

Approximate moment dynamics for polynomial and trigonometric stochastic systems

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Abstract—Stochastic dynamical systems often contain nonlinearities that make it hard to compute probability density functions or statistical moments of these systems. For the moment computations, nonlinearities lead to the well-known problem of unclosed moment dynamics, i.e., differential equations that govern the time evolution of moments up to a certain order may contain some moments of higher order. Moment closure techniques are used to find an approximate, closed system of equations for the moment dynamics, but their usage is rather limited for systems with continuous states particularly when the nonlinearities are non-polynomials. Here, we extend a moment closure technique based on derivative matching, which was originally proposed for polynomial stochastic systems with discrete states, to continuous state stochastic differential equations with both polynomial and trigonometric nonlinearities.

I. INTRODUCTION

Stochastic dynamical systems appear in numerous contexts in physics, engineering, finance, economics, and biology (see, e.g., [1]–[5]). In terms of mathematical characterization, the most useful quantity in analysis of stochastic systems is the probability density function (pdf). However, obtaining the pdf is analytically intractable for most systems. So, either numerical techniques, such as Monte Carlo simulation, are employed to compute the pdf [6], [7], or a less ambitious goal of computing only a few lower order moments (mean, variance, etc.) is pursued.

For stochastic systems defined over polynomials, the time evolution of its moments is given by a system of coupled ordinary differential equations (ODEs). However, a major drawback is that the ODEs for moments up to a given order may consist of terms involving higher-order moments. This is known as the problem of *moment closure*, and a typical approach to overcome it is to truncate the system of ODEs to a finite system of equations and *close* the moment equations using some sort of approximation for a given moment in terms of moments of lower order [8]–[13]. If the system under consideration involves nonlinearities such as trigonometric functions, then the differential equations describing the moments involve moments of nonlinear functions of the state. In such cases, usage of moment closure schemes is rather limited.

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Numerous moment closure techniques have been proposed for systems with polynomial dynamics. Some of these techniques make prior assumptions on the distribution of the system, while others attempt to find a linear or nonlinear approximation of the moment dynamics [14], [15]. One method that falls in the latter category is the derivative matching based closure [9]. Here, a nonlinear approximation of a given moment is obtained in terms of lower order moments by matching the derivatives of the original moment dynamics with the proposed approximate dynamics at some initial time. This method has been widely used in approximating moment dynamics of biochemical reaction systems that are described via discrete states [9]. Given the attention received by this approach and its better performance as compared to several other moment closure schemes [11], [16], we apply it to close moments for nonlinear stochastic systems described via stochastic differential equations (SDEs). We further extend the method to include trigonometric functions in the dynamics. Our results show that the derivative matching technique provides reasonably good approximation to the moment dynamics.

Remainder of the paper is organized as follows. In section II, we describe the moment dynamics for a stochastic system described via SDEs, and motivate the moment closure problem. In section III, we discuss the derivative matching moment closure technique for SDEs. We illustrate the technique via examples in section IV. The paper is concluded in section V, along with a few directions for future research.

Notation: Vectors and matrices are denoted in bold. The set of real numbers and non-negative integers are respectively denoted by \mathbb{R} and $\mathbb{Z}_{\geq 0}$. The expectation is represented by angled-brackets, $\langle \cdot \rangle$.

II. MOMENT DYNAMICS OF A STOCHASTIC SYSTEM

Consider a stochastic system described via the stochastic differential equation (SDE)

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t) dt + \mathbf{g}(\mathbf{x}, t) d\mathbf{w}_t, \quad (1)$$

where $\mathbf{x} = [x_1 \dots x_n]^\top \in \mathbb{R}^n$ is the state vector; $\mathbf{f}(\mathbf{x}, t) = [f_1(\mathbf{x}, t) \dots f_n(\mathbf{x}, t)]^\top : \mathbb{R}^n \times [0, \infty) \rightarrow \mathbb{R}^n$ and $\mathbf{g}(\mathbf{x}, t) = [g_1(\mathbf{x}, t) \dots g_n(\mathbf{x}, t)]^\top : \mathbb{R}^n \times [0, \infty) \rightarrow \mathbb{R}^n$ describe the system dynamics; and \mathbf{w}_t is the Wiener process satisfying

$$\langle d\mathbf{w}_t \rangle = \mathbf{0}, \quad \langle d\mathbf{w}_t d\mathbf{w}_t^\top \rangle = \mathbf{I} dt, \quad (2)$$

where \mathbf{I} is an $n \times n$ Identity matrix. We further assume that sufficient mathematical requirements for the existence of the solution to (1) are satisfied (see, e.g., [5]).

The moments of an SDE can be obtained using the well-known Itô formula [5]. This formula states that for any smooth scalar-valued function $h(\mathbf{x}(t))$

$$\frac{d}{dt} \langle h(\mathbf{x}(t)) \rangle = \left\langle \frac{\partial h(\mathbf{x}(t))}{\partial x} f(\mathbf{x}(t)) + \frac{1}{2} \text{Tr} \left(\frac{\partial^2 h(\mathbf{x}(t))}{\partial x^2} g(\mathbf{x}(t)) g(\mathbf{x}(t))^\top \right) \right\rangle, \quad (3)$$

where $\frac{\partial h(\mathbf{x}(t))}{\partial x}$ and $\frac{\partial^2 h(\mathbf{x}(t))}{\partial x^2}$ respectively denote the gradient and the Hessian of $h(\mathbf{x}(t))$ with respect to \mathbf{x} .

