# Simulation II: Dynamics on Networks
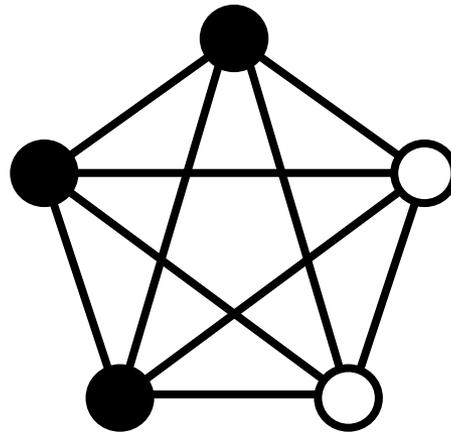
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Dynamics *on* networks

- **Dynamic state changes taking place on a static network topology**
  - Regulatory dynamics on gene/protein networks
  - Population dynamics on ecological networks
  - Disease infection on social networks
  - Information/culture propagation on organizational/social networks

Simple example:
Random walk on a network

- **An agent (or a set of agents) moving on a network**

- **An agent jumps randomly to one of the neighbor nodes at each time step**
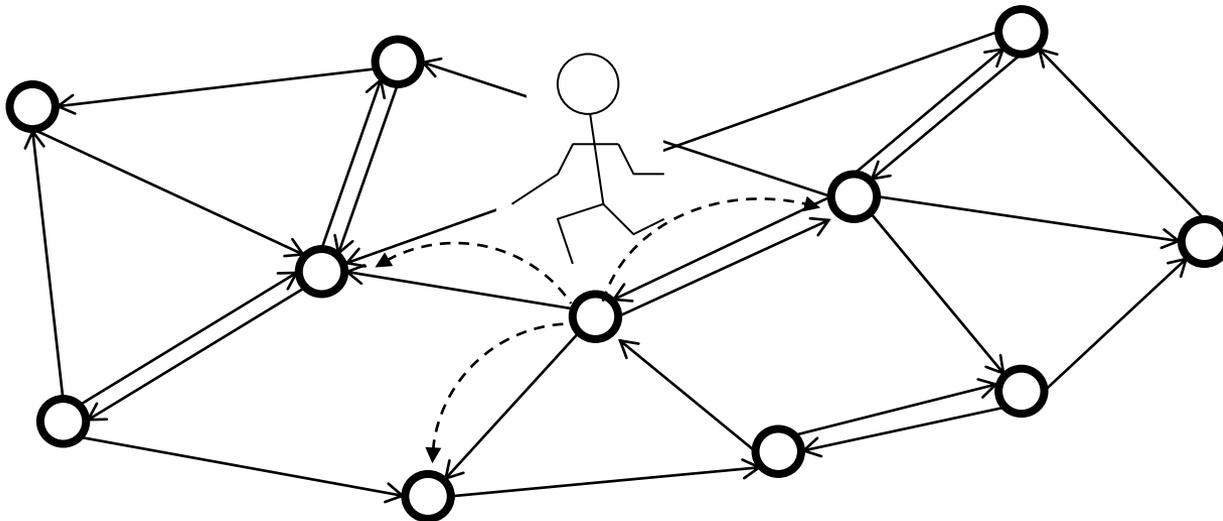
Exercise

- **Simulate random walk of an agent on a directed random network made of 50 nodes**

- **Count how many times each node was visited by the agent over time**

# TPM and asymptotic probability distribution (review)

- $|\lambda| <= 1$ for all eigenvalues

- **If the original network is strongly connected** (with some additional conditions), **the TPM has one and only one eigenvalue 1** (no degeneration)

$\rightarrow$ **This is a unique dominant eigenvalue; the probability vector will converge to its corresponding eigenvector**

Exercise

- **Construct the transition probability matrix of the random network used in the previous exercise**

- **Find its dominant eigenvector with $\lambda = 1$**

- **Compare the results with the previous "counting" results**

Dynamics on Networks with Discrete Node States

Opinion formation (Voter model)

