especially, the moment closure approximation is used when the statistical quantities such as moments (e.g. mean and variance) are sought [14, 15, 16, 17]. A difficulty in using the moment closure approximation is that the system of the ordinary differential equations of all moments is infinite dimensional if there are one or more nonlinear reactions in a reaction system, which is very common in real chemical systems. In [13], a moment closure approximation by truncation of the infinite system into a finite system has been introduced and the authors proved a formal error estimation for numerical consistency. However, since the solution of the infinite dimensional system is mostly unknown, a rigorous analytic estimation of the error generated by the truncation has not been reported yet, to the best of the authors' knowledge.

In this paper, we present a rigorous analytic error estimation generated by an approximation of infinite dimensional system into a finite dimensional system and apply it to a fundamental and important nonlinear chemical system, the dimerization model.

The outline of the paper is as follows. In Section 2, we develop an analytic estimation of the error generated from an approximation of an infinite dimensional system into a finite dimensional system. In Section 3, we apply the result of the error estimation to the stochastic dimerization reaction system and illustrate numerical results. Throughout this paper, we consider stochastically modeled chemical reaction systems with bounded state space (e.g. closed reaction system), to guarantee that all moments are bounded.

## 2. Error Estimation

We first consider a certain class of infinite ordinary differential equations arising from moment equations of stochastic reaction systems including the dimerization as follows; let us first denote the quadratic functions

$$f_{kj}(x_1) = \alpha_{kj,1}(x_1)^2 + \alpha_{kj,2}x_1 + \alpha_{kj,3}$$

for $k = 1, 2, \cdots$ and $j = 1, \cdots, k$. We define the infinite dimensional system (**S**) (here $f_1 = f_{11}$ for convenience for notation) as

$$\begin{aligned}
\dot{x}_1 &= f_1(x_1) + \beta_1 x_2 \\
\dot{x}_2 &= f_{21}(x_1) + f_{22}(x_1)x_2 + \beta_2 x_3 \\
\cdots &\quad \cdots \\
\dot{x}_n &= f_{n1}(x_1) + f_{n2}(x_1)x_2 + f_{n3}(x_1)x_3 + \cdots + f_{nn}(x_1)x_n + \beta_n x_{n+1}
\end{aligned}$$

$$\cdots \quad \cdots,$$

where $\dot{x}$ denotes the derivative of $x$ with respect to $t$. Note that $x_1(t)$ and $x_k(t), k \geq 2$, will denote the mean $\mu(t)$ and the $k$-th central moment $E[(X(t)-\mu(t))^k]$ of $X(t)$, respectively, where $X(t)$ is the random variable that denotes the number of molecule of a species in a chemical reaction system at time $t$.

Moreover, we consider the truncated closed system ($\mathbf{S}_n$) obtained by dropping the term $\beta_n x_{n+1}$ from the system (**S**):

$$\begin{aligned}
&\dot{y}_1 = f_1(y_1) + \beta_1 y_2\\
&\dot{y}_2 = f_{21}(y_1) + f_{22}(y_1)y_2 + \beta_2 y_3\\
&\cdots \quad \cdots\\
&\dot{y}_n = f_{n1}(y_1) + f_{n2}(y_1)y_2 + f_{n3}(y_1)y_3 + \cdots + f_{nn}(y_1)y_n.
\end{aligned}$$

Since $x_k$ denotes the $k$-th moment in a bounded system, we can assume that there exist constants $A_1 \leq A_2 \leq A_3 \leq \cdots$ such that $|x_k(t)| \leq A_k$ and $A_k \geq 1$. For $j \leq k$, we denote

$$m_{kj} = \max_{|t| \leq A_1} |f_{kj}(t)|, \quad m_k = \max_{j \leq k} m_{kj}. \tag{2.1}$$

Let $L_{kj}$ denote the Lipschitz constant of $f_{kj}$ on $[-A_1, A_1]$, so that

$$|f_{kj}(t) - f_{kj}(s)| \leq L_{kj}|t-s|, \quad \forall t, s \in [-A_1, A_1],\ j \leq k. \tag{2.2}$$

