

LECTURE #15

JOHN GOUTSIAS
WHITAKER BIOMEDICAL ENGINEERING INSTITUTE
THE JOHNS HOPKINS UNIVERSITY
BALTIMORE, MD 21218

EXAMPLE: NEURAL DYNAMICS

Neural Networks

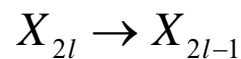
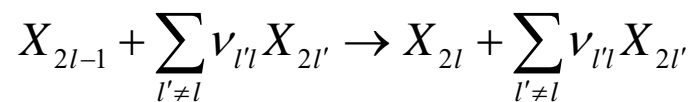
2

- We consider a model that consists of L neurons.
- Each neuron can be in either of two states: quiescent or active.
- X_{2l-1} denotes a quiescent neuron l .
- X_{2l} denotes an active neuron l .

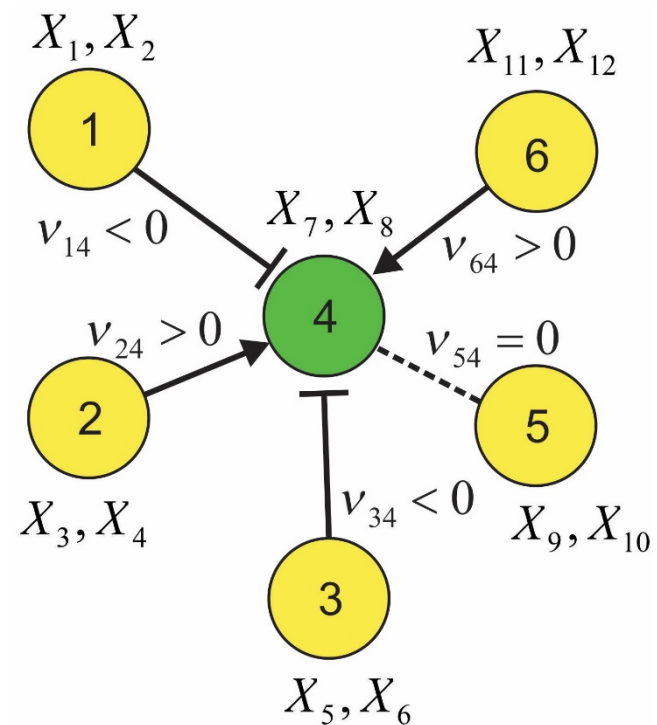
Neural Networks

3

- We assign the following two reactions to the l -th neuron:

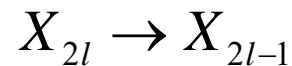
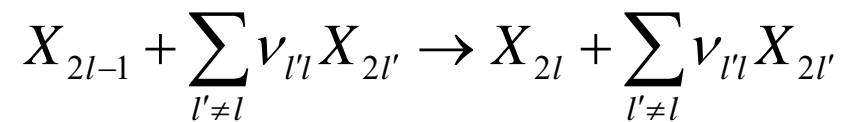


- ν_{ij} measures the synaptic weight between neurons i and j .
- A positive value of ν_{ij} indicates an excitatory synapsis and a negative value indicates an inhibitory synapsis.



Neural Networks

4



- The first reaction models transition of the l -th neuron from the quiescent to the active state.
- The second reaction models transition of the l -th neuron from the active to the quiescent state.
- We obtain a reaction network with $2L$ species and $2L$ reactions.

Neural Networks

5

- We can describe this system by a $2L \times 1$ state vector \mathbf{x} with binary-valued 0/1 elements x_{2l-1}, x_{2l} indicating the state of the l -th neuron (with 0 being quiescent and 1 being active).
- We must satisfy the “mass conservation” relationships:

$$x_{2l-1} + x_{2l} = 1, \quad \text{for } l = 1, 2, \dots, L$$

Neural Networks

6

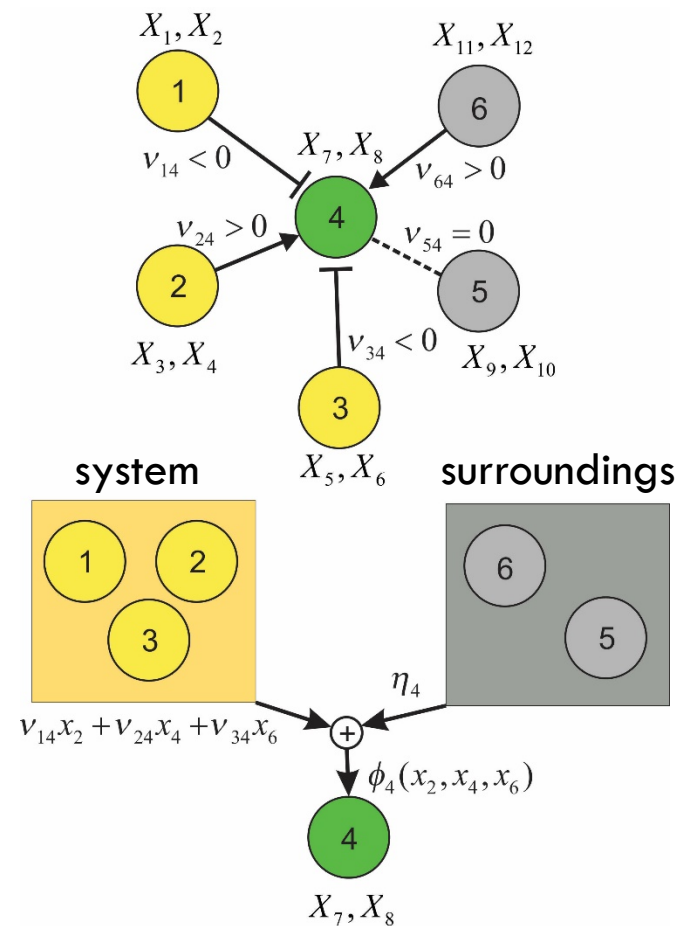
- It has been suggested that the probability of the l -th neuron becoming active during $[t, t + dt)$, given that the neuron is quiescent at time t , can be taken to be

$$x_{2l-1}[\phi_l(\mathbf{x}) > 0] \tanh[\phi_l(\mathbf{x})] dt$$

- $\phi_l(\mathbf{x})$ is the net synaptic input to the l -th neuron, given by

$$\phi_l(\mathbf{x}) = \sum_{l' \neq l} v_{ll'} x_{2l'} + \eta_l$$

external input



Neural Networks

7

$$X_{2l-1} + \sum_{l' \neq l} v_{l'l} X_{2l'} \rightarrow X_{2l} + \sum_{l' \neq l} v_{l'l} X_{2l'}$$
$$X_{2l} \rightarrow X_{2l-1}$$

- The propensity functions will now be given by

$$\pi_{2l-1}(\mathbf{x}) = x_{2l-1} [\phi_l(\mathbf{x}) > 0] \tanh[\phi_l(\mathbf{x})]$$
$$\pi_{2l}(\mathbf{x}) = \gamma_l x_{2l}$$

A Simplified Model

8

- Assume that the L neurons in the network can be divided into an equal number of $L/2$ excitatory and $L/2$ inhibitory neurons.
- Assume that all neurons synapse to all other neurons with excitatory and inhibitory weights $v_E \geq 0$ and $v_I \leq 0$.
- Consider the case in which the neurons are characterized by the same decay rate γ whereas, their external inputs take the same value η .