- A simple model of opinion formation in society
  - Opinions = discrete states
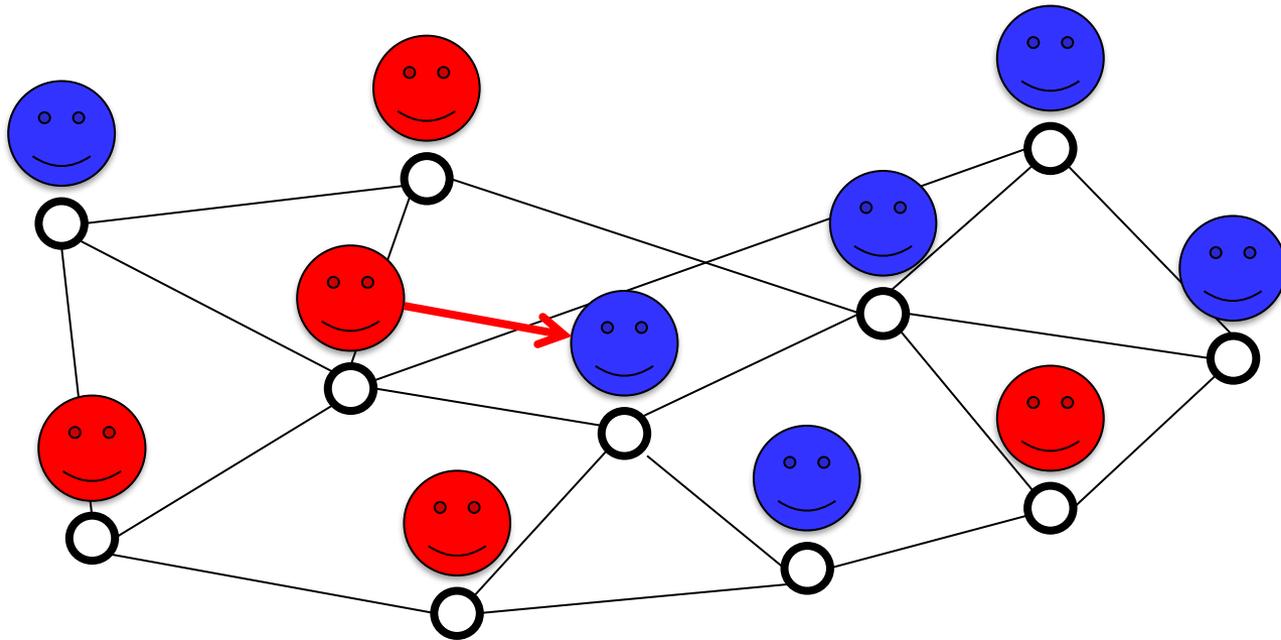
Three versions of voter models

- **Original voter model**
  - A randomly selected node copies the opinion of one of its neighbors
- **Reverse voter model**
  - A randomly selected node "pushes" its opinion into one of its neighbors
- **Link-based voter model**
  - An opinion is copied through a randomly selected link

Exercise

- **Simulate the three different versions of the voter model (original, reverse and link-based) on a Barabasi-Albert scale-free network**

- **Compare the speed of opinion homogenization between the three models**
  - **Why different?**

Epidemics (SIS/SIR model)

- **Initially, a small fraction of nodes are infected by a disease**

- If a susceptible node has an infected neighbor, it will be infected with probability p_i (per infected neighbor)

- An infected node will recover and become susceptible (SIS) or recovered (SIR) with probability p_r

Exercise

- **Study the effects of infection/ recovery probabilities on the fixation of a disease on a random social network**
  - In what condition will the disease remain within society?
  - In what condition will it go away?
 - Is the transition smooth, or sharp?

