

Energy consumption and entropy production in a stochastic formulation of BCM learning

L R de Oliveira, G Castellani and G Turchetti

Dip. di Fisica, Università di Bologna, Viale B. Pichat 6/2, 40126 Bologna IT

E-mail: lucianarenatadeoliveira@gmail.com

Abstract. Biochemical processes in living cells are open systems, therefore they exchange materials with their environment and they consume chemical energy. These processes are molecular-based and for that reason the role of fluctuations can not be ignored and the stochastic description is the most appropriate one. The chemical master equation describes in exact way the probabilistic dynamics of a given discrete set of states and helps us to understand and clarify the differences between closed and open systems. A closed system is related to a condition of detailed balance (DB), i.e. an equilibrium state. After a sufficiently long period, an open system will reach a non-equilibrium steady state (NESS) that is sustained by a flux of external energy. We demonstrate that two implementations of the BCM learning rule (BCM82) and (BCM92) are, respectively, always in DB, and never in DB. We define a one parameter parametrization of the BCM learning rule that interpolates between these two extremes. We compute thermodynamical quantities such as internal energy, free energy (both Helmholtz and Gibbs) and entropy. The entropy variation in the case of open systems (i.e. when DB does not hold) can be divided into internal entropy production and entropy exchanged with surroundings. We show how the entropy variation can be used to find the optimal value (corresponding to increased robustness and stability) for the parameter used in the BCM parametrization. Finally, we use the calculation of the work to drive the system from an initial state to the steady state as the parameter of the plasticity of the system.

1. Introduction

The BCM theory¹ was originally proposed to describe plasticity processes in visual cortex as observed by Hubel and Wiesel [1]. One of the main postulates of this theory is the existence of a critical threshold (the sliding threshold θ_M) and the BCM rule has been classically implemented in two ways: BCM82 [2] and BCM92 [3], depending on the definition of θ_M . In the BCM82, the neuron is assumed to be linear and θ_M is calculated as the power of the expectation value of the neuron postsynaptic activity c , that is $\theta_M = \langle c \rangle^2$ [2]. In order to have stable fixed points, the average used for θ_M in the BCM92 model is calculated with the square of the postsynaptic activity, $\theta_M = \langle c^2 \rangle$, as opposed to the original form, which squared the average of the output itself. If the expectation value of the output is zero, then the original form would have only trivial stable fixed points. This difference in the definition of θ_M leads to the possibility of deriving the rule from an energy function and of a statistical interpretation of these systems [3, 4].

¹ Named after E L Bienenstock, L N Cooper and P W Munro, the BCM rule is a physical theory of learning in the visual cortex developed in 1982.



A “natural” way to cope with the BCM theory is the so-called Chemical Master Equation (CME) approach [5] that executes in a precise manner the probabilistic dynamics of a finite number of states, and recovers, in the thermodynamic limit ($N \rightarrow \infty$), the mean field approximation. The CME can be viewed as a Markov process describing the temporal evolution of the probability of a given discrete set of states [5]. The CME approach offers the possibility of computing the thermodynamic state functions of both closed and open systems (i.e. whether they satisfy or not the detailed balance condition). The detailed balance condition (DB) states that in equilibrium the sum per unit time of all transitions into any state n must be balanced by the sum of all transitions from n into other states n' [5]. An interesting observation is that the two implementations of the BCM rule can either satisfy or not the DB condition.

Let \mathbf{m} be the synaptic weights and \mathbf{d} the input signals received by the synapses, the BCM synaptic modification rule for a single neuron [2] has the form

$$\dot{m}_j = \phi(c, \theta_M) d_j \quad (1)$$

where m_j is the j^{th} synaptic weight and d_j the j^{th} input signal. The modification function $\phi(c, \theta_M)$ depends on the neuron activity level $c \propto (\dots) \cdot \mathbf{d}$ (it is assumed a linear proportionality between the input \mathbf{d} and the output c) and on a moving threshold θ_M , which is a nonlinear function of the cell activity history [6]. For low values of d ($d < \theta_M$), ϕ is negative; for $d > \theta_M$, ϕ is positive. The possibility of computing thermodynamical functions such as entropy, free energy and entropy production gives the opportunity to quantify the grade of “openness” of a system. Nevertheless the entropy variation can be related to the stability and robustness of the system.

