Master-equation approach to stochastic neurodynamics

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A master-equation approach to the stochastic neurodynamics proposed by Cowan [in *Advances in Neural Information Processing Systems 3,* edited by R. P. Lippman, J. E. Moody, and D. S. Touretzky (Morgan Kaufmann, San Mateo, 1991), p. 62] is investigated in this paper. We deal with a model neural network that is composed of two-state neurons obeying elementary stochastic transition rates. We show that such an approach yields concise expressions for multipoint moments and an equation of motion. We apply the formalism to a $(1+1)$-dimensional system. Exact and approximate expressions for various statistical parameters are obtained and compared with Monte Carlo simulations.

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I. INTRODUCTION

Recently, Cowan introduced a model to describe stochastic neural networks [1] based on a master equation [2], which he called the "neural-network master equation" (NNME). The purpose of this paper is to investigate some of the properties of this equation for the case of networks composed of two-state neurons. We are especially interested in obtaining time-dependent expressions for one-point and many-point moments in a neural network, since such moments can presumably be used to study information processing in the brain [3].

In what follows, we first briefly review the NNME. We then derive equations for the moment-generating function. Explicit solutions to these equations are then obtained for a simple system composed of two neurons. The hierarchy of equations for moments is also derived using the NNME. In order to gain some insight into many neuron systems, we then discuss a special case of the NNME for a $(1+1)$-dimensional system, which is shown to be identical to the "contact process" [4]. For this system we study analytically, time-dependent bulk behavior using the moment equations. Analytical results are then compared with Monte Carlo simulations.

II. A NEURAL NETWORK MASTER EQUATION

The NNME is written using a second-quantization method for classical many-body systems originally formulated independently by Doi [5] and by Grassberger and Scheunert [6]. Cowan introduced two master equations: one to deal with two-state model neuron systems and the other for the more realistic case of three-state model neurons. However, in this paper we shall limit our discussion to systems composed of two-state neurons. Neurons at each site can thus be in one of two states, either "active" or "quiescent." We assume that the active state corresponds to firing and the quiescent to resting of a biological neuron. This assumption leads to a master equation based on spin operators differing from Doi's formulation based on boson operators.

In writing down the equation, we start with a set of elementary transition rates for each neuron in the network. Let us denote quiescent and active states by $|0\rangle$ and $|1\rangle$, respectively. We then assume the transition rates of the ith neuron from one state to the other to be given as follows:

$$|1\rangle \underset{\alpha}{\rightarrow} |0\rangle, \quad |0\rangle \underset{\phi(v_i)}{\rightarrow} |1\rangle \ , \tag{1}$$

where α is a uniform decay rate. (Since the cycle of an action potential lasts about 2 ms, this decay rate can be taken as roughly 500 Hz.) v_i is the sum of all inputs from active neurons connected to the ith neuron, and ϕ is the activation rate function. In general, this function ϕ is a nonlinear function of the total input current which has a sigmoid shape to reflect the upper bound in the activation rate due to the absolute refractory period [7,8].

Let us now denote states (or configurations) of network by $\{|\Omega\rangle\}$, which is the direct product space composed of all neural state vectors in the network:

$$|\Omega\rangle = |v_1\rangle |v_2\rangle \cdots |v_N\rangle, \quad v_i = 0 \text{ or } 1 \ . \tag{2}$$

We also define $P[\Omega,t]$ to be the probability to find the network in a particular state Ω at time t. Then, we can introduce the "neural state vector" for an N neuron network as

$$|\Phi(t)\rangle = \sum_{\{\Omega\}} P[\Omega,t]|\Omega\rangle \ , \tag{3}$$

where the sum is taken over all possible network states.

With these conditions, we can now write the NNME for a system which implements the transition rates given by (1), using creation and annihilation operators, σ_i^+ and σ_j^- in the Pauli spin formalism. [These anticommute at the same site $(i=j)$ to satisfy the physical assumption of single occupancy, and commute for different sites.]

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$$-\frac{\partial}{\partial t}|\Phi(t)\rangle = L|\Phi(t)\rangle \ . \tag{4}$$

The Liouvillian L is then given as

$$L=\alpha\sum_{i=1}^{N}(\sigma_i^+-1)\sigma_i^- + \sum_{i=1}^{N}(\sigma_i^--1)\sigma_i^+\phi\left[\frac{1}{n}\sum_{j=1}^{N}w_{ij}\sigma_j^+\sigma_j^-\right], \tag{5}$$

where n is the average number of connections to each neuron, and w_{ij} is the synaptic transmission strength from the jth to the ith neuron. This is one of the master equations formulated by Cowan. (The factor $1/n$ in the nonlinear function is introduced to normalize the input to each neuron.) In what follows we analyze some of the properties of this equation.