Exercise

- Do the same experiments with WS small-world networks and BA scale-free networks

- Compare their properties

Cascade of failure

- **Load on a failing node is divided and distributed to its neighbors**
- **If the load exceeds capacity of each node, it causes another node failure**
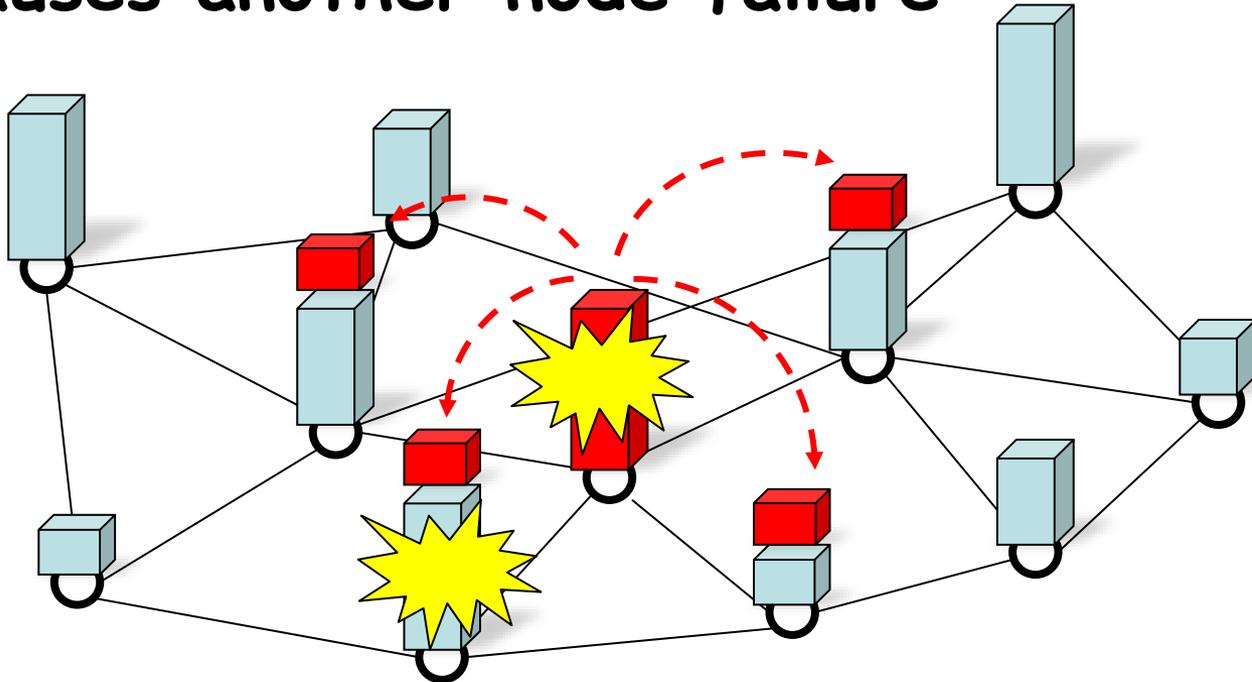
Exercise

- **Simulate a cascade of failure on a scale-free network made of 100 nodes with random node capacities and load assignments**