A Simplified Model

9

- Under the previous assumptions, it may not be of interest to track the state of individual neurons, since the excitatory or inhibitory neurons are identical to each other.
- Instead, it will be more appropriate to track the dynamics of the net number

$$A(t) \triangleq Y_1(t) + Y_2(t)$$

of active excitatory and inhibitory neurons, where

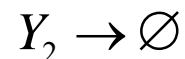
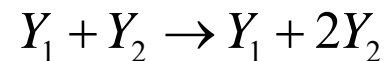
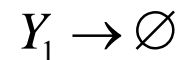
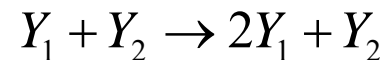
$$Y_1(t) \triangleq \sum_{l \in \mathcal{E}} X_{2l}(t) \quad \text{and} \quad Y_2(t) \triangleq \sum_{l \in \mathcal{I}} X_{2l}(t)$$

with \mathcal{E} and \mathcal{I} being the set of excitatory and inhibitory neurons, respectively.

Simplified Reactions

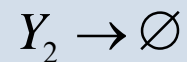
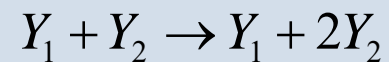
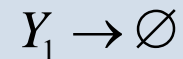
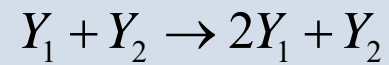
10

- It turns out that $Y_1(t)$ and $Y_2(t)$ can be modeled by a simple Markovian reaction network comprised of two species Y_1 and Y_2 that denote active excitatory and inhibitory neurons, respectively, which interact through the following reactions:



Simplified Reactions

11



- These reactions correspond to the activation/deactivation of an excitatory neuron (first and second reactions) and the activation/deactivation of an inhibitory neuron (third and fourth reactions).

Propensity Functions

12

- The propensity functions are given by

$$Y_1 + Y_2 \rightarrow 2Y_1 + Y_2$$

$$Y_1 \rightarrow \emptyset$$

$$Y_1 + Y_2 \rightarrow Y_1 + 2Y_2$$

$$Y_2 \rightarrow \emptyset$$

$$\pi_1(\mathbf{y}) = (L/2 - y_1)[\phi(\mathbf{y}) > 0] \tanh[\phi(\mathbf{y})]$$

$$\pi_2(\mathbf{y}) = \gamma y_1$$

$$\pi_3(\mathbf{y}) = (L/2 - y_2)[\phi(\mathbf{y}) > 0] \tanh[\phi(\mathbf{y})]$$

$$\pi_4(\mathbf{y}) = \gamma y_2$$

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

- y_1, y_2 take values in $\{0, 1, \dots, L/2\}$
- $[]$ is the Iverson bracket
- $\phi(\mathbf{y})$ is the synaptic input to each neuron, given by

$$\phi(\mathbf{y}) = v_E y_1 + v_I y_2 + \eta$$

Remarks

13

- Despite its simplified nature, the previous model has been shown to be effective for predicting experimentally observed, *in vitro* and *in vivo*, neural behavior, known as avalanching.
- This behavior is characterized by irregular and isolated bursts of neural activity during which many neurons fire simultaneously.
- We will use thermodynamic principles to explore this interesting behavior.
- For ease of computational analysis, we consider a moderately sized neural network comprised of $L = 100$ neurons.
- This allows us to numerically compute the solution of the underlying master equation using the KSA method.
- We assume that all neurons are initially at rest, i.e., $Y_1(0) = Y_2(0) = 0$.

Parameters

14

- We take

$$L = 100$$

$$\gamma = 0.1 \text{ ms}^{-1}$$

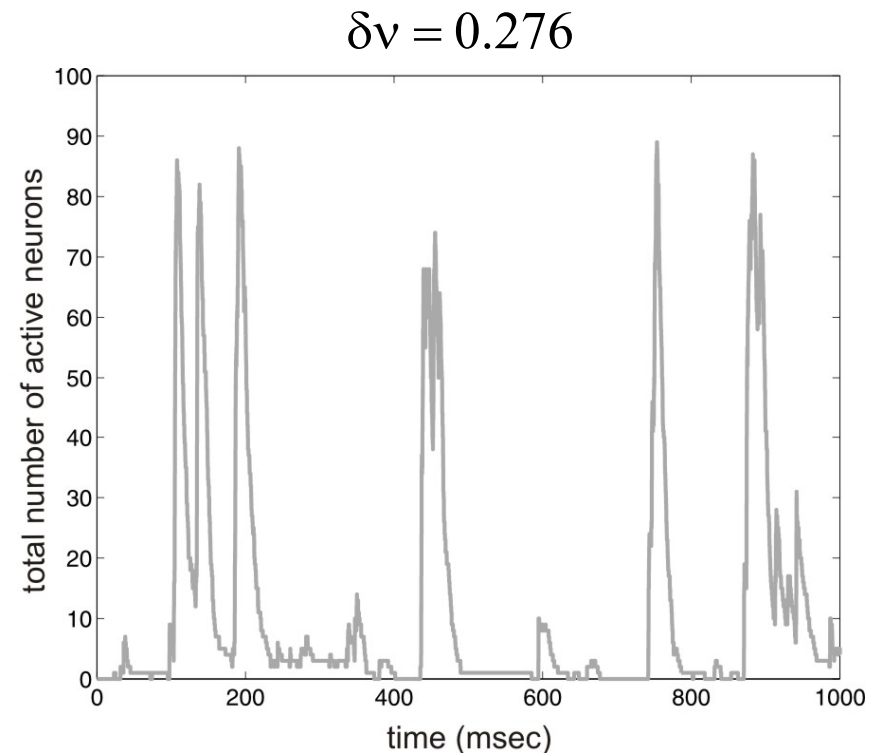
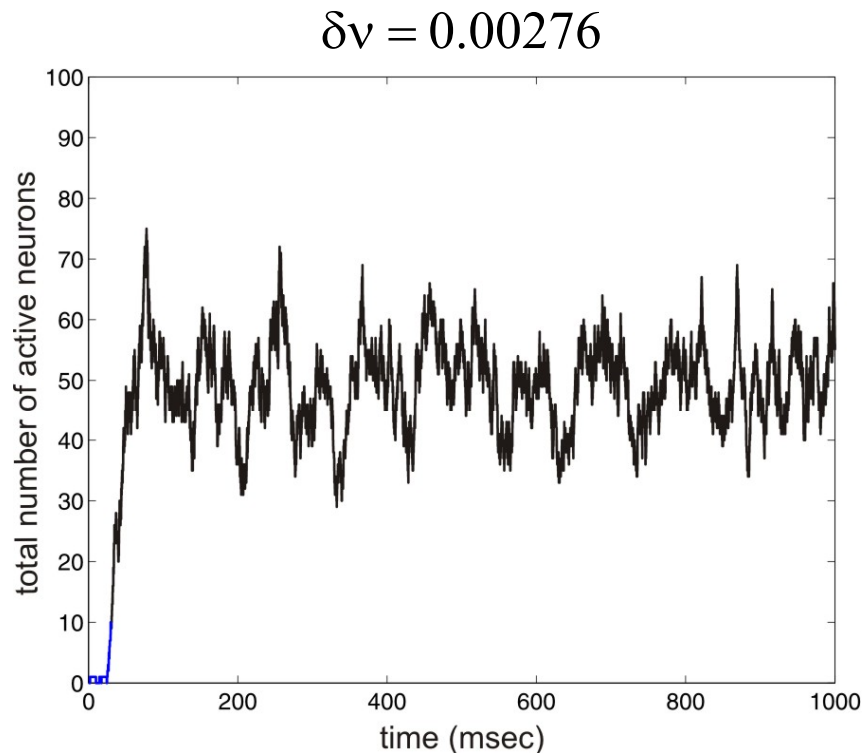
$$\eta = 0.001$$