III. MOMENT-GENERATING FUNCTION

In some recent studies of neural networks, one-point and many-point neural moments have gained attention as important quantities in signal processing. It can be shown that these quantities and their equations of motion are given in a concise form using the NNME and the spin-coherent states [9]:

$$\langle \mathbf{Z}| = \langle 0\|\exp\left[\sum_{i=1}^{N}Z_i\sigma_i^-\right] = \prod_{i=1}^{N}(\langle 0| + Z_i\langle 1|) \ , \tag{6}$$

where the product is taken as a direct product, Z_i are complex parameters, and

$$\langle 0\| = \langle 0|\langle 0|\langle 0+\cdots\langle 0| \ . \tag{7}$$

Introducing one-point and many-point moments as

$$\langle\langle v_i(t)\rangle\rangle = \sum_{\{\Omega\}} v_i P[\Omega,t] \ , \tag{8}$$

$$\langle\langle v_i v_j\cdots(t)\rangle\rangle = \sum_{\{\Omega\}}(v_i v_j\cdots)P[\Omega,t] \ , \tag{9}$$

it follows that

$$\langle\langle v_i(t)\rangle\rangle = \langle \mathbf{Z}=\mathbf{1}|\sigma_i^-|\Phi(t)\rangle \tag{10}$$

and

$$\langle\langle v_i v_j\cdots(t)\rangle\rangle = \langle \mathbf{Z}=1|(\sigma_i^-\sigma_j^-\cdots)|\Phi(t)\rangle \ . \tag{11}$$

Furthermore, the moment-generating function $G(\mathbf{Z},t)$ is given by

$$G(\mathbf{Z},t) = \langle \mathbf{Z}|\Phi(t)\rangle \tag{12}$$

from which we can recover the moments as

$$\langle\langle v_i(t)\rangle\rangle = \frac{\partial}{\partial Z_i}G(\mathbf{Z},t)|_{\mathbf{Z}=1} \ , \tag{13}$$

$$\langle\langle v_i v_j\cdots(t)\rangle\rangle = \frac{\partial}{\partial Z_i}\frac{\partial}{\partial Z_j}\cdots G(\mathbf{Z},t)|_{\mathbf{Z}=1} \ . \tag{14}$$

We obtain the equation for $G(\mathbf{Z},t)$ simply by projecting the NNME onto the spin-coherent states:

$$-\frac{\partial}{\partial t}G(\mathbf{Z},t) = \langle \mathbf{Z}|L|\Phi(t)\rangle \ . \tag{15}$$

We can also express this equation in oscillator-algebra form [10]:

$$-\frac{\partial}{\partial t}G(\mathbf{Z},t) = \left\{\alpha\sum_{i=1}^{N}(D_i^+-1)D_i^- + \sum_{i=1}^{N}(D_i^--1)D_i^+ \times\phi\left[\frac{1}{n}\sum_{j=1}^{N}w_{ij}D_j^+D_j^-\right]\right\}G(\mathbf{Z},\mathrm{t}) \ , \tag{16}$$

$$D_i^- = \frac{\partial}{\partial Z_i}, \quad D_i^+ = Z_i\left[1-Z_i\frac{\partial}{\partial Z_i}\right], \tag{17}$$

where we have used the relations

$$\langle \mathbf{Z}|\sigma_i^- = \frac{\partial}{\partial Z_i}\langle \mathbf{Z}|, \quad \langle \mathbf{Z}|\sigma_i^+ = Z_i\left[1-Z_i\frac{\partial}{\partial Z_i}\right]\langle \mathbf{Z}| \ . \tag{18}$$

We note here that our assumption of two states implies that $G(\mathbf{Z},t)$ is at most linear in each Z_i and that we can further simplify Eq. (16) by eliminating differential operators of second and higher orders, to obtain the equation

$$-\frac{\partial}{\partial t}G(\mathbf{Z},t) = \left\{\alpha\sum_{i=1}^{N}(Z_i-1)\frac{\partial}{\partial Z_i} - \sum_{i=1}^{N}(Z_i-1)\left[1-Z_i\frac{\partial}{\partial Z_i}\right]\phi\left[\frac{1}{n}\sum_{j=1}^{N}w_{ij}Z_j\frac{\partial}{\partial Z_j}\right]\right\}G(\mathbf{Z},\mathrm{t}) \ . \tag{19}$$