- **Investigate which node has the most significant impact when it fails**

Hopfield network

Input   Output
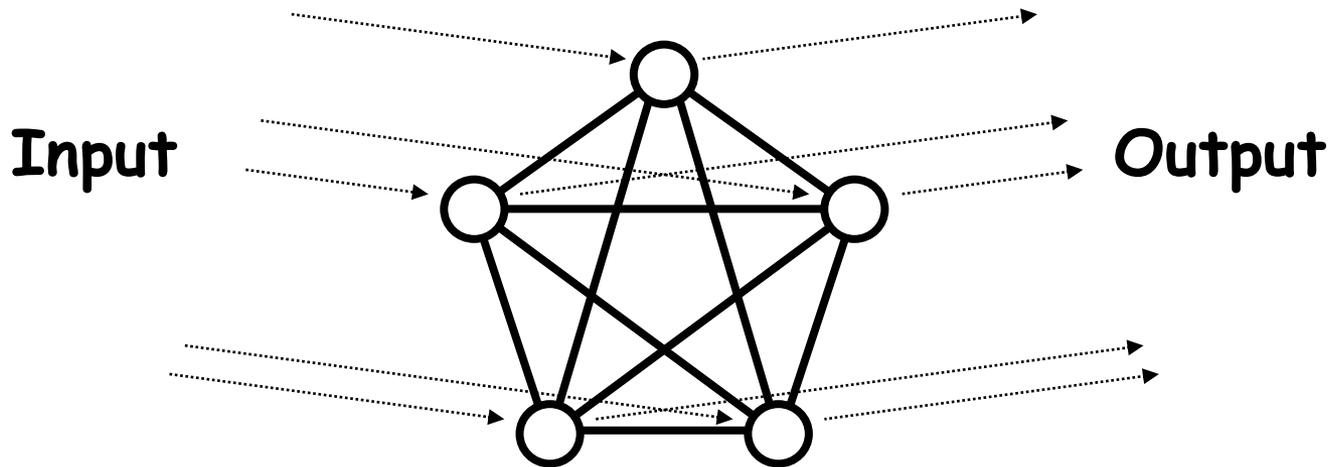
- A.k.a. "attractor network"
- Neurons connected in a shape of an undirected weighted complete graph
- Each neuron takes either 1 or -1, and updates its state in discrete time

State-transition rule

$$s_i(t+1) = \text{sign} \left(\sum_j w_{ij} \, s_j(t) \right)$$

- w_{ij} : connection weight between neuron i and neuron j
- $w_{ij} = w_{ji}$ (symmetric interaction)
- $w_{ii} = 0$ (no feedback to itself)

Setting weights by "imprinting"

$$w_{ij} = \Sigma_k \, s^k_i \, s^k_j$$

- **k** : index of patterns memorized
- s^k_i : state of neuron i in pattern k

  – e.g.

Pattern 1   Pattern 2

2   -2

0
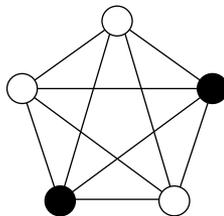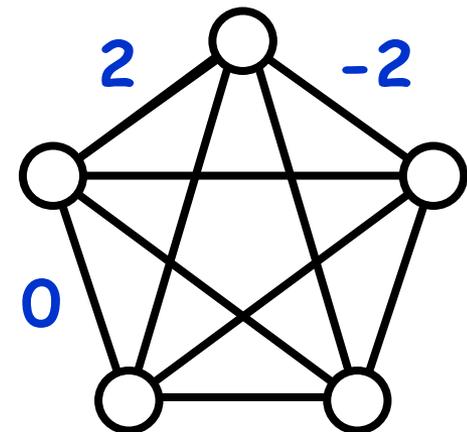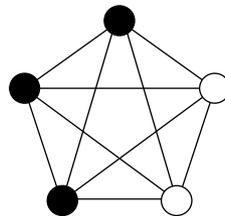
Recovering patterns

- **When started with some initial pattern, the network "remembers" the closest pattern in its memory (or its reversal)**
  - Can be applied to content addressable memory, pattern recognition, etc.