Let $h(\mathbf{x})$ be a monomial of the form

$$h(\mathbf{x}) = x_1^{m_1} x_2^{m_2} \dots x_n^{m_n} =: \mathbf{x}^{[\mathbf{m}]}, \quad (4)$$

where $\mathbf{m} = [m_1 \dots m_n]^\top \in \mathbb{Z}_{\geq 0}^n$, then $\langle h(\mathbf{x}) \rangle$ represents a moment of \mathbf{x} . For a given \mathbf{m} , we represent the moment by $\mu_{\mathbf{m}} = \langle \mathbf{x}^{[\mathbf{m}]} \rangle$. Using (3), dynamics of $\mu_{\mathbf{m}}$ evolves as per

$$\frac{d\mu_{\mathbf{m}}}{dt} = \sum_{i=1}^n \left\langle f_i \frac{\partial \mathbf{x}^{[\mathbf{m}]}}{\partial x_i} \right\rangle + \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \left\langle (g g^\top)_{ij} \frac{\partial^2 \mathbf{x}^{[\mathbf{m}]}}{\partial x_i \partial x_j} \right\rangle. \quad (5)$$

The sum $\sum_{j=1}^n m_j$ is referred to as the order of the moment.

As long as $\mathbf{f}(\mathbf{x}, t)$ and $\mathbf{g}(\mathbf{x}, t)$ are linear in \mathbf{x} , a moment of a certain order is a linear combination of other moments of the same or smaller order [15]. Hence, if we construct a vector $\boldsymbol{\mu}$ consisting of all moments up to the M^{th} order moments of \mathbf{x} , its time evolution is captured by the solution of the following system of linear differential equations:

$$\frac{d\boldsymbol{\mu}}{dt} = \mathbf{a} + \mathbf{A}\boldsymbol{\mu}. \quad (6)$$

Here, $\boldsymbol{\mu} = [\mu_{\mathbf{m}_1} \ \mu_{\mathbf{m}_2} \ \dots \ \mu_{\mathbf{m}_k}]^\top$, $\mathbf{m}_p \in \mathbb{Z}_{\geq 0}^n, \forall p \in \{1, 2, \dots, k\}$ is assumed to be a vector of k elements. The vector \mathbf{a} and the matrix \mathbf{A} are determined by the form of $\mathbf{f}(\mathbf{x}, t)$ and $\mathbf{g}(\mathbf{x}, t)$. Under some mild assumptions, standard tools from linear systems theory can be used to obtain solution to (6), and it is given by

$$\boldsymbol{\mu}(t) = -\mathbf{A}^{-1} \mathbf{a} + e^{\mathbf{A}t} (\boldsymbol{\mu}(0) + \mathbf{A}^{-1} \mathbf{a}). \quad (7)$$

Remark 1: It is easy to see that there are $(m+n-1)/(m!(n-1)!)$ moments of order m . Therefore, the dimension of the vector $\boldsymbol{\mu}$ in (6) is given by

$$k = \sum_{m=1}^M \frac{(m+n-1)!}{m!(n-1)!} = \frac{(M+n)!}{M!n!} - 1. \quad (8)$$

Without loss of generality, we can assume that the elements in $\boldsymbol{\mu}$ are stacked up in graded lexicographical order. That is, the first n elements in $\boldsymbol{\mu}$ are the moments of first order, next $n(n+1)/2$ elements are moments of the second order, and so on.

In general, when $\mathbf{f}(\mathbf{x}, t)$ and $\mathbf{g}(\mathbf{x}, t)$ are polynomials in \mathbf{x} , the time derivative of a moment might depend on moments

of order higher than it. The moment equations in (6) can be accordingly modified to a general form

$$\frac{d\boldsymbol{\mu}}{dt} = \mathbf{a} + \mathbf{A}\boldsymbol{\mu} + \mathbf{B}\bar{\boldsymbol{\mu}}, \quad (9)$$

where $\bar{\boldsymbol{\mu}} \in \mathbb{R}^r$ is a vector of moments of order greater than or equal to $M+1$.

The solution to (9) is generally obtained by approximating the higher order moments in $\bar{\boldsymbol{\mu}}$ as, possibly nonlinear, functions of lower order moments in $\boldsymbol{\mu}$. The approximation might be made by assuming some underlying distribution, or by applying some other physical principle [14], [15]. Essentially moment closure methods translate to finding an approximation of (9) by a system of equations

$$\frac{d\boldsymbol{\nu}}{dt} = \mathbf{a} + \mathbf{A}\boldsymbol{\nu} + \mathbf{B}\bar{\boldsymbol{\varphi}}(\boldsymbol{\nu}), \quad (10a)$$

$$\boldsymbol{\nu} = [\nu_{\mathbf{m}_1} \ \nu_{\mathbf{m}_2} \ \dots \ \nu_{\mathbf{m}_k}]^\top, \quad (10b)$$

where the function $\bar{\boldsymbol{\varphi}}: \mathbb{R}^k \rightarrow \mathbb{R}^r$ is chosen such that $\boldsymbol{\mu}(t) \approx \boldsymbol{\nu}(t)$. Here, M is called the order of truncation.