$$v_E + v_I = 0.004$$

- When the sum $v_E + v_I$ is kept fixed, the difference $\delta v \triangleq v_E - v_I$ controls avalanching.
- More particularly, as δv increases, the network transitions from asynchronous to synchronous neural firings that lead to avalanching.

Avalanching Example

15



Dynamic evolutions of the net number of active neurons drawn from the underlying master equation using exact sampling. The black trajectory indicates that neurons fire asynchronously, whereas the irregular and isolated bursts of net neural activity observed in the gray trajectory indicate that neurons fire synchronously resulting in avalanching.

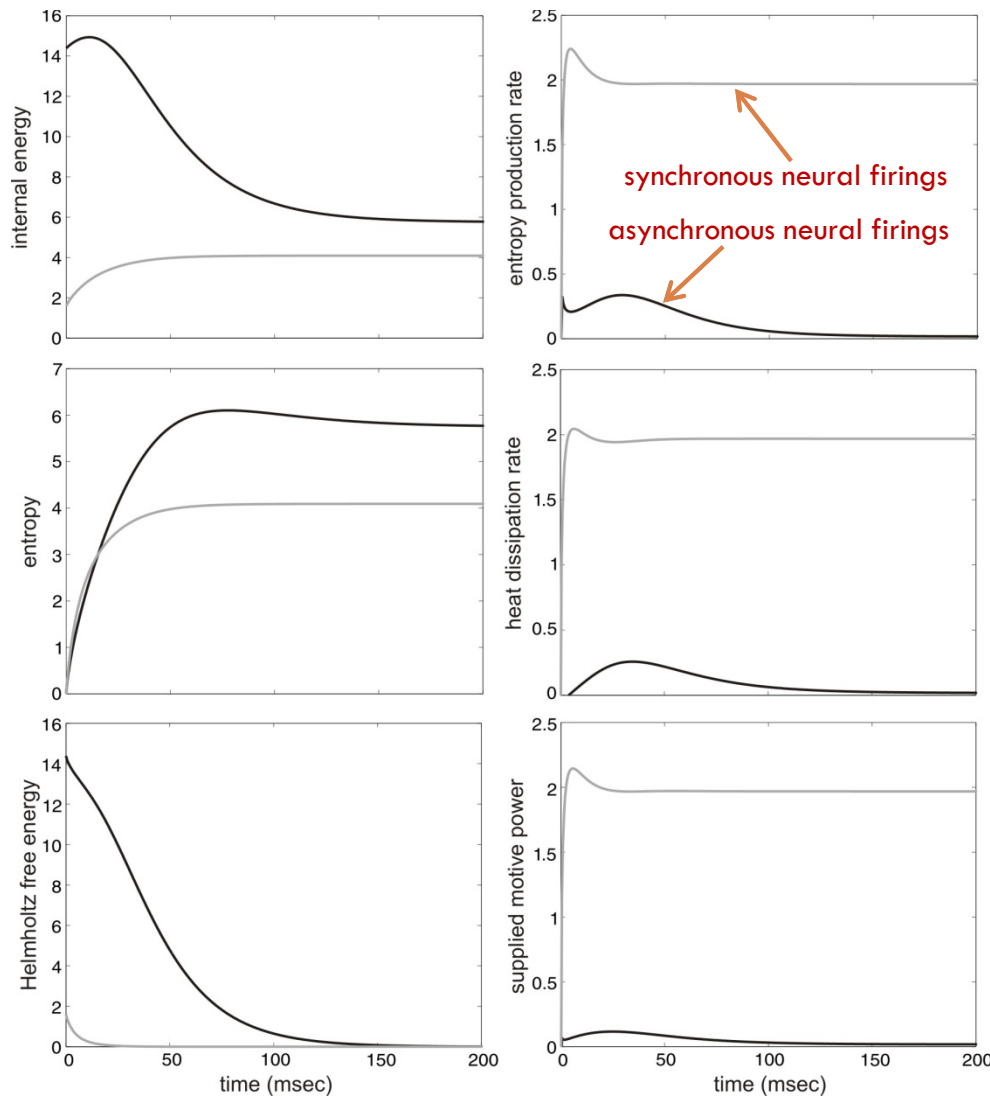
Non-equilibrium Steady-State (NESS)

16

- Most biological systems of interest reach a state of homeostasis, wherein the system is maintained at a given stable operating point.
- Mathematically, we can describe this point by a stable steady state.
- From a thermodynamic perspective such a system must operate away from thermodynamic equilibrium at steady-state, since living organisms require transfer of energy and mass with their surroundings in order to consume nutrients and excrete waste.
- To achieve this, nonzero motive power must be supplied to the system at steady-state, which implies, by virtue of the first law of thermodynamics, that an equal amount must be dissipated to the surroundings in the form of heat.
- Consequently, the state of homeostasis at which biological systems operate is often referred to as non-equilibrium steady-state (NESS).
- Naturally, the neural network example must also operate at a NESS.