Let us denote $L_k = \max_{j \leq k} L_{kj}$ and $a(n) = \max\limits_{1 \leq j \leq k \leq n} \max\limits_{\ell=1,2,3} \{|\alpha_{kj,\ell}|\}$. Then, as easy to check, one can choose $L_k$ and $m_k$ such that

$$L_k \leq 3a(k)A_1, \quad m_k \leq 3a(k)A_1^2. \tag{2.3}$$

Now we will use the following version of Gronwall's inequality.

**Lemma 1.** *Let $h(t)$ be a continuous real-valued function such that*

$$|h(t)| \leq M \int_0^t |h(s)|ds + C.$$

*Then*

$$|h(t)| \leq Ce^{Mt}.$$

Before we proceed further, we explain why one cannot apply Gronwall's inequality directly for $h(t) := |(x_1, \cdots, x_n) - (y_1, \cdots, y_n)|$: Typically for $h(t)$, unless $L_k$ and $m_k$ are very small, one has

$$h(t) \leq M_n \int_0^t h(s)ds + C_n$$

with some constants $C_n$ and $M_n$ with the property that $C_n, M_n \to \infty$ as $n \to \infty$. In this case, Lemma 1 only leads to

$$h(t) \leq C_n e^{M_n t} \to \infty \quad \text{as} \quad n \to \infty.$$

Thus, the approximation by the truncated system does not work well in general. To avoid this problem, we construct an alternative system for

$$\bar{x}_k(t) := \frac{x_k(t)}{g(k)},$$

where $\{g(k)|k = 1, 2, \cdots\}$ is an increasing sequence such that $g(1) = 1$: We first note that $\forall k, j$,

$$|\bar{x}_k| \le \frac{A_k}{g(k)}, \qquad \frac{x_k}{g(j)} = \frac{g(k)}{g(j)}\bar{x}_k.$$

Using this relation and dividing the equation for $x_k$ in system (**S**) by $g(k)$, one obtains the system ($\bar{\mathbf{S}}_n$) for $\bar{X}_n := (\bar{x}_1, \cdots, \bar{x}_n)$ :

$$\begin{aligned}
\dot{\bar{x}}_1 &= \frac{g(1)}{g(1)} f_1(\bar{x}_1) + \beta_1 \frac{g(2)}{g(1)} \bar{x}_2 \\
\dot{\bar{x}}_2 &= \frac{g(1)}{g(2)} f_{21}(\bar{x}_1) + \frac{g(2)}{g(2)} f_{22}(\bar{x}_1)\bar{x}_2 + \beta_2 \frac{g(3)}{g(2)} \bar{x}_3 \\
\cdots & \quad \cdots \\
\dot{\bar{x}}_n &= \frac{g(1)}{g(n)} f_{n1}(\bar{x}_1) + \frac{g(2)}{g(n)} f_{n2}(\bar{x}_1)\bar{x}_2 \cdots + \frac{g(n)}{g(n)} f_{nn}(\bar{x}_1)\bar{x}_n + \beta_n \frac{1}{g(n)} x_{n+1}.
\end{aligned}$$

Next we introduce a closed system which is basically almost same as the above system ($\bar{\mathbf{S}}_n$) except the last term $\beta^n x_{n+1}/g(n)$. Since we do not know a prior if the solution to closed system has a similar upper bound as $\bar{X}_n$ or not, we do some minor adjustments as follows: We define

$$h_k(t) = \begin{cases} \frac{A_k}{g(k)} & : t \ge \frac{A_k}{g(k)} \\ t & : t \in [-\frac{A_k}{g(k)}, \frac{A_k}{g(k)}] \\ -\frac{A_k}{g(k)} & : t \le -\frac{A_k}{g(k)}. \end{cases}$$