If the functions $\mathbf{f}(\mathbf{x}, t)$ are not polynomials, then it may not be possible to obtain a convenient form like (9) for the moments. In Section IV, we will consider a system with trigonometric nonlinearities and perform moment closure for it. In the next section, we first discuss the derivative matching closure scheme for SDEs.

III. DERIVATIVE MATCHING MOMENT CLOSURE TECHNIQUE FOR SDES

In this section, we describe the derivative matching based moment closure technique for SDEs. As the name suggests, the closure is performed by matching time derivatives of $\boldsymbol{\mu}(t)$ and $\boldsymbol{\nu}(t)$. This technique has been widely applied to discrete-state continuous-time systems [9], [17]. The derivative matching technique attempts to approximate $\boldsymbol{\mu}(t)$ by some $\boldsymbol{\nu}(t)$ such that a sufficiently large number of their derivatives match point-wise. The idea being that if the values of these two vectors at some time t_0 are equal, and their derivatives up to certain order also match, then they would closely follow each other for some time interval after t_0 . More precisely, for each $\delta > 0$ and $N \in \mathbb{Z}_{\geq 0}$, $\exists T \in \mathbb{R}$ such that if

$$\boldsymbol{\mu}(t_0) = \boldsymbol{\nu}(t_0) \implies \left. \frac{d^i \boldsymbol{\mu}(t)}{dt^i} \right|_{t=t_0} = \left. \frac{d^i \boldsymbol{\nu}(t)}{dt^i} \right|_{t=t_0}, \quad (11)$$

hold for some $t_0 \in [0, \infty)$ and $i = 1, 2, \dots, N$, then

$$\|\boldsymbol{\mu}(t) - \boldsymbol{\nu}(t)\| \leq \delta, \quad \forall t \in [t_0, T]. \quad (12)$$

Further, one can obtain the bound in (12) for the interval $[t_0, \infty)$ under appropriate asymptotic conditions [18].

To construct the closed moment dynamics, we follow similar steps as [9]. Consider a vector $\bar{\mathbf{m}} \in \mathbb{Z}_{\geq 0}^n$ such that $\mu_{\bar{\mathbf{m}}}$ is an element in $\bar{\boldsymbol{\mu}}$. We approximate $\mu_{\bar{\mathbf{m}}}$ as a function of elements in the vector $\boldsymbol{\mu}$. Denoting the corresponding

approximation of $\mu_{\bar{m}}$ in $\bar{\varphi}(\mu)$ by $\phi_{\bar{m}}(\mu)$, the following separable form is considered

$$\phi_{\bar{m}}(\mu) = \prod_{p=1}^k (\mu_{m_p})^{\alpha_p}, \quad (13)$$

where α_p are appropriately chosen constants. Generally speaking, (11) is a strong requirement and it is not possible to find the coefficients α_p such that it holds for every initial condition. We, therefore, consider a relaxation of this by seeking α_p such that the derivatives match for a deterministic initial condition $x(t_0) = x_0$.

Next, we state a theorem showing that the coefficients α_p can be obtained by solving a system of linear equations. Before that, we define a short-hand notation that is used in the theorem. For two vectors $\hat{m} = [\hat{m}_1 \ \hat{m}_2 \ \dots \ \hat{m}_n]^\top \in \mathbb{Z}_{\geq 0}^n$ and $\check{m} = [\check{m}_1 \ \check{m}_2 \ \dots \ \check{m}_n]^\top \in \mathbb{Z}_{\geq 0}^n$, we have the following notation

$$C_{\hat{m}}^{\check{m}} := C_{\hat{m}_1}^{\check{m}_1} C_{\hat{m}_2}^{\check{m}_2} \dots C_{\hat{m}_n}^{\check{m}_n}, \quad (14a)$$

where

$$C_l^h = \begin{cases} \frac{h!}{l!(h-l)!}, & h \geq l, \\ 0, & h < l. \end{cases} \quad (14b)$$

Theorem 1: For each element $\mu_{\bar{m}}$ of the vector $\bar{\mu}$, assume that the corresponding moment closure function $\phi_{\bar{m}}(\mu)$ in the vector $\bar{\varphi}(\mu)$ is chosen according to equation (13) with the coefficients α_p chosen as the unique solution to the following system of linear equations

$$C_{[\bar{m}_s]}^{[\bar{m}]} = \sum_{p=1}^k \alpha_p C_{[m_s]}^{[m_p]}, \quad s = 1, 2, \dots, k. \quad (15)$$

Then, for every initial condition $x(t_0) = x_0 \in \mathbb{R}^n$, we have that

$$\mu(t_0) = \nu(t_0) \implies \left. \frac{d\mu(t)}{dt} \right|_{t=t_0} = \left. \frac{d\nu(t)}{dt} \right|_{t=t_0} \quad (16a)$$

$$\implies \left. \frac{d^2\mu(t)}{dt^2} \right|_{t=t_0} = \left. \frac{d^2\nu(t)}{dt^2} \right|_{t=t_0}. \quad (16b)$$

Proof: It is sufficient to prove that for each element $\mu_{\bar{m}}$ of $\bar{\mu}$ and its corresponding moment closure function $\phi_{\bar{m}}(\mu)$, we have the following:

$$\mu_{\bar{m}}(t_0) = \phi_{\bar{m}}(\mu(t_0)), \quad (17a)$$

$$\left. \frac{d\mu_{\bar{m}}(t)}{dt} \right|_{t=t_0} = \left. \frac{d\phi_{\bar{m}}(\mu(t))}{dt} \right|_{t=t_0}. \quad (17b)$$