Non-equilibrium Steady-State (NESS)

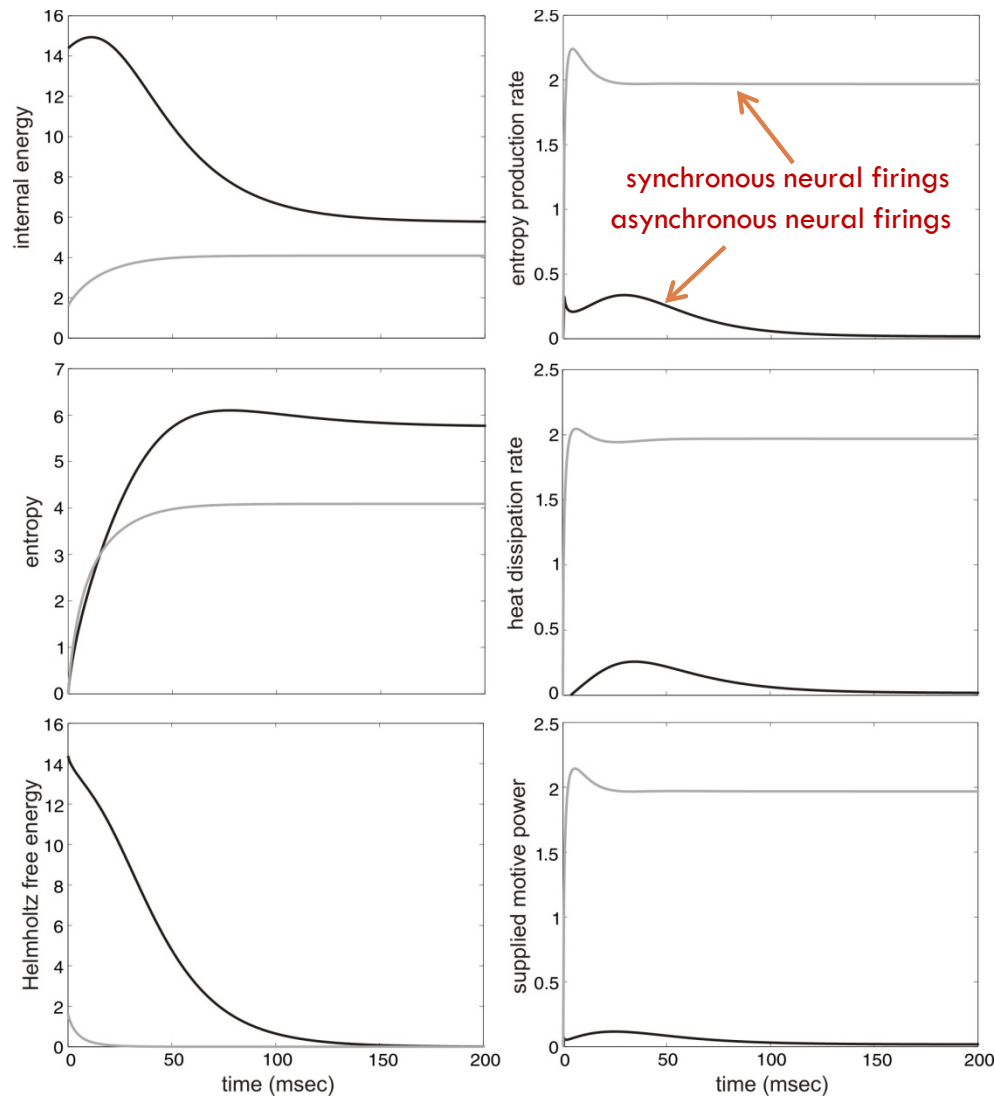
17



- All thermodynamic quantities reach stationarity, with the entropy production rate, heat dissipation rate, and supplied motive power converging to the same value in each case, in agreement with the first and second law of thermodynamics.
- This stationary value is nonzero in both cases (although it is close to zero in the asynchronous case) which shows that the system operates away from thermodynamic equilibrium at steady-state regardless of the type of neural firings involved.

System Entropy

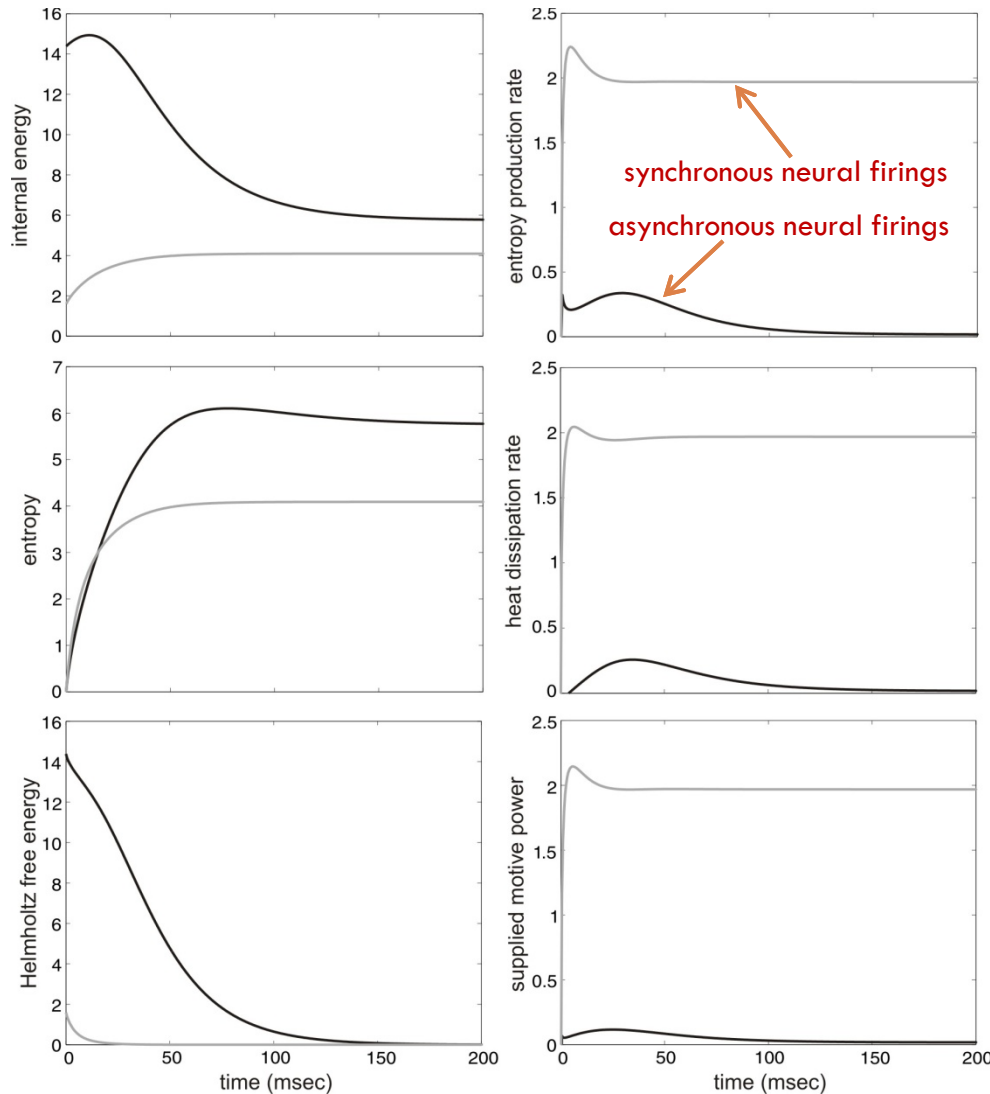
18



- The system entropy is in general smaller when neurons fire synchronously than when they fire asynchronously.
- This indicates an expected degree of predictability in neural activity when neurons fire synchronously.