Then, obviously $\bar{x}_k = h_k(\bar{x}_k)$, and for all $t, s \in \mathbb{R}$ (not only for $t, s \in [-A_1, A_1]$),

$$|h_k(t)| \le \frac{A_k}{g(k)}, \quad |h_k(t) - h_k(s)| \le |t - s|, \quad |f_{kj}(h_1(t)) - f_{kj}(h_1(s))| \le L_k |t - s|, \quad (j \le k) \tag{2.4}$$

and

$$\frac{g(k)}{g(j)} h_k(t) \le \frac{g(k)}{g(j)} \frac{A_k}{g(k)} \le \frac{A_k}{g(j)}, \quad \forall k, j.$$

Replacing $\bar{x}_k$ by $h_k(\bar{x}_k)$ in the system ($\bar{\mathbf{S}}_n$), we consider the closed system ($\hat{\mathbf{S}}_n$):

$$\begin{aligned}
\dot{\bar{y}}_1 &= \frac{g(1)}{g(1)} f_1(h_1(\bar{y}_1)) + \beta_1 \frac{g(2)}{g(1)} h_2(\bar{y}_2) =: F_1(\bar{Y}_n), \\
\dot{\bar{y}}_k &= \frac{g(1)}{g(k)} f_{k1}(h_1(\bar{y}_1)) + \left( \sum_{j=2}^{k} \frac{g(j)}{g(k)} f_{kj}(h_1(\bar{y}_1)) h_j(\bar{y}_j) \right) + \beta_k \frac{g(k+1)}{g(k)} h_{k+1}(\bar{y}_{k+1})
\end{aligned}$$

$$=: F_k(\bar{Y}_n), \quad \text{for} \quad (2 \le k \le n-1),$$

$$\dot{\bar{y}}_n = \frac{g(1)}{g(n)} f_{n1}(h_1(\bar{y}_1)) + \sum_{j=2}^{n} \frac{g(j)}{g(n)} f_{nj}(h_1(\bar{y}_1)) h_j(\bar{y}_j) =: F_n(\bar{Y}_n).$$

By (2.1), (2.2), (2.4) and the inequality

$$|f(t)g(t) - f(s)g(s)| \le \sup_t |f| \cdot |g(t) - g(s)| + \sup_t |g| \cdot |f(t) - f(s)|,$$

we have

$$|F_1(t_1,t_2) - F_1(s_1,s_2)| \le L_1|t_1 - s_1| + \beta_1 g(2)|t_2 - s_2|,$$

and similarly for $2 \le k \le n-1$ and $\mathbf{T} = (t_1, \cdots, t_n)$ and $\mathbf{S} = (s_1, \cdots, s_n)$,

$$\begin{aligned} |F_k(\mathbf{T}) - F_k(\mathbf{S})| &\le \frac{g(1)}{g(k)} L_{k1}|t_1 - s_1| + \sum_{j=2}^{k} \left( \frac{g(j)}{g(k)} L_{kj} \frac{A_j}{g(j)} |t_1 - s_1| + \frac{g(j)}{g(k)} m_{kj} |t_j - s_j| \right) \\ &\quad + |\beta_k| \frac{g(k+1)}{g(k)} |t_{k+1} - s_{k+1}| \\ &\le \frac{1}{g(k)} \sum_{j=1}^{k} L_{kj} A_j |t_1 - s_1| + \frac{1}{g(k)} \sum_{j=2}^{k} m_{kj} g(j) |t_j - s_j| \\ &\quad + |\beta_k| \frac{g(k+1)}{g(k)} |t_{k+1} - s_{k+1}|. \end{aligned}$$

Moreover, for $k = n$, we have

$$|F_n(\mathbf{T}) - F_n(\mathbf{S})| \le \frac{1}{g(n)} \sum_{j=1}^{n} L_{nj} A_j |t_1 - s_1| + \frac{1}{g(n)} \sum_{j=2}^{n} m_{nj} g(j) |t_j - s_j|.$$