We first show that equation (17a) holds. Since initial conditions are $x(t_0) = x_0$ with probability one, we have

$$\mu_{\bar{m}}(t_0) = x_0^{[\bar{m}]}, \quad (18a)$$

$$\phi_{\bar{m}}(\mu(t_0)) = \prod_{p=1}^k (x_0^{[m_p]})^{\alpha_p} = x_0^{[\sum_{p=1}^k \alpha_p m_p]}. \quad (18b)$$

Recall Remark 1, that without loss of generality, the moments in vector μ can be assumed to be stacked in graded

lexicographical order. Thus, the first n elements of μ are moments of order one. This allows us to write

$$\bar{m} = [C_{m_1}^{\bar{m}}, C_{m_2}^{\bar{m}}, \dots, C_{m_n}^{\bar{m}}]^\top, \quad (19a)$$

$$m_p = [C_{m_1}^{m_p}, C_{m_2}^{m_p}, \dots, C_{m_n}^{m_p}]^\top, \forall p = 1, 2, \dots, k, \quad (19b)$$

where a vector $m_i \in \mathbb{Z}_{\geq 0}^n, i = 1, 2, \dots, n$ has 1 at the i^{th} position, and rest of the elements are zero. Using these relations, and (14a) for $s = 1, 2, \dots, n$, we obtain

$$\bar{m} = \sum_{p=1}^k \alpha_p m_p. \quad (20)$$

Substituting this result in (18a) proves equation (17a).

Next, we prove that (17b) holds. For this part, we assume that $x_0 = [x_{01}, x_{02}, \dots, x_{0n}]^\top \in \mathbb{R}^n$. Consider

$$\left. \frac{d\phi_{\bar{m}}(\mu(t))}{dt} \right|_{t=t_0} \quad (21a)$$

$$= \phi_{\bar{m}}(\mu(t_0)) \sum_{p=1}^k \alpha_p \frac{\left. \frac{d\mu_{m_p}(t)}{dt} \right|_{t=t_0}}{\mu_{m_p}(t_0)} \quad (21b)$$

$$= \sum_{p=1}^k \alpha_p x_0^{[\bar{m}-m_p]} \left. \frac{d\mu_{m_p}(t)}{dt} \right|_{t=t_0}. \quad (21c)$$

Assuming $m_p = [m_{p1} \ m_{p2} \ \dots \ m_{pn}]^\top \in \mathbb{Z}_{\geq 0}^n$, we can use equation (5) to obtain the expression for $\frac{d\mu_{m_p}(t)}{dt} = \frac{d\langle x^{[m_p]} \rangle}{dt}$. This enables us to write

$$\left. \frac{d\phi_{\bar{m}}(\mu(t))}{dt} \right|_{t=t_0} \quad (22a)$$

$$\begin{aligned} &= x_0^{[\bar{m}]} \sum_{i=1}^n \frac{\sum_{p=1}^k \alpha_p m_{pi}}{x_{0i}} f_i(x_0, t_0) + \\ &\frac{1}{2} x_0^{[\bar{m}]} \sum_{i=1}^n \frac{\sum_{p=1}^k \alpha_p m_{pi}(m_{pi} - 1)}{x_{0i}^2} (g(x_0, t_0) g^\top(x_0, t_0))_{ii} + \\ &\frac{1}{2} x_0^{[\bar{m}]} \sum_{\substack{i,j=1 \\ i \neq j}}^n \frac{\sum_{p=1}^k \alpha_p m_{pi} m_{pj}}{x_{0i} x_{0j}} (g(x_0, t_0) g^\top(x_0, t_0))_{ij}. \end{aligned} \quad (22b)$$

Comparing this with the expression for $\frac{d\mu_{\bar{m}}}{dt}$ computed at $t = t_0$, which can be calculated from (5) and assuming $\bar{m} = [\bar{m}_1, \bar{m}_2, \dots, \bar{m}_n]^\top \in \mathbb{Z}_{\geq 0}^n$, we require:

$$\sum_{p=1}^k \alpha_p m_{pi} = \bar{m}_i, \quad (23a)$$

$$\sum_{p=1}^k \alpha_p \frac{m_{pi}(m_{pi} - 1)}{2} = \frac{\bar{m}_i(\bar{m}_i - 1)}{2}, \quad (23b)$$

$$\sum_{p=1}^k \alpha_p \frac{m_{pi} m_{pj}}{2} = \frac{\bar{m}_i \bar{m}_j}{2}. \quad (23c)$$

Note that (23a) is nothing but the relation in (20) written element-wise. Further, we had assumed that the vector μ has its elements stacked up in graded lexicographical order (Remark 1). In particular, the moments of second order start with the $(n+1)^{th}$ element. In that case, the equality in (23b) follows when relations in (19a)–(19b) are used in (14a) for $s = n+1, 2n+1, \dots, n^2+1$ (i.e., the second order moments with one of the exponents as 2 and rest of them as zeros). Likewise, (23c) holds for the rest of the second order moments wherein two exponents are 1 and rest are zeros. ■

Remark 2: It is worth noting that when the derivative-matching technique is applied for a discrete-state process, there is an error in matching the first two derivatives [9]. However, in case of a continuous state stochastic differential equation, the first two derivatives are matched exactly. Another important difference between discrete state systems, and continuous state systems is that in the latter, the first two derivatives are matched exactly regardless of the form of f and g whereas in the former, one needs to assume polynomial form for the rates at which the states are changed.