Helmholtz Free Energy

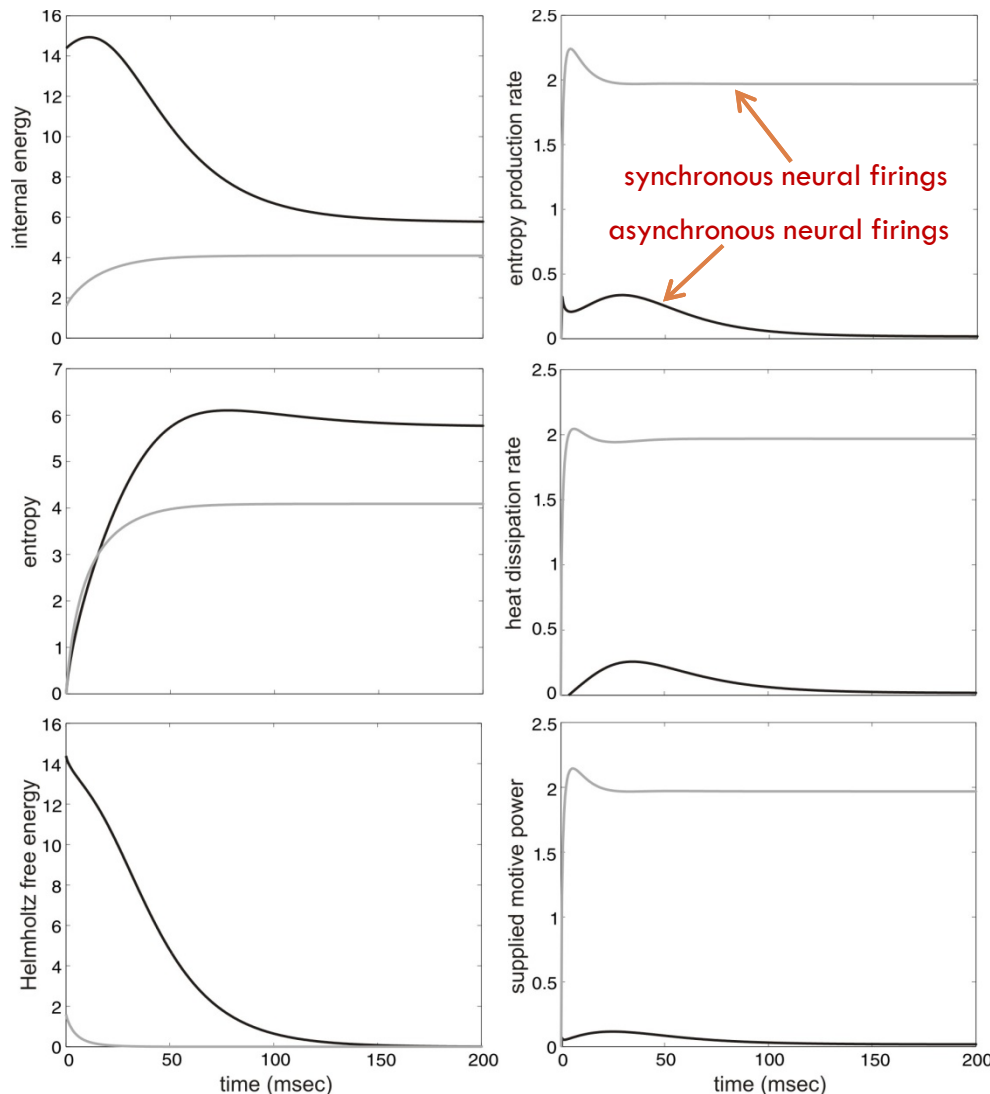
19



- The initial Helmholtz free energy associated with asynchronous neural firings is almost an order of magnitude larger than that associated with synchronous firings.
- In both cases the Helmholtz free energy becomes zero at steady-state, as expected.
- This indicates that, under constant temperature and volume, appreciable more work must be done when the neurons fire asynchronously to reach steady-state than when the neurons fire synchronously.
- It is therefore expected that when neurons fire synchronously, the system will reach steady-state much faster than when neurons fire asynchronously.
- We may therefore postulate that synchronous neural firing is, among other things, necessary for a neural network to quickly reach a state of homeostasis.

Motive Power

20



The stationary value of the supplied motive power (as well as the stationary values of the entropy production and heat dissipation rates) is appreciably larger in the case of synchronous neural firings than asynchronous firings.

This difference is well predicted by the theory of dissipative structures according to which self-organization of a system to an ordered internal state requires that the system is sufficiently driven by external sources and dissipates appreciable heat to its surroundings.