Thus, we have for $\mathbf{F}_n = (F_1, \cdots, F_n)$,

$$|\mathbf{F}_n(\mathbf{T}) - \mathbf{F}_n(\mathbf{S})| \le N_{n,1}|t_1 - s_1| + N_{n,2}|t_2 - s_2| + \cdots + N_{n,n}|t_n - s_n|,$$

where

$$N_{n,1} := \sum_{k=1}^{n} \frac{1}{g(k)} \sum_{j=1}^{k} L_{kj} A_j,$$

and for $2 \le k \le n$,

$$N_{n,k} := |\beta_{k-1}| \frac{g(k)}{g(k-1)} + g(k) \sum_{\ell=k}^{n} \frac{1}{g(\ell)} m_{\ell k}.$$

If we define

$$\mathbf{M}_n := \sup_{1 \le k \le n} N_{n,k}, \tag{2.5}$$

then it follows that

$$|F_n(\mathbf{T}) - F_n(\mathbf{S})| \le \mathbf{M}_n |\mathbf{T} - \mathbf{S}|, \quad \forall \mathbf{T}, \mathbf{S}.$$

Now let $\bar{Y}_n = (\bar{y}_1, \cdots, \bar{y}_n)$. Then, since $\bar{X}_n - \bar{Y}_n = 0$ when $t = 0$, we have for $Z_n = \bar{X}_n - \bar{Y}_n$,

$$\begin{aligned} |Z_n(t)| &= |\int_0^t \mathbf{F}_n(\bar{X}_n) - \mathbf{F}_n(\bar{Y}_n)ds + \int_0^t \beta_n x_{n+1}(s)(g(n))^{-1}ds| \\ &\leq \mathbf{M}_n \int_0^t |Z_n(s)|ds + |\beta_n| T \frac{A_{n+1}}{g(n)}. \end{aligned}$$

Thus by Gronwall's inequality,

$$|\bar{X}_n(t) - \bar{Y}_n(t)| \leq T|\beta_n| \frac{A_{n+1}}{g(n)} e^{\mathbf{M}_n t} =: \mathcal{E}_n(t), \qquad \forall\, t \leq T.$$

Up to now, we have proved the following result:

**Theorem 2.** *Let $(x_1, x_2, \cdots)$ be a solution to the infinite system (*$\mathbf{S}$*) and assume there exists an increasing sequence of constants $A_n, n = 1, 2, \dots$ such that $|x_n(t)| \leq A_n$. Also we let $\{g(n) : n \geq 1\}$ be an increasing sequence satisfying $g(1) = 1$ and let $\bar{Y}_n = (\bar{y}_1, \cdots, \bar{y}_n)$ be the solution of the closed system (*$\hat{\mathbf{S}}_n$*). Then for $\bar{X}_n = (x_1, x_2 g^{-1}(2), \cdots, x_n g^{-1}(n))$, we have*

$$|\bar{X}_n(t) - \bar{Y}_n(t)| \leq T|\beta_n| \frac{A_{n+1}}{g(n)} e^{\mathbf{M}_n t}, \quad \forall t \leq T, \tag{2.6}$$

*where $\mathbf{M}_n$ is the constant defined in (2.5).*

**Remark 3.** *If we assume there are constants $N, K_1, K_2 > 0$ such that*

$$A_k \leq N^k, a(n) \leq K_1 n, |\beta(n)| \leq K_2 n,$$

*then, taking $g(n) = e^{n-1}N^{n-1}$ and using (2.3) and (2.6), one can show*

$$\mathcal{E}_n(t) \leq C e^{-n[1 - t(3eNK_2 + 3eN^2K_1)]},$$

*where $C$ is a constant depending on $T$. Hence the approximation error goes exponentially fast as $n \to \infty$ if $t < (3eNK_2 + 3eN^2K_1)^{-1}$.*