IV. NUMERICAL VALIDATION

In this section, we illustrate the derivative matching technique on two examples. The first example is a Van der Pol oscillator that frequently arises in many engineering applications [19]. In this case, the system dynamics consists of polynomial functions of the state vector. The second example is a swinging pendulum subject to white noise. In this example, the dynamics consist of polynomial functions in one state and a trigonometric function for the other state. We show that the derivative matching technique can be straightforwardly applied to the second example.

A. Van der Pol oscillator

In the deterministic setting, the Van der Pol oscillator is governed by the following second-order differential equation

$$\frac{d^2x}{dt^2} - \epsilon(1 - x^2)\frac{dx}{dt} + \omega_n^2 x = A \cos(\omega_g t), \quad (24)$$

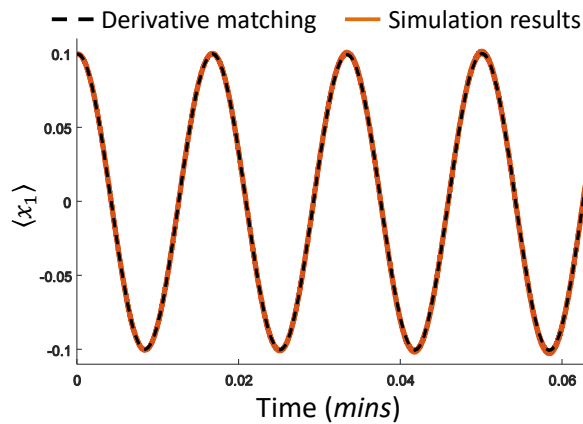


Fig. 1. Derivative matching technique replicates the oscillations of the Van der Pol oscillator quite reasonably. For this plot, the parameters values are $A = 2.5$, $\omega_n = \omega_g = 120\pi$, and $\epsilon = 0.1$. The initial conditions are taken as $x_1(0) = x_2(0) = 0.1$.

where ϵ is the bifurcation parameter, ω_n is the natural frequency, ω_g is the force frequency and A is the force amplitude. A possible stochastic description of the oscillator could be to assume that the force is noisy, i.e., the actuators that apply the force also add a zero mean noise to the system. By choosing $x_1 = x$ and $x_2 = \frac{dx}{dt}$, the oscillator dynamics could be written as

$$dx_1 = x_2 dt, \quad (25a)$$

$$dx_2 = (\epsilon(1 - x_1^2)x_2 - \omega_n^2 x_1) dt + (A \cos(\omega_g t) dt + A dw_t). \quad (25b)$$

Suppose we are interested in the dynamics of $\langle x_1 \rangle$. To this end, we write moment dynamics of this oscillator up to order two

$$\frac{d\langle x_1 \rangle}{dt} = \langle x_2 \rangle, \quad (26a)$$

$$\frac{d\langle x_2 \rangle}{dt} = \epsilon(\langle x_2 \rangle - \langle x_1^2 x_2 \rangle) - \omega_n^2 \langle x_1 \rangle + A \cos(\omega_g t), \quad (26b)$$

$$\frac{d\langle x_1^2 \rangle}{dt} = 2\langle x_1 x_2 \rangle, \quad (26c)$$

$$\begin{aligned} \frac{d\langle x_2^2 \rangle}{dt} &= 2\epsilon(\langle x_2^2 \rangle - \langle x_1^2 x_2^2 \rangle) - 2\omega_n^2 \langle x_1 x_2 \rangle \\ &\quad + 2A\langle x_2 \rangle \cos(\omega_g t) + A^2, \end{aligned} \quad (26d)$$

$$\begin{aligned} \frac{d\langle x_1 x_2 \rangle}{dt} &= \langle x_1^2 x_2 \rangle + \epsilon(\langle x_1 x_2 \rangle - \langle x_1^3 x_2 \rangle) - \omega_n^2 \langle x_1^2 \rangle \\ &\quad + A\langle x_1 \rangle \cos(\omega_g t). \end{aligned} \quad (26e)$$

As expected, the nonlinearities in the dynamics manifest in unclosed moment dynamics, and the moment equations up to order two depend upon third and fourth order moments. In terms of notations in (9), we have $\mu = [\langle x_1 \rangle \ \langle x_2 \rangle \ \langle x_1^2 \rangle \ \langle x_1 x_2 \rangle \ \langle x_2^2 \rangle]^\top$, and $\bar{\mu} = [\langle x_1^2 x_2 \rangle \ \langle x_1^2 x_2^2 \rangle \ \langle x_1^3 x_2 \rangle]^\top$.