We can solve this equation explicitly for networks comprising a few neurons. Consider the two-neuron case, whose Liouvillian L is given by

$$L_2 = \alpha\sum_{i=1}^{2}(\sigma_i^+-1)\sigma_i^- + \sum_{i=1}^{2}(\sigma_i^--1)\sigma_i^+\sum_{j=1}^{2}\phi(w_{ij}\sigma_j^+\sigma_j^-)$$

$$= \alpha\{(\sigma_1^+-1)\sigma_1^- + (\sigma_2^+-1)\sigma_2^-)\} + (\sigma_1^--1)\sigma_1^+\phi(w_{12})\sigma_2^+\sigma_2^- + (\sigma_2^--1)\sigma_2^+\phi(w_{21})\sigma_1^+\sigma_1^- \ . \tag{20}$$

[In obtaining the last expression, we have assumed that $\phi(x)$ can be expanded in a Taylor series about $x=0$, and that $\phi(0)=0$. Physically, this assumption excludes "self-activation".] We obtain the general form of the moment-generating function as follows [for $\phi(w_{12})\neq\phi(w_{21})$]:

$$G(Z_1,Z_2,t)=S_0+\sum_{i=1}^{3} S_i e^{-\alpha m_i t}\left\{-\frac{1}{m_i}\left[\frac{1}{k_1-m_i}+\frac{1}{k_2-m_i}\right]+\frac{1}{k_2-m_i}Z_1+\frac{1}{k_1-m_i}Z_2+Z_1Z_2\right\}, \tag{21}$$

where

$$k_1=1+\frac{\phi(w_{12})}{\alpha},\quad k_2=1+\frac{\phi(w_{21})}{\alpha}, \tag{22}$$

and m_i are solutions of

$$m^3-(2+k_1+k_2)m^2+(2+k_1+k_2+k_1k_2)m-(k_1+k_2)=0 . \tag{23}$$

The S_i ($i=0,1,2,3$) are constants determined by the initial conditions.

In the special case that $\phi(w_{12})=\phi(w_{21})\equiv\phi$, the solution is given by the simpler form.

$$G(Z_1,Z_2,t)=A+B(Z_1-Z_2)e^{-(\alpha+\phi)t}+Ce^{-\gamma_+ t}\left[-\frac{2\alpha}{\gamma_+}+Z_1+Z_2+\frac{2\phi}{2\alpha-\gamma_+}Z_1Z_2\right]$$
$$+De^{-\gamma_- t}\left[-\frac{2\alpha}{\gamma_-}+Z_1+Z_2+\frac{2\phi}{2\alpha-\gamma_-}Z_1Z_2\right] . \tag{24}$$

Again A,B,C,D are constants determined by the initial conditions, and

$$\gamma_\pm=\tfrac{1}{2}\{(3\alpha+\phi)\pm\sqrt{\alpha^2+6\alpha\phi+\phi^2}\} . \tag{25}$$

Finding a solution to the many-neuron case can be done in principle by trial function methods [11]. However, it is not an easy task in practice and some approximation scheme is necessary.

IV. THE HIERARCHY OF MOMENT EQUATIONS

In addition to the equation for the moment-generating function, we can obtain equations for the moments themselves. As is typical in the case of many-body problems, we obtain an analog of the BBGKY hierarchy of equations [12]:

$$-\frac{\partial}{\partial t}\langle\langle v_i\rangle\rangle=\alpha\langle\langle v_i\rangle\rangle+\langle\langle(v_i-1)\phi\left[\frac{1}{n}\sum_{j=1}^{N}w_{ij}v_j\right]\rangle\rangle , \tag{26}$$

$$-\frac{\partial}{\partial t}\langle\langle v_iv_j\rangle\rangle=2\alpha\langle\langle v_iv_j\rangle\rangle+\langle\langle(v_i-1)v_j\phi\left[\frac{1}{n}\sum_{k=1}^{N}w_{ik}v_k\right]\rangle\rangle+\langle\langle(v_j-1)v_i\phi\left[\frac{1}{n}\sum_{k=1}^{N}w_{jk}v_k\right]\rangle\rangle \tag{27}$$