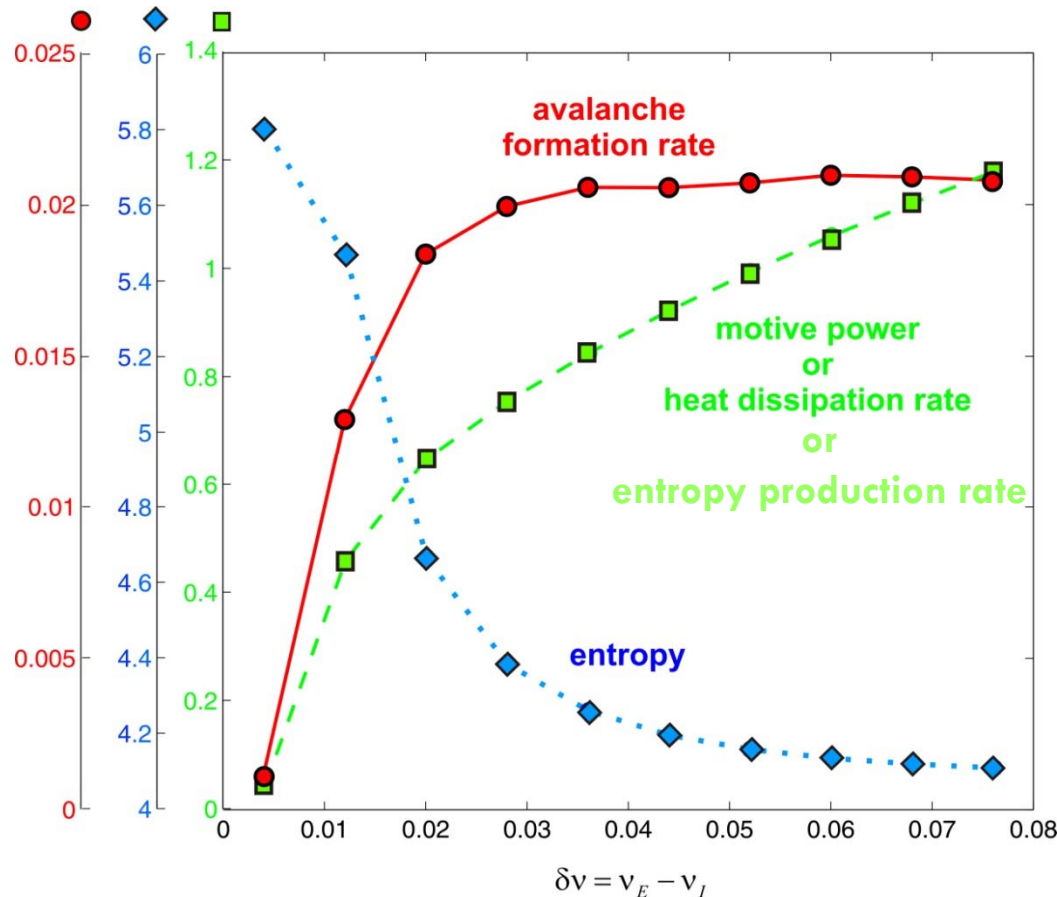
Appreciable amounts of supplied motive power and heat dissipation is required to achieve avalanching behavior, which leads to an ordered stationary state, quantified by a lower entropy.

We may therefore conclude that the emergence of avalanches in a neural network is a consequence of externally driven self-organization accompanied by appreciable heat dissipation.

Self-organization and Avalanching

21

Emergence of avalanches in a neural network is a consequence of externally driven self-organization accompanied by appreciable heat dissipation.



The (average) rate of avalanche formation (number of avalanches per unit time), the supplied motive power (or heat dissipation), and the system entropy at steady-state

Thermodynamic Analysis

22

- Characterize stability, robustness, and critical behavior of a neural network when neurons are removed (or added) from the network.
- Potential energy at steady-state

$$\bar{V}(\mathbf{y}; \Omega) = -\frac{1}{\Omega} \ln \left[\frac{\bar{p}(\mathbf{y}; \Omega)}{\bar{p}(\mathbf{y}_*; \Omega)} \right]$$

- Entropy at steady-state

$$\bar{S}(\Omega) = \mathbb{E}[-\ln \bar{p}(\mathbf{Y}; \Omega)]$$

- The network size Ω is given by

$$\Omega = \frac{L}{L_0}$$

where

$$L_0 \gg 1 \quad (L_0 = 200)$$

Thermodynamic Analysis

23

- Internal potential energy

$$\bar{U}(\Omega) = \Omega \mathbb{E}[\bar{V}(\mathbf{Y}; \Omega)]$$

- Free potential energy

$$\bar{H}(\Omega) = \bar{U}(\Omega) - \bar{S}(\Omega)$$

- Pressure

$$\bar{P}(\Omega) = -\frac{\partial \bar{H}(\Omega)}{\partial \Omega}$$

Measures the portion of energy available in the neural network to do work.

- Bulk modulus

$$\bar{B}(\Omega) = -\Omega \frac{\partial \bar{P}(\Omega)}{\partial \Omega}$$

Quantifies the rate of change in free potential energy w.r.t. a change in the number of nodes.

Measures the network resistance to changing pressure.

Thermodynamic Stability

24

- It turns out that

$$\bar{U}(\Omega) = \Omega \mathbb{E}[\bar{V}(\mathbf{Y}; \Omega)] = \bar{S}(\Omega) + \ln \bar{p}(\mathbf{y}_*; \Omega) = \mathbb{E}[I_{\Omega}(\mathbf{Y}; \Omega)] - I_{\Omega}(\mathbf{y}_*; \Omega)$$

where

$$I(\mathbf{y}; \Omega) = -\ln \bar{p}(\mathbf{y}; \Omega)$$

is the self-information of state \mathbf{y} .

- The self-information quantifies the amount of information associated with the occurrence of state \mathbf{y} at steady-state.

https://en.wikipedia.org/wiki/Information_content

Thermodynamic Stability

25

$$\bar{U}(\Omega) = \Omega E[\bar{V}(\mathbf{Y}; \Omega)] = \bar{S}(\Omega) + \ln \bar{p}(\mathbf{y}_*; \Omega) = E[I_\Omega(\mathbf{Y}; \Omega)] - I_\Omega(\mathbf{y}_*; \Omega)$$

- The internal potential energy measures how far the self-information of the most-likely state is from the expected self-information of all network states (which is the entropy).
- Since

$$\bar{U}(\Omega) = \bar{S}(\Omega) + \ln \bar{p}(\mathbf{y}_*; \Omega) = - \sum_{\mathbf{y}} \bar{p}(\mathbf{y}; \Omega) \ln \bar{p}(\mathbf{y}; \Omega) + \ln[\bar{p}(\mathbf{y}_*; \Omega)],$$

zero internal potential energy is achieved (for $\Omega > 0$) when $\bar{p}(\mathbf{y}_*; \Omega) = 1$, in which case the neural network will be at the most-likely state with probability one.

- We may consider the internal potential energy as a thermodynamic measure of “stability” of a particular ground state of the potential energy landscape, with smaller values indicating increasing thermodynamic stability of that state.

Thermodynamic Robustness

26

$$\bar{P}(\Omega) = -\frac{\partial \bar{H}(\Omega)}{\partial \Omega}$$

- We can use the pressure as a measure of thermodynamic “robustness” of the neural network w.r.t. network size Ω .
- The neural network is “robust” against variations in size if there is no appreciable change in pressure when adding or removing neurons.
- The neural network is “robust” if the derivative

$$\bar{B}(\Omega) = -\Omega \frac{\partial \bar{P}(\Omega)}{\partial \Omega} \quad \text{BULK MODULUS}$$

of the pressure is small.

- A “robust” network resists changes in pressure.