Applying the derivative matching closure as described in Section III, we seek approximations of each element of $\bar{\mu}$ in terms of those of μ as in (13). Solving (15) for each of these yields the following approximations

$$\langle x_1^2 x_2 \rangle \approx \frac{\langle x_1^2 \rangle \langle x_1 x_2 \rangle^2}{\langle x_1 \rangle^2 \langle x_2 \rangle}, \quad (27a)$$

$$\langle x_1^2 x_2^2 \rangle \approx \frac{\langle x_1^2 \rangle \langle x_1 x_2 \rangle^4 \langle x_2^2 \rangle}{\langle x_1 \rangle^4 \langle x_2 \rangle^4}, \quad (27b)$$

$$\langle x_1^3 x_2 \rangle \approx \frac{\langle x_1^2 \rangle^3 \langle x_1 x_2 \rangle^3}{\langle x_1 \rangle^6 \langle x_2 \rangle^2}. \quad (27c)$$

Using the approximations from (27) in (26), we obtain a closed set of moment equations. Fig. 1 compares the solution of $\langle x_1 \rangle$ with that of numerical simulations. Our results show an almost perfect match between the system with closure approximation and numerical simulations.

A caveat of the proposed derivative matching approximation is that, as in (27), the means of states appear in the denominator. Since the oscillator states repeatedly cross zero, it is possible that some of these moments approach zero. To avoid this, we add a small term δ to the denominator of approximations.

B. Swinging Pendulum

In the deterministic setting, dynamics of a simple pendulum are given by

$$\frac{d^2\theta}{dt^2} + \frac{k}{m} \frac{d\theta}{dt} + \frac{g}{l} \sin \theta = 0, \quad (28)$$

where g is the acceleration due to gravity, l is the length of the pendulum, and θ is the angular displacement [20]. We also consider friction in our system, with friction constant k . In the stochastic formulation, we could consider that the dynamics are affected by white noise that arises due to random interaction of the pendulum with air molecules. This term scales inversely with mass of the pendulum m , i.e., the interaction with gas particles is negligible for a large mass. By choosing $x_1 = \theta$ and $x_2 = \frac{d\theta}{dt}$, the dynamics of the pendulum can be represented as

$$dx_1 = x_2 dt, \quad (29a)$$

$$dx_2 = \left(-\frac{k}{m} x_2 - \frac{g}{l} \sin x_1 \right) dt + \frac{1}{m} dw_t. \quad (29b)$$

Here we have the trigonometric function $\sin x_1$, which gives rise to nonlinear behavior. To illustrate how derivative matching closure can be used in this context, we approximate $\langle \sin x_1 \rangle$. To this end, we use Euler's relation

$$\sin x_1 = \frac{e^{jx_1} - e^{-jx_1}}{2j}, \quad (30)$$

and carry out a change of variables in the Itô formula to write the moment dynamics such that the moments of x_2 appear in the form of monomials, and moments of x_1 appearing in the form of complex exponentials.

$$\frac{d\langle e^{jx_1} \rangle}{dt} = j \langle e^{jx_1} x_2 \rangle, \quad (31a)$$

$$\frac{d\langle e^{-jx_1} \rangle}{dt} = -j \langle e^{-jx_1} x_2 \rangle, \quad (31b)$$

$$\frac{d\langle x_2 \rangle}{dt} = -\frac{k}{m} \langle x_2 \rangle + \frac{j}{2} \frac{g}{l} \langle e^{jx_1} \rangle - \frac{j}{2} \frac{g}{l} \langle e^{-jx_1} \rangle \quad (31c)$$

$$\begin{aligned} \frac{d\langle e^{jx_1} x_2 \rangle}{dt} &= j \langle e^{jx_1} x_2^2 \rangle - \frac{k}{m} \langle e^{jx_1} x_2 \rangle \\ &\quad + \frac{j}{2} \frac{g}{l} \langle e^{2jx_1} \rangle - \frac{j}{2} \frac{g}{l}, \end{aligned} \quad (31d)$$

$$\begin{aligned} \frac{d\langle e^{-jx_1} x_2 \rangle}{dt} &= -j \langle e^{-jx_1} x_2^2 \rangle - \frac{k}{m} \langle e^{-jx_1} x_2 \rangle \\ &\quad - \frac{j}{2} \frac{g}{l} \langle e^{-2jx_1} \rangle + \frac{j}{2} \frac{g}{l}, \end{aligned} \quad (31e)$$

$$\begin{aligned} \frac{d\langle x_2^2 \rangle}{dt} &= -2\frac{k}{m} \langle x_2^2 \rangle + j\frac{g}{l} \langle e^{jx_1} x_2 \rangle \\ &\quad - j\frac{g}{l} \langle e^{-jx_1} x_2 \rangle + \frac{1}{m^2}, \end{aligned} \quad (31f)$$

$$\frac{d\langle e^{2jx_1} \rangle}{dt} = 2j \langle e^{2jx_1} x_2 \rangle, \quad (31g)$$

$$\frac{d\langle e^{-2jx_1} \rangle}{dt} = -2j \langle e^{-2jx_1} x_2 \rangle. \quad (31h)$$

One way to interpret the above mixed complex exponential monomial moment dynamics is to think that since

all moments of x_2 are generated by taking expectations of the monomials $1, x_2, x_2^2, \dots$, we could consider the terms e^{jx_1} and e^{-jx_1} as two different variables. The mixed moments can then be generated by taking expectation of the products of the complex exponentials $1, e^{-jx_1}, e^{-2jx_1}, \dots$ (or $1, e^{jx_1}, e^{2jx_1}, \dots$) with the monomials $1, x_2, x_2^2, \dots$. The order of the mixed moment can be thought of as the sum of powers of the monomials and complex exponentials.