and so on, with the equation for the Mth-order moment given as

$$-\frac{\partial}{\partial t}\langle\langle v_{p_1}v_{p_2}\cdots v_{p_M}\rangle\rangle=M\alpha\langle\langle v_{p_1}v_{p_2}\cdots v_{p_M}\rangle\rangle+\sum_{s=1}^{M}\langle\langle(v_{p_1}v_{p_2}\cdots v_{p_M}\left[1-\frac{1}{v_{p_s}}\right]\times\phi\left[\frac{1}{n}\sum_{j=1}^{N}w_{p_sj}v_j\right]\rangle\rangle . \tag{28}$$

The main point to note in this hierarchy is that as is common the nonlinearity of ϕ makes interdependency of these equations more involved than hierarchies arising from a linear interaction (like the one obtained by Doi). More specifically, nonlinearity in the interaction makes the equation of motion for the (m)th moment depend not only on the $(m+1)$th and the $(m-1)$th moments, but also on higher and lower moments as well. In the following, we present a way to visualize this hierarchy using Venn diagrams. Let us define the set $\|v_i\|$ as $\{P[\Omega(v_i=1),t]\}$, i.e., $\|v_i\|$ is a set of probabilities summed to obtain $\langle\langle v_i\rangle\rangle$ in the definition (8). We can define sets corresponding to higher moments in a similar fashion,

$$\|v_iv_j\cdots\|=\{P[\Omega(v_i=v_j=\cdots 1),t]\} . \tag{29}$$

It is straightforward to represent the relationships between these sets with Venn diagrams. The higher moments can be visualized as an overlap of relevant lower moments. In such diagrams, we can visualize which factors are involved given the equation for a given moment. We have not found a way to utilize these diagrams other than for visualization purposes. However, it makes apparent some simple relationships, which may prove useful in approximation schemes, e.g.,

$$\langle\langle v_i\rangle\rangle\geq\langle\langle v_iv_j\rangle\rangle\geq\langle\langle v_iv_jv_k\rangle\rangle\geq\cdots . \tag{30}$$

V. (1+1)-DIMENSIONAL SYSTEM

To gain some insight into the NNME, we devote the rest of this paper to the study of a special case, a one-dimensional ring of excitatory neurons. As shown schematically in Fig. 1, each neuron in this system interacts with its two neighbors via a uniform excited synapic strength w. We also assume that the activation rate function is linear. (It should be kept in mind that

FIG. 1. Schematic diagram of a one-dimensional chain system of neurons.

this is a rather unrealistic model for biological neural networks.) More precisely, we impose the following conditions on Eqs. (4) and (5):

$$\phi(x)=x, \quad w_{ij}=w(\delta_{i,i+1}+\delta_{i+1,i}) \quad (N+1=1) . \tag{31}$$

It turns out that with this condition our model is isomorphic to the contact process [4] with suitable rescaling, the equations of which can be written as

$$-\frac{\partial}{\partial t}|\Phi(t)\rangle=\left\{\lambda\sum_{i=1}^{N}(\sigma_i^+-1)\sigma_i^- +\tfrac{1}{2}\sum_{i=1}^{N}(\sigma_i^--1)\sigma_i^+\sum_{j=1}^{N}\sigma_j^+\sigma_j^-\right\}|\Phi(t)\rangle . \tag{32}$$

This system has been studied by several groups using both computer simulations and analytical methods [13–15]. It appears to possess an active steady state for $\lambda<\lambda_c$ (in the limit of infinitely many neurons) and a totally quiescent (vacuum) steady state for $\lambda>\lambda_c$ with a continuous transition at $\lambda_c\approx 0.304$ [13]. Here, we shall investigate the time-dependent behavior of this model using the moment equations which in this case are (up to second order)

$$-\frac{\partial}{\partial t}\langle\langle v_i\rangle\rangle=\lambda\langle\langle v_i\rangle\rangle-\tfrac{1}{2}\{(\langle\langle v_{i+1}\rangle\rangle-\langle\langle v_iv_{i+1}\rangle\rangle)+(\langle\langle v_{i-1}\rangle\rangle-\langle\langle v_{i-1}v_i\rangle\rangle)\} , \tag{33}$$

$$-\frac{\partial}{\partial t}\langle\langle v_iv_{i+1}\rangle\rangle=2\lambda\langle\langle v_iv_{i+1}\rangle\rangle+\tfrac{1}{2}(\langle\langle v_{i-1}v_iv_{i+1}\rangle\rangle-\langle\langle v_{i-1}v_{i+1}\rangle\rangle+\langle\langle v_iv_{i+1}\rangle\rangle-\langle\langle v_{i+1}\rangle\rangle) +\tfrac{1}{2}(\langle\langle v_iv_{i+1}v_{i+2}\rangle\rangle-\langle\langle v_iv_{i+2}\rangle\rangle+\langle\langle v_iv_{i+1}\rangle\rangle-\langle\langle v_i\rangle\rangle) . \tag{34}$$