Initial pattern   Memorized pattern

Imprinting   Recovery
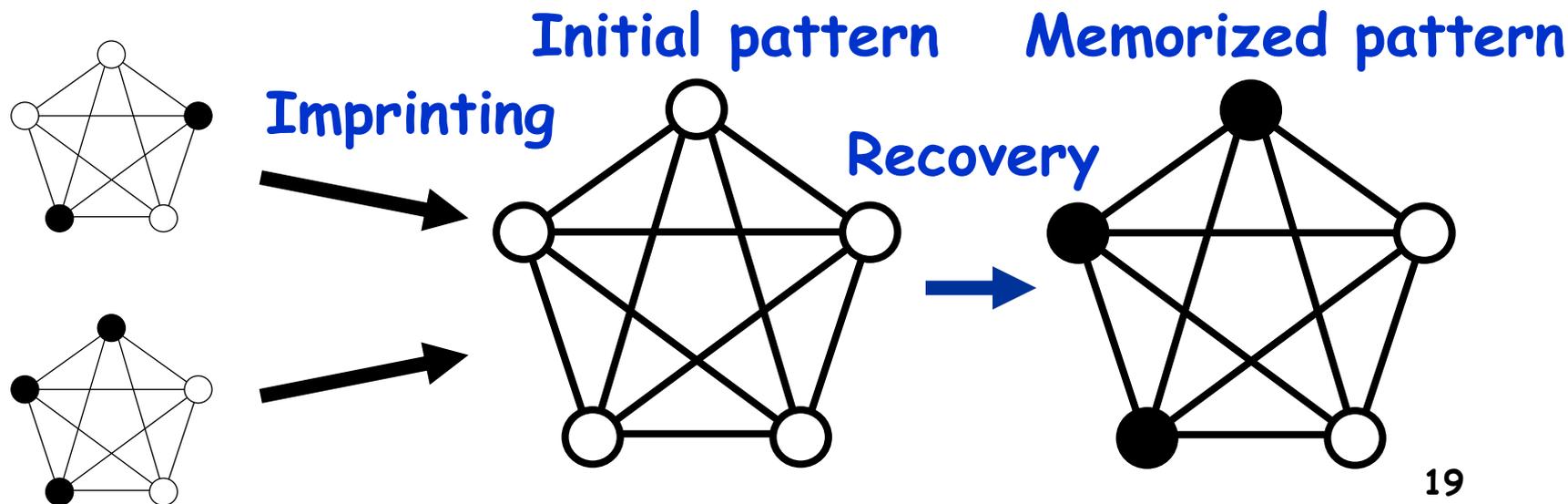
Exercise

- **Simulate the behavior of the following Hopfield network**
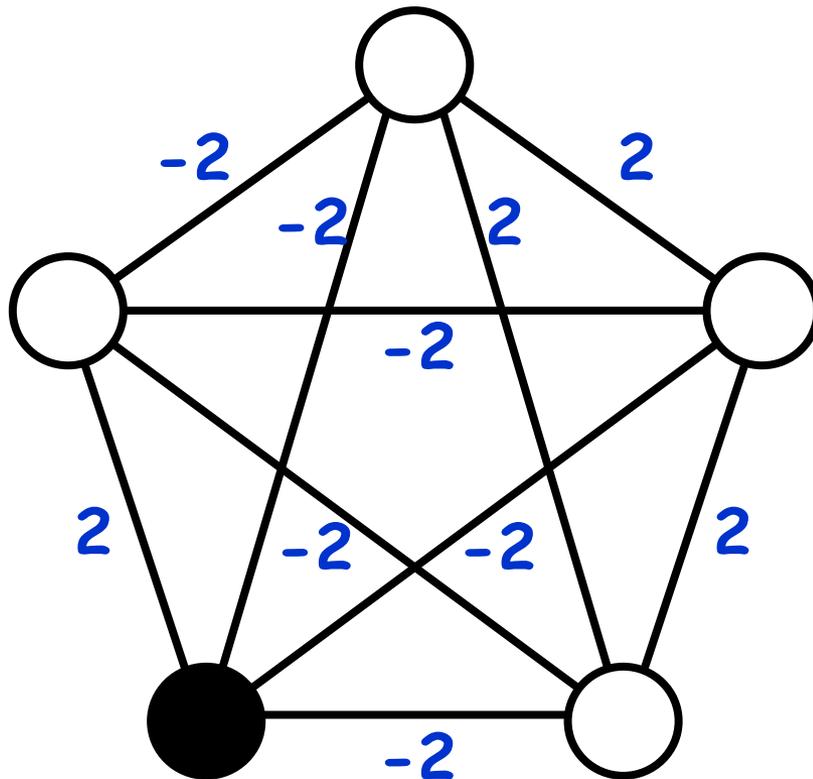
○ : +1