Given the above interpretation, the moment dynamics in (31) are not closed. As per notation in (9), we have $\boldsymbol{\mu} = [\langle e^{jx_1} \rangle \langle e^{-jx_1} \rangle \langle x_2 \rangle \dots \langle x_2^2 \rangle]^\top$, and $\bar{\boldsymbol{\mu}} = [\langle e^{jx_1} x_2^2 \rangle \langle e^{-jx_1} x_2^2 \rangle \langle e^{2jx_1} x_2 \rangle \langle e^{-2jx_1} x_2 \rangle]^\top$. An important point to note is that since $e^{-jx_1} e^{jx_1} = 1$, there is no need to consider their cross-moments. Thus, we only consider cross moments of e^{-jx_1} with x_2 , and e^{jx_1} with x_2 .

Next, we use the derivative matching scheme to approximate moments in $\bar{\boldsymbol{\mu}}$ as nonlinear functions of moments up to order 2. For instance, consider the moment $\langle e^{jx_1} x_2^2 \rangle$. The aim of closure is to approximate this moment as

$$\langle e^{jx_1} x_2^2 \rangle \approx \langle e^{jx_1} \rangle^{\alpha_1} \langle e^{jx_1} x_2 \rangle^{\alpha_2} \langle x_2 \rangle^{\alpha_3} \langle x_2^2 \rangle^{\alpha_4}. \quad (32)$$

Performing derivative matching approach as explained in Section III results in

$$\langle e^{jx_1} x_2^2 \rangle \approx \frac{\langle x_2^2 \rangle}{\langle e^{jx_1} \rangle} \frac{\langle e^{jx_1} x_2 \rangle^2}{\langle x_2 \rangle^2}. \quad (33)$$

With a similar approach, we can approximate the other moments in the vector $\bar{\boldsymbol{\mu}}$

$$\langle e^{-jx_1} x_2^2 \rangle \approx \frac{\langle x_2^2 \rangle}{\langle e^{-jx_1} \rangle} \frac{\langle e^{-jx_1} x_2 \rangle^2}{\langle x_2 \rangle^2}, \quad (34a)$$

$$\langle e^{2jx_1} x_2 \rangle \approx \frac{\langle e^{2jx_1} \rangle}{\langle x_2 \rangle} \frac{\langle e^{jx_1} x_2 \rangle^2}{\langle e^{jx_1} \rangle^2}, \quad (34b)$$

$$\langle e^{-2jx_1} x_2 \rangle \approx \frac{\langle e^{-2jx_1} \rangle}{\langle x_2 \rangle} \frac{\langle e^{-jx_1} x_2 \rangle^2}{\langle e^{-jx_1} \rangle^2}. \quad (34c)$$

The results show that derivative matching provides reasonably accurate approximation of the moment dynamics (Fig. 2).

V. CONCLUSION

In this paper, we extended the derivative matching based moment approximation method to stochastic dynamical systems with continuous state. We further illustrated that the method is not limited to polynomial dynamics, and it can be used to study systems that contain trigonometric functions. It would be interesting to extend the technique to other forms of mixed functions, and also include differential algebraic inequalities. This would open possibilities of using the moment closure techniques to study a variety of nonlinearities, and has potential applications in power systems analysis. In addition, while in this paper we just considered continuous dynamics modeled through SDEs, many models contain both continuous dynamics and random discrete events [21]–[24]. Deriving derivative matching closure for such hybrid systems will be another avenue of research. Finally, we

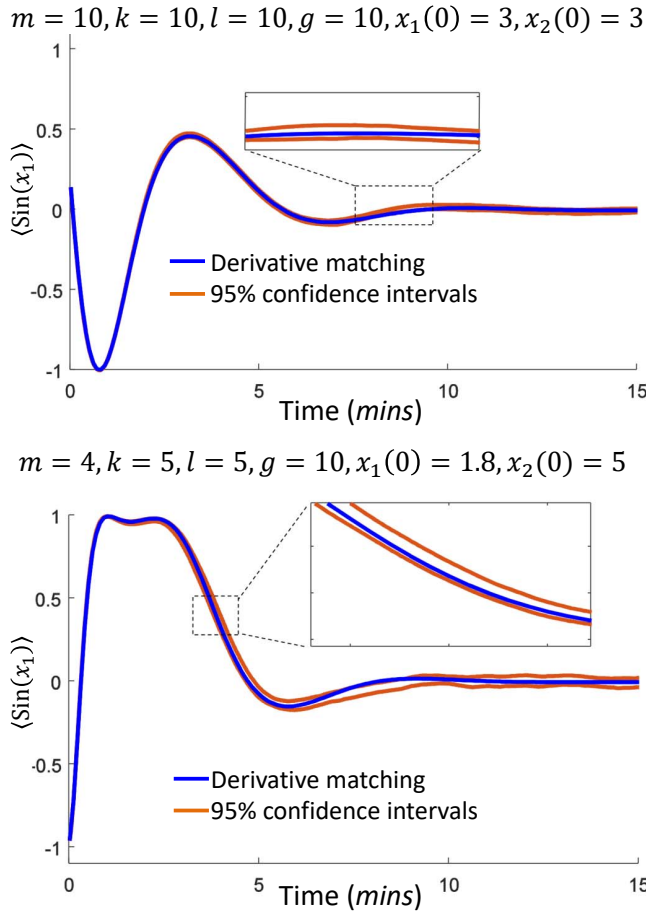


Fig. 2. Derivative Matching provides accurate approximation of the nonlinear function $\langle \sin(x_1) \rangle$. For comparison purpose, 95% confidence interval of the dynamics as obtained from numerical simulation.

note that despite the promising results obtained by closure approximations, generally there are no guarantees on the errors of the closure approximation. Future work will carry out a detailed error analysis using other methods of finding bounds on moments [25], [26].