We are faced with the hierarchy problem mentioned earlier in solving these sets of equations. But we can use these equations to compute statistical parameters of the time-dependent behavior of this network.

One such parameter is Δ, the "total activation difference," between even-numbered and odd-numbered neurons in the ring. We define Δ as

$$\Delta=\frac{1}{N}\left[\sum_{i=\text{even}}\langle\langle v_i\rangle\rangle-\sum_{i=\text{odd}}\langle\langle v_i\rangle\rangle\right]\equiv\chi_e-\chi_0 . \tag{35}$$

It follows from Eq. (33) that the equation for Δ is given *exactly* for a system with even N as

$$-\frac{\partial}{\partial t}\Delta=(\lambda+1)\Delta . \tag{36}$$

This equation is almost exact for systems with odd N with the extra term $1/N\langle\langle v_Nv_1\rangle\rangle$, which is negligible for large N.

A Monte Carlo algorithm designed for master equations [16] was used to simulate Eq. (32) with 10 000 neurons in the ring. The initial condition for each run was set so that all even-numbered neurons are active and all odd-numbered ones are quiescent. For each run with a given λ, we computed the difference between the numbers of active neurons on even and odd sites at sample time

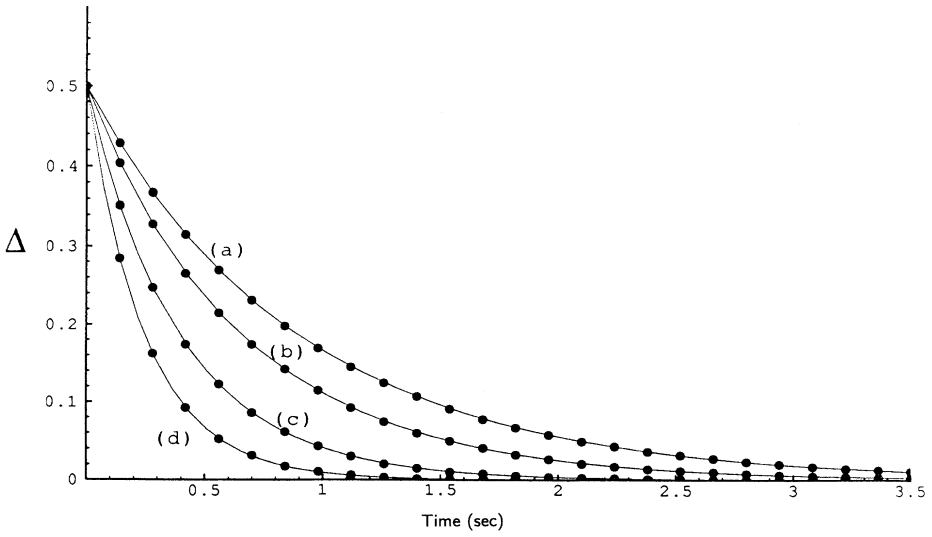

FIG. 2. Examples from comparison of Eq. (32) (solid line) with Monte Carlo simulations (dots) for values of λ given as (a) 0.1, (b) 0. 5, (c) 1.5, and (d) 3.0.

steps. Twenty runs were made for each λ and the differences were averaged at each sampled time step in order to obtain the numerical dynamics of Δ.