● : -1

2, -2 : weights

Gene regulatory network

- **Each gene is activated or inhibited by other genes**
  - **Forming a network of "logic gates"**
  - **Each gene takes binary state (on/off)**
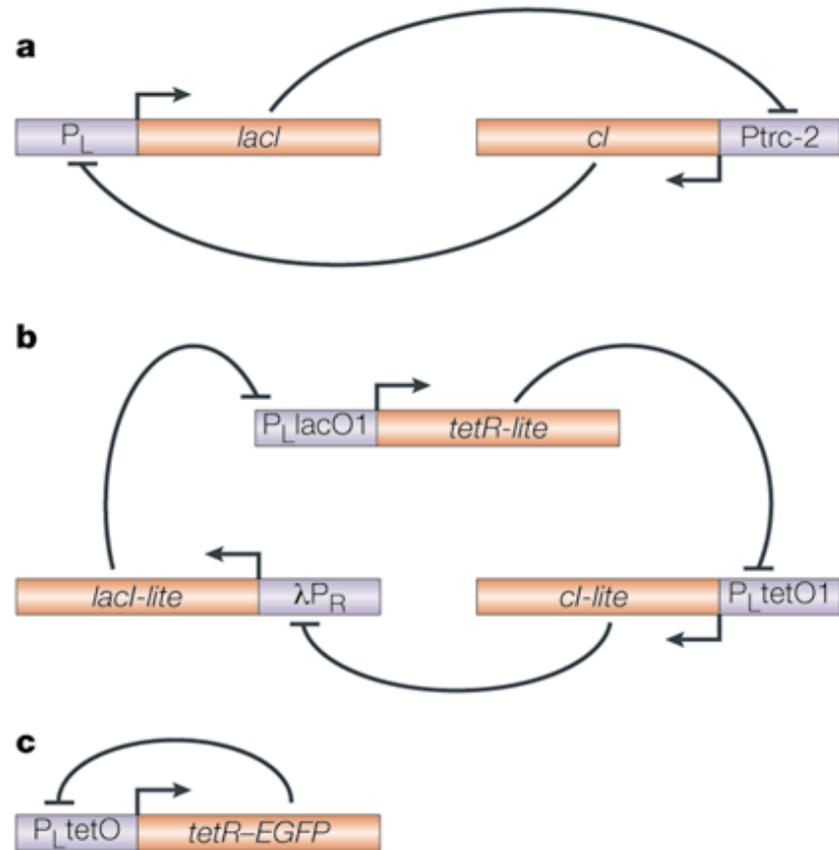
Nature Reviews | Genetics

(from Hasty et al., Nature Reviews Genetics 2, 268-279, 2001)

Boolean network

- **Mathematical abstraction of gene regulatory networks**
  - Binary node states
  - Each node determines next state using its own Boolean state transition function (referring to neighbors' states)
- **Random Boolean network:**
  - Network topology and state transition functions are both randomly generated

Example of transition functions

- 2-input functions ($2^{2^2}=16$ possibilities)

X	Y	Z	Z	Z	Z	Z	Z	Z	Z	Z	Z	Z	Z	Z	Z	Z	Z
0	0	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1
0	1	0	0	1	1	0	0	1	1	0	0	1	1	0	0	1	1
1	0	0	0	0	0	1	1	1	1	0	0	0	0	1	1	1	1
1	1	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1

Kauffman's NK networks

- N: # of nodes
- K: # of inputs to each node
  - Topologies and state-transition functions are both random
  - Similar to, but not the same as, the NK fitness landscape (NK model) often used in mathematical biology and management sciences