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REFERENCES

- [1] E. Allen, *Modeling with Itô stochastic differential equations*, vol. 22. Springer Science & Business Media, 2007.
- [2] R. Lande, S. Engen, and B.-E. Saether, *Stochastic population dynamics in ecology and conservation*. Oxford University Press on Demand, 2003.
- [3] A. G. Malliaris, *Stochastic methods in economics and finance*, vol. 17. North-Holland, 1982.
- [4] C. Gardiner, "Handbook of stochastic methods for physics, chemistry and the natural sciences," *Applied Optics*, vol. 25, p. 3145, 1986.
- [5] B. Øksendal, *Stochastic differential equations*. Springer, 2003.
- [6] J. P. Hespanha, "A model for stochastic hybrid systems with application to communication networks," *Nonlinear Analysis: Theory, Methods & Applications*, vol. 62, pp. 1353–1383, 2005.

- [7] A. Julius and G. Pappas, "Approximations of stochastic hybrid systems," *IEEE Transactions on Automatic Control*, vol. 54, pp. 1193–1203, 2009.
- [8] C. H. Lee, K. Kim, and P. Kim, "A moment closure method for stochastic reaction networks," *Journal of Chemical Physics*, vol. 130, p. 134107, 2009.
- [9] A. Singh and J. P. Hespanha, "Approximate moment dynamics for chemically reacting systems," *IEEE Transactions on Automatic Control*, vol. 56, pp. 414–418, 2011.
- [10] C. S. Gillespie, "Moment closure approximations for mass-action models," *IET Systems Biology*, vol. 3, pp. 52–58, 2009.
- [11] M. Soltani, C. A. Vargas-Garcia, and A. Singh, "Conditional moment closure schemes for studying stochastic dynamics of genetic circuits," *IEEE Transactions on Biomedical Systems and Circuits*, vol. 9, pp. 518–526, 2015.
- [12] J. Zhang, L. DeVille, S. Dhople, and A. Dominguez-Garcia, "A maximum entropy approach to the moment closure problem for stochastic hybrid systems at equilibrium," in *Proc. of the 53rd IEEE Conf. on Decision and Control, Los Angeles, CA*, pp. 747–752, 2014.
- [13] A. Singh and J. P. Hespanha, "Stochastic analysis of gene regulatory networks using moment closure," in *Proc. of the 2007 Amer. Control Conference, New York, NY*, 2006.
- [14] C. Kuehn, *Moment Closure—A Brief Review*. Understanding Complex Systems, Springer, 2016.
- [15] L. Socha, *Linearization Methods for Stochastic Dynamic Systems*. Lecture Notes in Physics 730, Springer-Verlag, Berlin Heidelberg, 2008.
- [16] M. Soltani, C. A. Vargas-Garcia, N. Kumar, R. Kulkarni, and A. Singh, "Approximate statistical dynamics of a genetic feedback circuit," *Proc. of the 2015 Amer. Control Conference, Chicago, IL*, pp. 4424–4429, 2015.
- [17] A. Singh and J. P. Hespanha, "Lognormal moment closures for biochemical reactions," in *Proceedings of the 45th Conference on Decision and Control*, pp. 2063–2068, 2006.
- [18] J. P. Hespanha, "Polynomial stochastic hybrid systems," in *Hybrid Systems: Computation and Control*, pp. 322–338, 2005.
- [19] S. H. Strogatz, *Nonlinear dynamics and chaos: with applications to physics, biology, chemistry, and engineering*. Westview press, 2014.
- [20] H. K. Khalil, *Nonlinear systems*, vol. 3. Prentice Hall, NJ, 1996.
- [21] J. Hespanha, "Modelling and analysis of stochastic hybrid systems," *IEE Proceedings Control Theory and Applications*, vol. 153, pp. 520–535, 2006.
- [22] A. R. Teel, A. Subbaraman, and A. Sferlazza, "Stability analysis for stochastic hybrid systems: A survey," *Automatica*, vol. 50, no. 10, pp. 2435–2456, 2014.
- [23] J. Hu, J. Lygeros, and S. Sastry, "Towards a theory of stochastic hybrid systems," in *Hybrid Systems: Computation and Control*, Lecture Notes in Computer Science, pp. 160–173, Springer, 2000.
- [24] M. Soltani and A. Singh, "Moment-based analysis of stochastic hybrid systems with renewal transitions," *Automatica*, vol. 84, pp. 62–69, 2017.
- [25] K. R. Ghusinga, C. A. Vargas-Garcia, A. Lamperski, and A. Singh, "Exact lower and upper bounds on stationary moments in stochastic biochemical systems," *Physical Biology*, vol. 14, 2017.
- [26] A. Lamperski, K. R. Ghusinga, and A. Singh, "Analysis and control of stochastic systems using semidefinite programming over moments," *arXiv preprint arXiv:1702.00422*, 2017.