The results, some of which are shown in Fig. 2, indicate that Eq. (36) indeed captures the dynamical evolution of Δ very well for all ranges of λ. (The unit of λ is taken to be $\sec^{-1}$.) Hence, as long as Δ is concerned, the many-body behavior of this model can be identified with that of a two-neuron system: one being odd-numbered neurons collectively, and the other being even-numbered neurons collectively. We can derive Eq. (36) using the moment-generating function for the two-neuron case

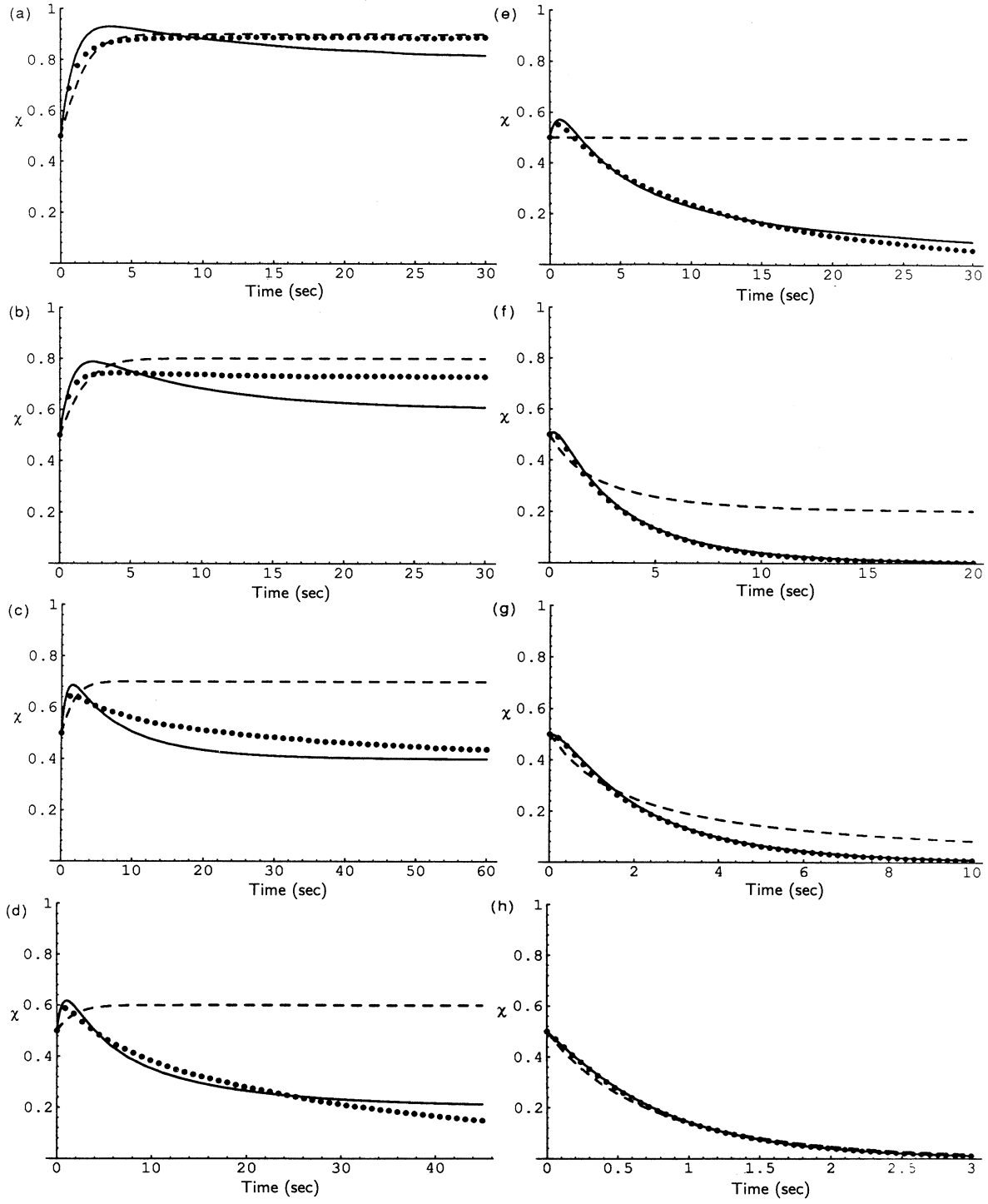

FIG. 3. Comparison of Monte Carlo simulations (dots) with the SMF (dashed line) and the 2 ML (solid line) approximations for χ. The values of λ are given as (a) 0.1, (b) 0.2, (c) 0.3, (d) 0.4, (e) 0.5, (f) 0.8, (g) 1.0, and (h) 2.0.

given in (24) with definition (35), and identification of parameters as $\alpha=\lambda$ and $\phi=1$.

This identity to the two-neuron system does not hold so well when we consider the total activation, $\chi=\chi_e+\chi_o$, which is of more interest in studies of this model. We do not have an exact equation for χ, and need to resort to some form of approximation.