## 3. Application: Dimerization

We consider the stochastic dimerization model

$$A_1 + A_2 \underset{k_2}{\overset{k_1}{\rightleftarrows}} A_3.$$

Let $X_i(t), i = 1, 2, 3$ denote the number of molecules of species $A_i$ at time $t$ and let $k_i, i = 1, 2$ denote the reaction probability constant. Using conservation relations $X_1(t) + X_3(t) = A$ and $X_2(t) + X_3(t) = B$ for some constant $A, B > 0$, one obtains the equations for $E[X_1(t)] := \mu(t)$ and $m^{th}$ central moment $M_m := E[(X_1 - \mu)^m]$ for $m \geq 2$,

$$\frac{d\mu}{dt} = (-1)\Big(k_1\mu(B - A + \mu) + k_1 M_2\Big) + k_2(A - \mu) \tag{3.1}$$

$$\begin{aligned}\frac{dM_m}{dt} &= k_1\mu(B-A+\mu)\Big(\sum_{k=0}^{m-1}\binom{m}{k}(-1)^{m-k}M_k\Big)\\ &+k_1(B-A+2\mu)\Big(\sum_{k=0}^{m-1}\binom{m}{k}(-1)^{m-k}M_{k+1}\Big)\\ &+k_1\Big(\sum_{k=0}^{m-1}\binom{m}{k}(-1)^{m-k}M_{k+2}\Big)+k_2(A-\mu)\Big(\sum_{k=0}^{m-1}\binom{m}{k}M_k\Big)\\ &-k_2\Big(\sum_{k=0}^{m-1}\binom{m}{k}M_{k+1}\Big)-m\mu' M_{m-1},\end{aligned}$$

where $M_0(t) = E[1] = 1$ and $M_1(t) = E[X_1 - \mu] = 0$ for all $t \geq 0$ [13].

Let us denote $\mu(t)$ and $M_k(t)$ by $x_1(t)$ and $x_k(t)$ for $k \geq 2$ in the system (3.1). Then one sees that the system (3.1) is of the form of the infinite system (**S**), and its truncated system by the moment closure is of the form of the system ($\mathbf{S}_n$) if the highest-order moment term $-k_1 m M_{m+1}$ is dropped off by the moment closure method [13]. Let us assume that $k_1 = 1, k_2 = 1$ and $A = 10, B = 5$. Then, for example, we can obtain the following ODE system for $x_k(t), 1 \leq k \leq 10$ from the 10-th order moment closure approximation of (3.1);

$$\begin{aligned}
\dot{x}_1 &= \Big(10+4x_1-(x_1)^2\Big)-x_2\\
\dot{x}_2 &= \Big(10-6x_1+(x_1)^2\Big)+\Big(9-4x_1\Big)x_2-2x_3\\
\dot{x}_3 &= \Big(10+4x_1-(x_1)^2\Big)+\Big(11+18x_1-3(x_1)^2\Big)x_2+\Big(15-6x_1\Big)x_3-3x_4\\
\dot{x}_4 &= \Big(10-6x_1+(x_1)^2\Big)+\Big(77-44x_1+6(x_1)^2\Big)x_2+\Big(28x_1-4(x_1)^2\Big)x_3\\
&\quad+\Big(22-8x_1\Big)x_4-4x_5\\
\dot{x}_5 &= \Big(10+4x_1-(x_1)^2\Big)+\Big(69+50x_1-10(x_1)^2\Big)x_2+\Big(145-80x_1+10(x_1)^2\Big)x_3\\
&\quad+\Big(20+40x_1-5(x_1)^2\Big)x_4+\Big(30-10x_1\Big)x_5-5x_6\\
\dot{x}_6 &= \Big(10-6x_1+(x_1)^2\Big)+\Big(175-102x_1+15(x_1)^2\Big)x_2+\Big(104+110x_1-20(x_1)^2\Big)x_3\\
&\quad+\Big(245-130x_1+15(x_1)^2\Big)x_4+\Big(-50+54x_1-6(x_1)^2\Big)x_5+\Big(39-12x_1\Big)x_6-6x_7\\
\dot{x}_7 &= \Big(10+4x_1-(x_1)^2\Big)+\Big(167+98x_1-21(x_1)^2\Big)x_2+\Big(441-252x_1+35(x_1)^2\Big)x_3\\
&\quad+\Big(119+210x_1-35(x_1)^2\Big)x_4+\Big(385-196x_1+21(x_1)^2\Big)x_5\\
&\quad+\Big(-91+70x_1-7(x_1)^2\Big)x_6+\Big(49-14x_1\Big)x_7-7x_8
\end{aligned}$$