2. Parametrization of the bidimensional case of the BCM rule

It turns out that the bidimensional version of BCM rule, with two orthogonal inputs is indicative of the general case of stochastic high-dimensional non-orthogonal inputs. Analysis that connects both has been given in [2, 3, 6]. The averaged version of the BCM learning rule, in the bidimensional case is:

$$\frac{d}{dt} \begin{pmatrix} m_1 \\ m_2 \end{pmatrix} = (PD)^T \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \quad (2)$$

where m_1 and m_2 are the synaptic weights, P is the diagonal matrix with the inputs probability of the inputs p_1 and p_2 , D is the inputs matrix (a matrix whose rows are the input vectors \vec{d}_1 and \vec{d}_2), and the neuronal output in the linearity region is $c = \vec{m} \cdot \vec{d}$. The vector $\vec{\phi} = (\phi_1, \phi_2)$, is defined as $(\phi(\vec{m} \cdot \vec{d}_1, \theta), \phi(\vec{m} \cdot \vec{d}_2, \theta))$.

The BCM learning rule can be formulated in two ways: BCM82 [2] and BCM92 [3], based on two definitions of the moving threshold θ . It is possible to find a parametrization that interpolates with continuity between these two extremes by a suitable definition of θ_α

$$\theta_\alpha = \langle c^{1+\alpha} \rangle^{2-\alpha} \quad (3)$$

in this way we obtain for $\alpha = 0 \Rightarrow \theta_0 = \langle c \rangle^2$ and for $\alpha = 1 \Rightarrow \theta_1 = \langle c^2 \rangle$.

As was done in the work of Bienenstock et al. 1982 [2], we consider two special input vectors as $d_1 = (1, 0)$, $d_2 = (0, 1)$, with equal probability of appearing $p_1 = p_2 = 1/2$ and the definition of θ as in equation 3, in this way the the BCM rule becomes²:

$$\begin{aligned} \dot{m}_1 &= \frac{1}{2} \phi(m_1, \theta) = \frac{m_1}{2} (m_1 - \theta) \\ \dot{m}_2 &= \frac{1}{2} \phi(m_2, \theta) = \frac{m_2}{2} (m_2 - \theta) \end{aligned} \quad (4)$$

² A detailed description is given by Cooper et al. 2004 [6].

3. BCM rule and CME

Both systems (BCM82 and BCM92) can be studied by the CME because the number of synapses can be small, and the role of fluctuations can not be neglected. On the other hand, if these numbers increase, the CME approaches the deterministic equations (mean field limit). Another motivation for the CME approach is that we can state conditions for the validity of the detailed balance, and if we can compute the stationary distribution, we can also compute all the relevant thermodynamic quantities as free energy and entropy. The CME formalism allows us to deal with “discrete synapses”, that are synapses with non-continuous values, as pointed out by several authors [2, 3, 4, 6, 7]. The CME for the system defined in equation 4 is:

$$\begin{aligned}\dot{p}_{m_1, m_2} &= (\mathbb{E}_{m_1} - 1)r_{m_1, m_2}^{(m_1)}p_{m_1, m_2} + (\mathbb{E}_{m_1}^{-1} - 1)g_{m_1, m_2}^{(m_1)}p_{m_1, m_2} \\ &+ (\mathbb{E}_{m_2} - 1)r_{m_1, m_2}^{(m_2)}p_{m_1, m_2} + (\mathbb{E}_{m_2}^{-1} - 1)g_{m_1, m_2}^{(m_2)}p_{m_1, m_2}.\end{aligned}\quad (5)$$