Critical Behavior

27

- We can use the bulk modulus

$$\bar{B}(\Omega) = -\Omega \frac{\partial \bar{P}(\Omega)}{\partial \Omega}$$

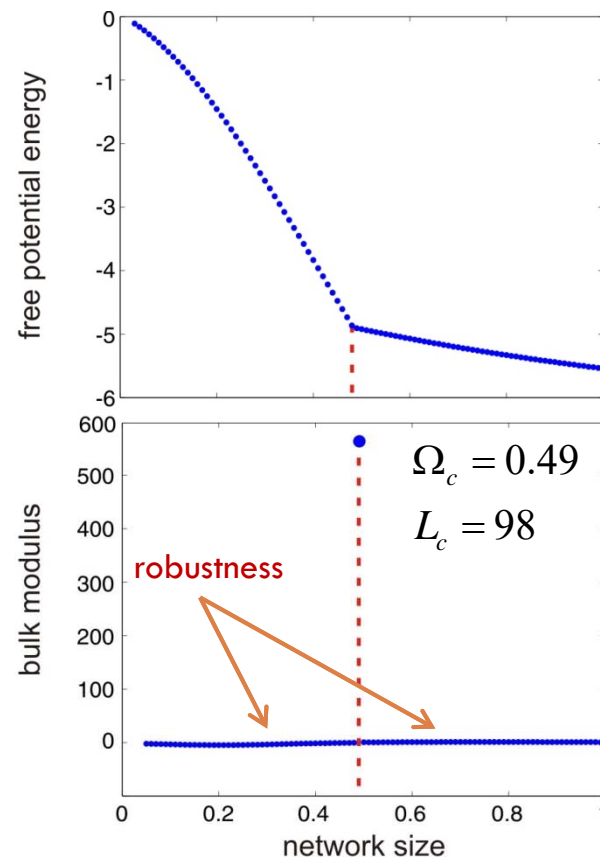
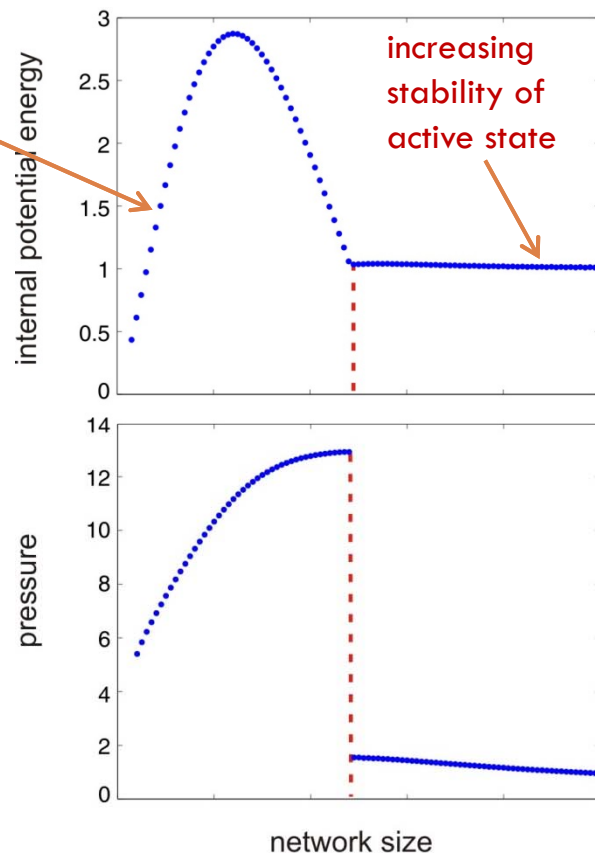
to detect network sizes at which the neural network exhibits critical behavior.

- The bulk modulus may experience a sharp discontinuity as the network size varies past a critical value !
- If the pressure experiences such a discontinuity as the network size varies past a critical value Ω_c , then the bulk modulus will effectively capture this discontinuity by a pulse located at Ω_c .
- This will indicate that the network experiences phase transition at Ω_c .

Thermodynamic Analysis

28

increasing
stability of
inactive state



Thermodynamic Analysis

29

- **What is the underlying cause of this critical behavior?**
- Loss of network robustness near Ω_c indicates that there is a change in the ground state (global minimum) of the stationary potential energy landscape at Ω_c .
- Critical behavior is caused by the ground state changing from (0.5032,0.5032) to (0,0) at $\Omega_c = 0.49$.