$$
\begin{aligned}
\dot{x}_8 = &\Big(10 - 6x_1 + (x_1)^2\Big) + \Big(313 - 184x_1 + 28(x_1)^2\Big)x_2 + \Big(384 + 280x_1 - 56(x_1)^2\Big)x_3 \\
&+ \Big(952 - 532x_1 + 70(x_1)^2\Big)x_4 + \Big(84 + 364x_1 - 56(x_1)^2\Big)x_5 \\
&+ \Big(574 - 280x_1 + 28(x_1)^2\Big)x_6 + \Big(-144 + 88x_1 - 8(x_1)^2\Big)x_7 + \Big(60 - 16x_1\Big)x_8 - 8x_9 \\
\dot{x}_9 = &\Big(10 + 4x_1 - (x_1)^2\Big) + \Big(305 + 162x_1 - 36(x_1)^2\Big)x_2 + \Big(993 - 576x_1 + 84(x_1)^2\Big)x_3 \\
&+ \Big(720 + 672x_1 - 126(x_1)^2\Big)x_4 + \Big(1848 - 1008x_1 + 126(x_1)^2\Big)x_5 \\
&+ \Big(-42 + 588x_1 - 84(x_1)^2\Big)x_6 + \Big(822 - 384x_1 + 36(x_1)^2\Big)x_7 \\
&+ \Big(-210 + 108x_1 - 9(x_1)^2\Big)x_8 + \Big(72 - 18x_1\Big)x_9 - 9x_{10} \\
\dot{x}_{10} = &\Big(10 - 6x_1 + (x_1)^2\Big) + \Big(491 - 290x_1 + 45(x_1)^2\Big)x_2 + \Big(920 + 570x_1 - 120(x_1)^2\Big)x_3 \\
&+ \Big(2625 - 1500x_1 + 210(x_1)^2\Big)x_4 + \Big(1140 + 1428x_1 - 252(x_1)^2\Big)x_5 \\
&+ \Big(3318 - 1764x_1 + 210(x_1)^2\Big)x_6 + \Big(-312 + 900x_1 - 120(x_1)^2\Big)x_7 \\
&+ \Big(1140 - 510x_1 + 45(x_1)^2\Big)x_8 + \Big(-290 + 130x_1 - 10(x_1)^2\Big)x_9 \\
&+ \Big(85 - 20x_1\Big)x_{10} - 10x_{11}
\end{aligned}
$$

Since $X_1 \leq 10$, one can show that

$$|x_1| \leq 10 := A_1, |x_k| \leq 20^k =: A_k$$

for $k \geq 2$ by Minkowski inequality and $|\beta_k| = k$. If we take $g(k) = 20^{k-1}e^{k-1}$, then one can check $\mathbf{M}_n = 20e(n-1)$ for $n = 2, 3, \cdots, 10$. Now let $\bar{x}_k(t) := x_k(t)g^{-1}(k)$ and let $\bar{y}_k(t)$ ($k = 1, 2, \cdots, 10$) denote the solution of the closed system $\hat{\mathbf{S}}_n$. Then, by (2.6), for any $t < 1$ and $n = 2, 3, \cdots$, we obtain

$$|\bar{X}_n(t) - \bar{Y}_n(t)| \leq n20^2 e^{-(n-1)(1-20et)}.$$

Thus, $\mathcal{E}_n(t) = |\bar{X}_n(t) - \bar{Y}_n(t)|$ gets smaller as $n$ grows for any $t < 1/(20e) \approx 0.0184$.