This CME is derived under the condition of a one-step Poisson process [5], \mathbb{E} and \mathbb{E}^{-1} are the forward and backward step operators, whose effect on an arbitrary function $f(n)$ is defined as $\mathbb{E}_n f(n) = f(n+1)$, $\mathbb{E}_n^{-1} f(n) = f(n-1)$. The generation and recombination terms respectively are $g_{m_1, m_2}^{(m_i)} = \frac{m_i^2}{2N^2}$, $r_{m_1, m_2}^{(m_i)} = \frac{m_i \theta_\alpha}{2N^2}$, $i = 1, 2$, and N is the maximum value of the synaptic weight (proportional to the maximum number of molecules). To verify if the DB condition holds, we define a quantity that we call “commutator” $\mathcal{C}_\alpha(m_1, m_2)$, because it is the difference between the two possible paths (i.e. by joining the bottom left vertex with the upper right vertex) in an unitary square. The validity of this definition relies on the structure of the CME, which does not contain diagonal terms (i.e. there are no terms with simultaneous variations of m_1 and m_2)

$$\mathcal{C}_\alpha(m_1, m_2) = \frac{g_{m_1-1, m_2-1}^{(m_2)} \cdot g_{m_1-1, m_2}^{(m_1)}}{r_{m_1-1, m_2}^{(m_2)} \cdot r_{m_1, m_2}^{(m_1)}} - \frac{g_{m_1-1, m_2-1}^{(m_1)} \cdot g_{m_1, m_2-1}^{(m_2)}}{r_{m_1, m_2-1}^{(m_1)} \cdot r_{m_1, m_2}^{(m_2)}}. \quad (6)$$

If $\mathcal{C}_\alpha(m_1, m_2) = 0$, the DB condition always holds, whereas if $\mathcal{C}_\alpha(m_1, m_2) \neq 0$ the DB does not hold.

4. Thermodynamics quantities from CME:

In order to make a non equilibrium thermodynamics approach in terms of the chemical master equation, we have to know some concepts from the statistical mechanics of equilibrium. For the canonical ensemble one can define the Gibbs entropy S , the total energy U and the Helmholtz free energy F

$$S = -k_B \sum_{i=1}^N p_i \ln p_i, \quad U = \sum_{i=1}^N p_i u_i \quad \text{and} \quad F = U - TS \quad (7)$$

In this paper we will assume that k_B and the temperature T are equal to 1.

Considering that the Gibbs entropy (equation 7) can be written as function of time and taking its time derivate³

$$\frac{dS(t)}{dt} = - \sum_{i=1}^N \frac{dp_i}{dt} \ln p_i - \frac{d}{dt} \sum_{i=1}^N p_i = - \sum_{i=1}^N \frac{dp_i}{dt} \ln p_i \quad (8)$$

we take into account the generic master equation $\frac{dp_i(t)}{dt} = \sum_{j=1}^N (p_j(t)q_{ij} - p_i(t)q_{ji})$, where q_{ij} are the transition rates and $p_i(t)$ is the probability that the system is in the i_{th} state. In equation 8

³ The term $\frac{d}{dt} \sum_{i=1}^N p_i$ does not contribute since $\sum_{i=1}^N p_i = 1$.

the term $\frac{dp_i}{dt}$ can be replaced by the master equation and then we can write the time variation of entropy as [8, 9]

$$\frac{dS(t)}{dt} = -\frac{1}{2} \sum_{i,j=1}^N (p_j q_{ij} - p_i q_{ji}) \ln \frac{p_i q_{ji}}{p_j q_{ij}} + \frac{1}{2} \sum_{i,j=1}^N (p_i q_{ij} - p_j q_{ji}) \ln \frac{q_{ji}}{q_{ij}} \quad (9)$$