NK network's attractors

- **Total # of macro-states: 2^N**
- **The network eventually falls into one of its "attractors"**
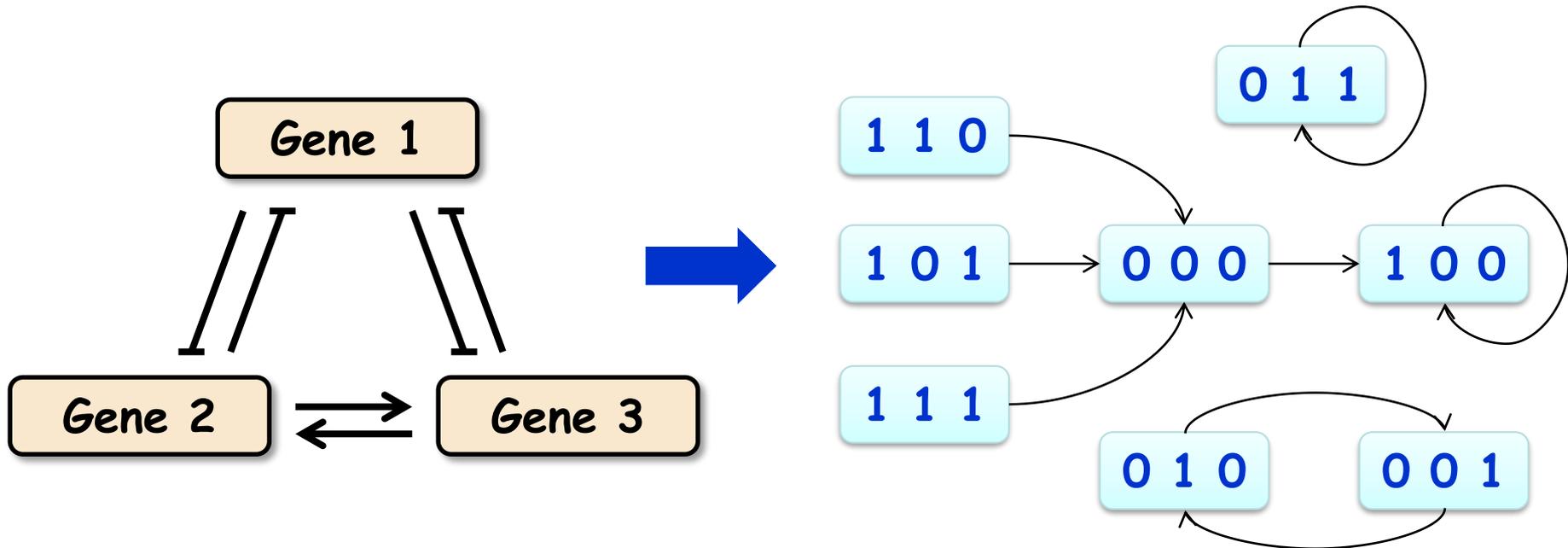
Exercise

- **Create a Python code that generates the NK network's state-transition diagram (i.e., a directed network whose nodes are the network's macro-states)**

- **Count how many attractors exist**

- **Study how # of attractors change when you vary N and K**

Dynamics on Networks with Continuous Node States

Simple diffusion

- **Individually:**

$$\frac{ds_i}{dt} = D \ \Sigma_{j \ in \ N_i} \ (s_j - s_i)$$

- **Collectively (with Laplacian L):**

$$\frac{ds}{dt} = - D \ L \ s$$

Exercise

- **Simulate a diffusion process of continuous node states on a Barabasi-Albert scale-free networks with n = 100 and m = 1**

Exercise

- **Calculate the eigenvalues and eigenvectors of Laplacian matrices of several different network topologies**

- **Interpret their meanings in the context of diffusion**

- **Confirm your interpretation by numerical simulation of the diffusion processes**

Synchronization

- **Linear coupling model:**

$$\frac{ds_i}{dt} = F(s_i) + \Sigma_j \left(c_{ij} \, H(s_j) \right)$$

- $F(s)$: internal dynamics
- $C = (c_{ij})$: coupling matrix
- $H(s)$: output function

  - **If $s_i(t) = s(t)$ for all i, then the network is synchronized**

Synchronization and Laplacian

- **If coupling depends only on the difference of outputs across a link:**

$$\frac{ds_i}{dt} = F(s_i) + \sigma \, \Sigma_{j \text{ in } N_i} \, (H(s_j) - H(s_i))$$

- I.e., $C = -\sigma L$

- Laplacian's "spectral gap" (first non-zero eigenvalue) is critical in determining synchronizability of the network