The single-site mean-field (SMF) approximation [13] (or, equivalently the Bragg-Williams approximation [17,18]) can be obtained by assuming the following:

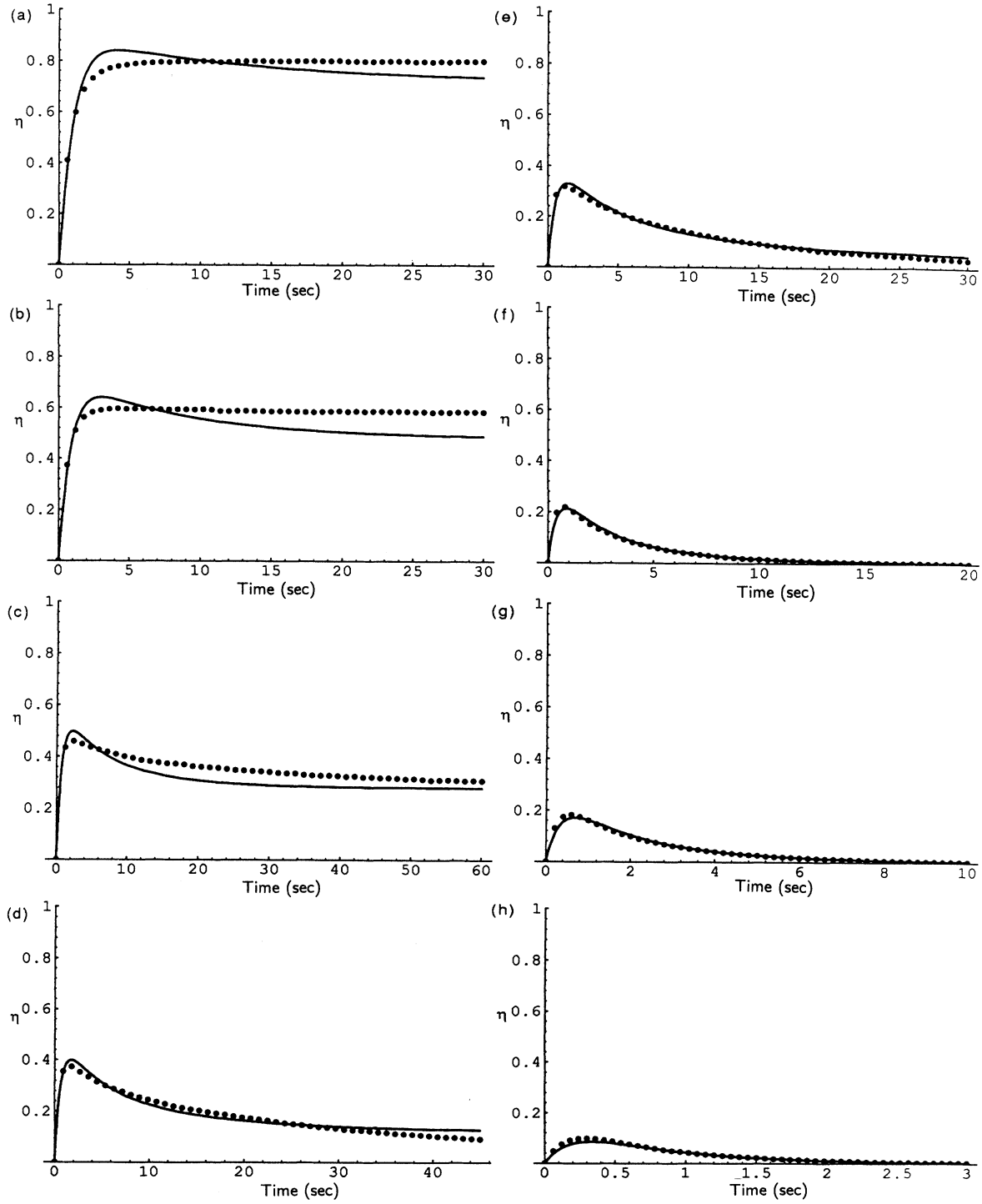

FIG. 4. Comparison of Monte Carlo simulation (dots) with the 2 ML (solid line) approximation for η. The values of λ are given as (1) 0.1, (b) 0.2, (c) 0.3, (d) 0.4, (e) 0.5, (f) 0.8, (g) 1.0, and (h) 2.0.