This derivation is in agreement with the classical definition of the entropy variation and may be written as the sum of two terms [10]:

$$\frac{dS(t)}{dt} = h_d - e_p \quad (10)$$

Where e_p is the entropy production rate, i.e. the entropy produced inside the system due to spontaneous process and h_d is the heat dissipation rate, i.e. the entropy supplied to the system by its surroundings. According to the second law of thermodynamics e_p must be zero for reversible (or equilibrium) transformations and positive for irreversible transformations of the system. The entropy supplied, h_d , may be positive, zero or negative depending on the interaction of the system with its surroundings [10].

We can still relate h_d and e_p to the thermodynamic variables at equilibrium. If we consider the definition of the Helmholtz free energy (equation 7), the entropy variation (equation 10) can be expressed as $\frac{dS(t)}{dt} = \frac{dU(t)}{dt} - \frac{dF(t)}{dt}$. Therefore, we identify

$$h_d = \frac{dU(t)}{dt} \quad \text{and} \quad e_p = \frac{dF(t)}{dt} \quad (11)$$

In this way we have the mathematical formulation for the thermodynamic variables in terms of the master equation. When the system presents detailed balance condition, for $t \rightarrow \infty$ it reaches an equilibrium state with $e_p = h_d = \frac{dS(t)}{dt} = 0$. In contrast to systems in equilibrium, systems in NESS present fluxes of physical quantities, such as particles or energy. Thus, DB is violated and energy is pumped into the system to sustain the NESS [9, 11, 12]: e_p and h_d are not null, but equal. This is necessary to ensure that S is finite asymptotically and $\frac{dS(t)}{dt} = 0$.

Using the result in equation 11, we can calculate the work to drive the system from an initial state to the stationary (or equilibrium) state as

$$\frac{dW_{h_d}}{dt} = \frac{dU(t')}{dt'} - \frac{dU(\infty)}{dt'} \quad (12)$$

$$W_{h_d} = \lim_{t \rightarrow \infty} \int_0^t (h_d(t') - h_d(\infty)) dt' = \lim_{t \rightarrow \infty} \left[\int_0^t h_d(t') dt' - t h_d(\infty) \right]$$

and

$$\frac{dW_{e_p}}{dt} = \frac{dF(t')}{dt'} - \frac{dF(\infty)}{dt'} \quad (13)$$

$$W_{e_p} = \lim_{t \rightarrow \infty} \int_0^t (e_p(t') - e_p(\infty)) dt' = \lim_{t \rightarrow \infty} \left[\int_0^t e_p(t') dt' - t e_p(\infty) \right]$$

The total work (work of entropy) is written as

$$W_S = W_{h_d} - W_{e_p} \quad (14)$$

Hence, we use the calculation of the work as the parameter of the plasticity of the system (where each value of e_p and h_d represents a probability configuration for the system).

5. Results

In this section we are going to compare the behavior of the different formulations of the BCM rule, through the calculation of the thermodynamic variables. More specifically, we are interested in determining which model is more plastic, studying the differences between DB and NESS. We have to determine if systems with $\alpha \neq 0$ and $\mathcal{C}_\alpha(m_1, m_2) \neq 0$ are in a NESS condition. We can do this by the calculation of h_d , e_p and $\frac{dS}{dt}$, because as we enunciated in section 4 NESS is characterized by a sustained energy input and $h_d = e_p \neq 0$ in the stationary state. We simulate the time evolution of h_d and e_p for $0 \leq \alpha \leq 1$ and we verify that for $\alpha = 1$ (BCM92) the system presents $h_d = e_p = 0.0013465$ and for $\alpha = 0$ (BCM82) $h_d = e_p = 0$. We can infer that the BCM82 reaches an equilibrium state and the BCM92 reaches a NESS.