Energy Landscape

30



see video-13-1.mov

Energy Landscape

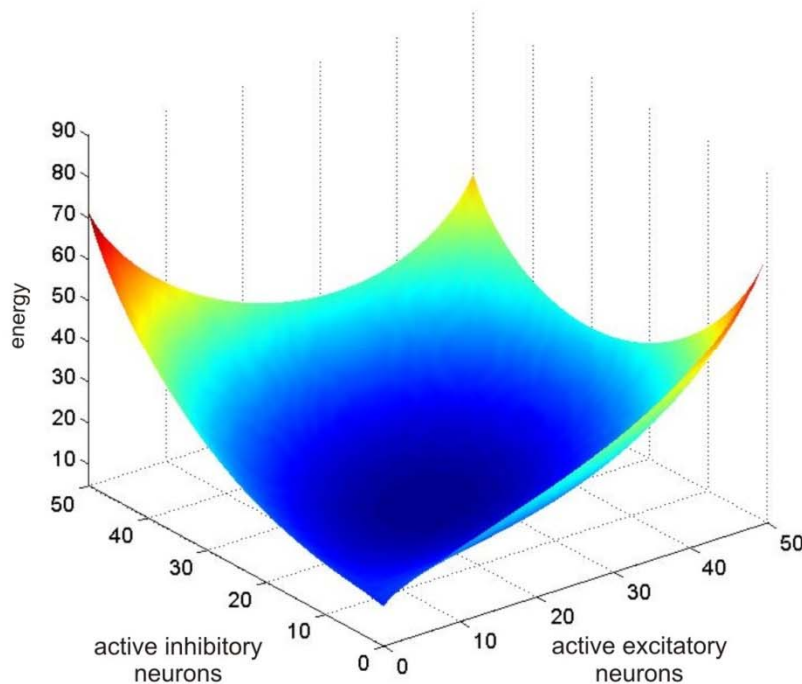
31



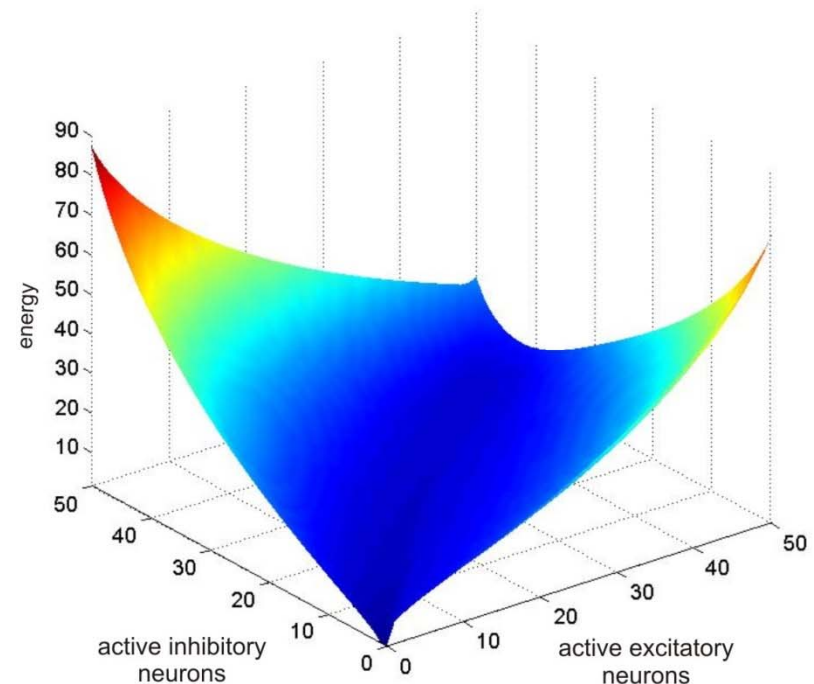
see video-13-2.mov

Energy Landscape

32



ASYNCHRONOUS NEURAL FIRINGS

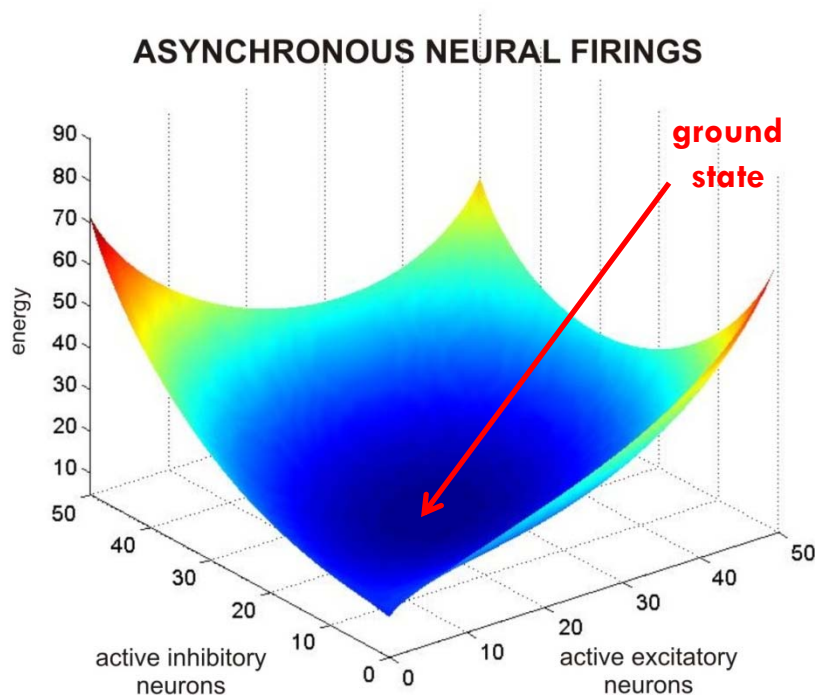


SYNCHRONOUS NEURAL FIRINGS

The stationary dynamics of neural activity may be thought of as a random walk on the energy landscape, where the most likely steps follow a path from higher to lower energy states (i.e., the preference is to move downhill), with occasional (low probability) jumps from lower to higher energy states.

Energy Landscape

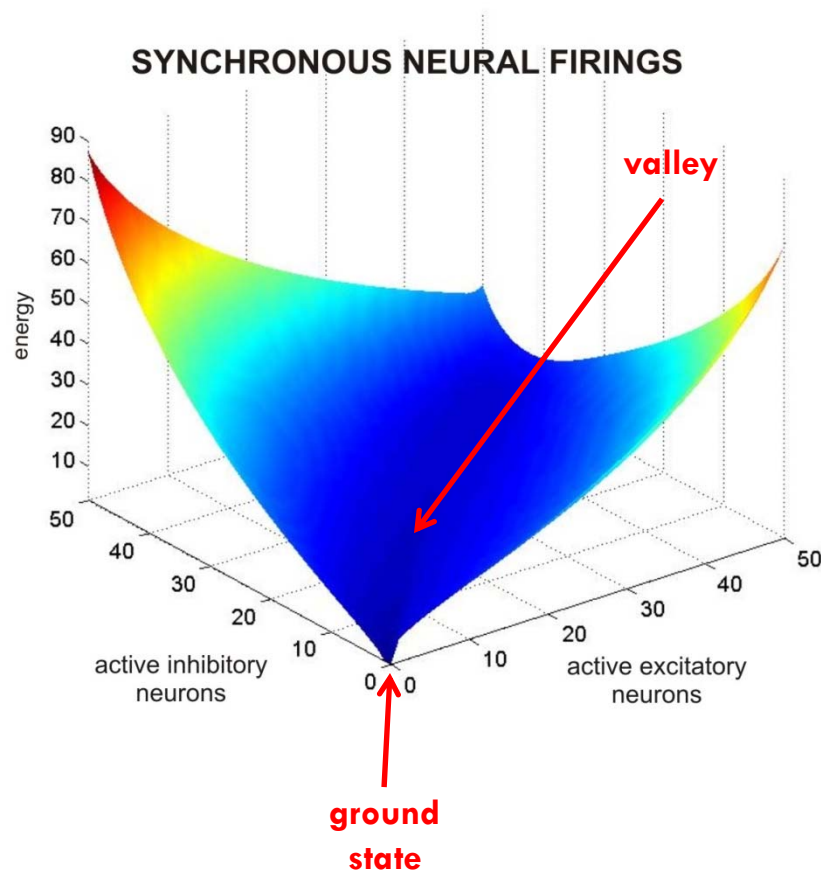
33



- The ground state (global minimum) of the energy landscape occurs away from the origin at which neural activity is zero.
- Consequently, the system spends most time in Gaussian-like fluctuations about the ground state.
- The system can jump out of the energy well surrounding the ground state and reach the origin, but with very small probability, due to its large width.
- Therefore, avalanche formation in this system is a rare event.
- This behavior agrees with a finding that neural networks may simultaneously support synchronous and asynchronous dynamics, switching between these two modes of operation spontaneously.

Energy Landscape

34



- The energy landscape of the system with synchronous neural firings contains a valley along the line $Y_1 = Y_2$ of equal excitatory and inhibitory activities, which slopes down to the ground state that is now located at the origin.
- Thus, from any point on this landscape, the most likely trajectory rolls downhill until it reaches the origin.
- From this point, the dynamics of excitatory and inhibitory neural activities may again reach the valley by randomly jumping away in an uphill motion that overcomes the steep and narrow energy well surrounding the origin.
- This mechanism results in avalanching, which can be thought of as a random sequence of zero (or almost zero) net neural activity at points in the well surrounding the origin followed by nonzero net neural activity at points proximal to the valley.