$$\langle\langle v_i v_{i+1}\rangle\rangle \approx \langle\langle v_i\rangle\rangle \chi \ . \tag{37}$$

Then from (33),

$$-\frac{\partial}{\partial t}\chi=(\lambda-1)\chi+\chi^2 \ . \tag{38}$$

This equation shows a critical value of $\lambda_c^{(1)}=1$, and a steady state

$$\chi\to 1-\lambda \ \ (\lambda<1), \ \ \chi\to 0 \ \ (\lambda>1) \ . \tag{39}$$

Thus, the SMF approximation poses a problem in describing the behavior of the system with $\lambda_c \approx 0.304 < \lambda < \lambda_c^{(1)}=1$.

To improve the approximation, we utilize both (33) and (34) and introduce the variable η, the total neighbors moment:

$$\eta=\frac{1}{N}\sum_{i=1}^{N}\langle\langle v_i v_{i+1}\rangle\rangle \ . \tag{40}$$

We assume that next nearest neighbors which are not directly connected are statistically independent, though we retain the two-point correlation of nearest neighbors. In addition, we assume that three-point moments factor into a product of one- and two-point moments. More precisely, we assume that

$$\langle\langle v_i v_{i+1} v_{i+2}\rangle\rangle \approx \langle\langle v_i v_{i+1}\rangle\rangle \chi \ , \ \ \langle\langle v_i v_{i+2}\rangle\rangle \approx \langle\langle v_i\rangle\rangle \chi \ . \tag{41}$$

With these assumptions, coupled nonlinear equations for χ and η are obtained using (33) and (34),

$$-\frac{\partial}{\partial t}\chi=(\lambda-1)\chi+\eta \ , \tag{42}$$

$$-\frac{\partial}{\partial t}\eta=-\chi+(2\lambda+1)\eta+\chi\eta-\chi^2 \ . \tag{43}$$

We call this approximation the second-moment level (2ML) approximation. With the 2ML approximation, the critical value of λ is improved to $\lambda_c^{(2)}=0.5$ and the steady states are given as

$$\chi\to 1-2\lambda \ (\lambda<0.5), \ \ \chi\to 0 \ (\lambda>0.5) \ . \tag{44}$$

We now compare Monte Carlo simulations with the time dependence of χ given by (38) and (42) and of η by (43). Some of the results are shown in Figs. 3 and 4. (The procedures of simulation are the same as before. Similar results are obtained for different initial conditions.) The result shows that for $\lambda \gtrsim 0.5$, the 2ML approximation scheme captures the time-dependent changes in χ and η very well. As seen in (44), the 2ML approximation predicts a steady state with nonzero χ for $\lambda_c<\lambda<\lambda_c^{(2)}$, which does not match simulation results. Even in this range of λ, however, improvement over the SMF approximation is obtained.

Thus, the 2ML approximation captures the dynamics of χ in the range of λ where the SMF approximation does not work well. It should be stressed, however, that merely going to higher order in the moment equation hierarchy is not sufficient to obtain a better approximation for χ. First, we note that there is a range of λ ($\lesssim 0.2$) where the 2ML approximation does not work as well as the SMF approximation. Second, we made a *particular* choice to retain certain correlations and neglected others to close the hierarchy, and to obtain the 2ML approximation which works for $\lambda \gtrsim 0.5$. It turns out that our choice of this closure of the hierarchy can be formulated as an extension of the Vlasov equation [19] to the second moments. A general formulation of this extension suited for the hierarchy given in Eqs. (26)–(28) with applications to more complex networks is currently being investigated.

VI. SUMMARY AND DISCUSSION

In this paper, we have described a neural-network master equation that enables us to derive dynamical equations for statistical quantities associated with the network in a concise form. In analyzing the resulting dynamics of stochastic neural networks, we are faced with two aspects of the usual many-body problem: one is the difficulty in solving equations of motion for moment-generating functions and the other in dealing with the hierarchy of equations of motion for the moments. We have studied a special case of the NNME for a (1+1)-dimensional system, which is shown to be isomorphic to a dynamical contact process. One way to go beyond the single-site mean-field approximation was derived and limited improvement was seen. Even though there exist some results [1,12,20] which suggest possible approaches toward systematic time-dependent approximations for dealing with the hierarchy of moment equations (or equivalently with the moment-generation function), such theories still need to be adapted for stochastic neurodynamics.

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