We will compute the work done by the system to reach the equilibrium configuration. To do this we compute W_{h_d} , W_{e_p} and W_S according to equations 12, 13 and 14 by numerical integration of the CME over a time span sufficiently long to reach the stationary distribution.

A first comparison between the two BCM models reveals that the work done to reach the stationary distribution is lower in the case of DB violation (see figure 1).

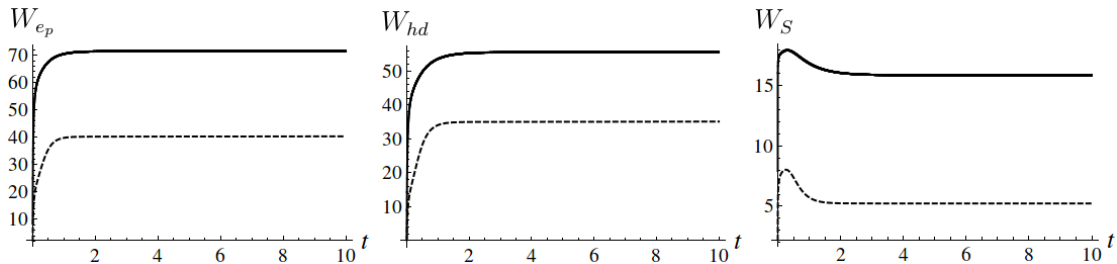


Figure 1. Change of W_{h_d} , W_{e_p} , W_S for BCM82 (black line) and BCM92 (dashed line). The simulations are performed for $N = 31$ and the initial condition $p_{m_1, m_2} = \delta_{m_1, 31} \delta_{m_2, 31}$

We confirm this trend by plotting the value of entropy work in the stationary state (W_S^s) as a function of α (see figure 2).

We note that the value of these quantities is dependent on the choice of the initial conditions. This dependence on the initial conditions is easily explainable for the W_S from the definition

$$W_S = \int_0^\infty \frac{dS}{dt'} dt' = \int_0^\infty (e_p(t') - h_d(t')) dt' = W_{e_p} - W_{h_d} = S(\infty) - S(0) : \quad (15)$$

the entropy variation depends on the initial value. If for example we choose the initial conditions as: $p_{m_1, m_2} = \delta_{m_1, \bar{m}_1} \delta_{m_2, \bar{m}_2}$, the initial entropy is zero, hence $W_{e_p} - W_{h_d}$ is simply $S(\infty)$.

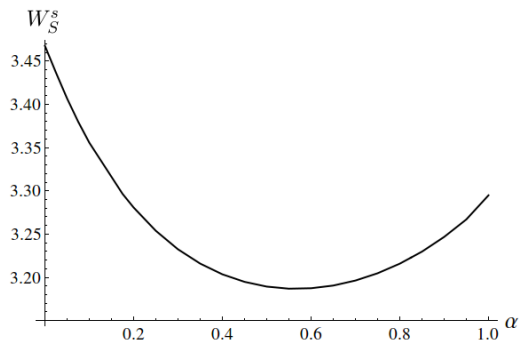


Figure 2. Change of W_S^s when α is varied from 0 to 1. The simulations are performed for $N = 31$ and the initial condition $p_{m_1, m_2} = \delta_{m_1, 15} \delta_{m_2, 15}$.

In figure 2 we show W_S^s as a function of the parameter α . It is possible to see that the entropy variation shows a minimum for $\alpha \approx 0.6$.

6. Conclusions

Our results show that when the system is not in the detailed balance condition, the work necessary to reach the stable state is less than that requested when the detailed balance holds. This means that the system requires less energy to memorize a pattern when the detailed balance is not satisfied. Hence the system is more plastic: a part of the energy that is requested to maintain the NESS is recovered when the system learns and develops selectivity to input pattern. We believe that this can be an hallmark of biological systems and that this can explain why these systems spend a large part of their metabolic energy to maintain NESS states; this energy is recovered during crucial developmental steps such as differentiation and learning.

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