Figure 1 illustrates the errors in $\log_{10}$ between approximate means and variances computed by Euler method in time interval $[0, 0.02]$. Here the errors are very small and so we use the errors in $\log_{10}$ to illustrate the error graphs clearly. Moreover, in Table 1, we compare $L^2$ error between approximate mean and variance in the time interval $[0, 0.02]$. In Figure 1 and Table 1, one can see that the errors become smaller and converge to zero as the order of approximation is increased, which is a consequence of Theorem 2.

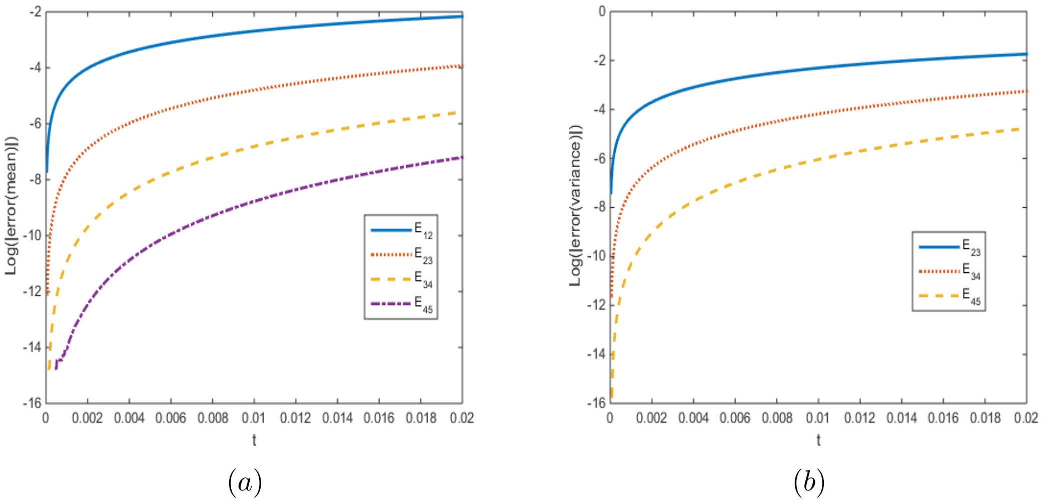


FIGURE 1. Comparison of errors in $\log_{10}$ between approximate solutions obtained by using Euler method with time step $h = 2 \times 10^{-5}$ in $[0, 0.02]$. (a) $E_{ij} = \log_{10}($ | mean by $i$-th order moment approximation - mean by $j$-th order moment approximation |). (b) $E_{ij} = \log_{10}($ | variance by $i$-th order moment approximation - variance by $j$-th order moment approximation |).

TABLE 1. $L_2$ errors in time interval $[0, 0.02]$. $LE_{ij} = L_2$ error between solutions of $i$-th order and $j$-th order moment approximation. The $L_2$ error between $x(t)$ and $y(t)$ is defined by $\sqrt{\sum_t (x(t) - y(t))^2}$

| $L_2$ Error | Mean | Variance |
|---|---|---|
| $LE_{12}$ | 0.1031 | N/A |
| $LE_{23}$ | 0.0014 | 0.2666 |
| $LE_{34}$ | 2.7301e-05 | 0.0066 |
| $LE_{45}$ | 5.8851e-07 | 1.7597e-04 |
| $LE_{56}$ | 0 | 0 |
| $LE_{67}$ | 0 | 0 |

## 4. CONCLUSION

In this paper, we presented the approximation of the solution of an infinite dimensional ODE system motivated from moment equations of stochastic reaction systems. We obtained a rigorous analytic estimation of the error between the solutions of the infinite system and the truncated finite system (Theorem 2). As an example, we applied it to the stochastic dimerization model and illustrated the numerical results.

This work is a first report for an analytic estimation of the error generated by the moment closure approximation, and the result presented in this paper has a limitation in that it can be applied to a certain class of the chemical reaction systems with the type of moment equations similar to the system (**S**). As a future work, we plan to extend the result to general stochastic chemical reaction systems with multi-dimensional variables.

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