Exercise

- **Simulate the following nonlinear Kuramoto model:**

$$\frac{ds_i}{dt} = w_i + K/|N_i| \ \Sigma_{j \ in \ N_i} \ sin(s_j - s_i)$$

- w_i: inherent angular velocity
- N_i: neighbors of node I

– **What kind of networks synchronize most easily?**

Exercise

- **Measure and plot the following "phase coherence" in the simulation of the Kuramoto model:**

$$r = \left| \Sigma_j \, e^{i\theta_j} \, / \, n \right|$$

Synchronizability

Synchronizability

- **Synchronizability of a simple coupled dynamical network can be studied by conducting stability analysis**

$$\frac{dx_i}{dt} = R(x_i) + \alpha \sum_{j \in N_i} (H(x_j) - H(x_i))$$

R(x): Local reaction term (homogeneous)
H(x): Output function

Exercise

- **Consider adding a small perturbation to the general solution of the dynamical equation (w/o interactions)**

$$\frac{dx}{dt} = R(x) \quad \rightarrow \quad x_s(t)$$

- **Conduct stability analysis by assuming:**

$$x_i(t) = x_s(t) + \Delta x_i(t)$$

Condition for synchronizability

- **Solution $x_s(t)$ is stable (i.e., the network is synchronized) if**

$$\alpha \, \lambda_i \, H'(x_s(t)) > R'(x_s(t))$$

for all i and t
**(you need to consider only λ_2 and λ_n)**

Exercise

- **Analyze the synchronizability condition of the following coupled oscillator model:**

$$\frac{d\theta_i}{dt} = \beta\theta_i + \alpha \sum_{j \in N_i} (\theta_j - \theta_i)$$

Mean-Field Approximation

Mean-field approximation

- An approximation to **drastically reduce the dimensions of the system** by reformulating the dynamics in terms of "a state of one node" and "the average of all the rest (= mean field)"

MFA

Healthy

A node

Sick
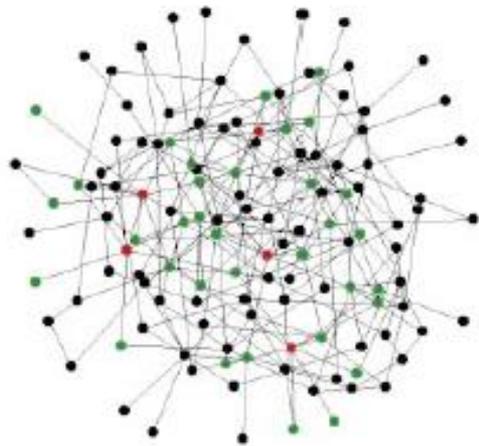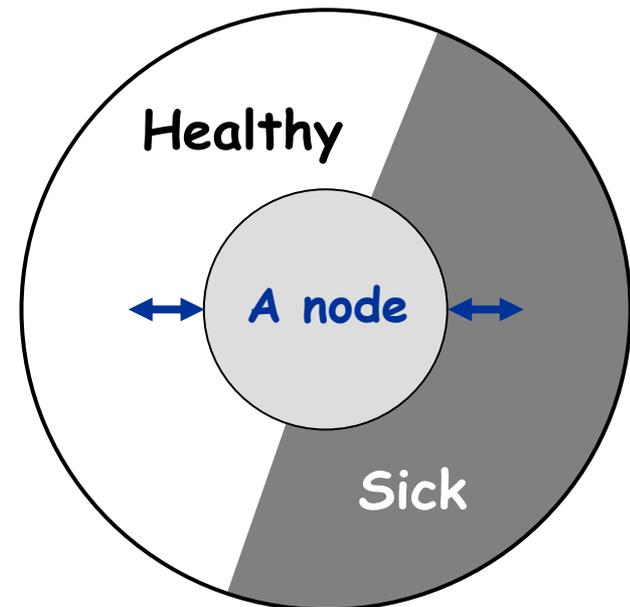
How MFA works
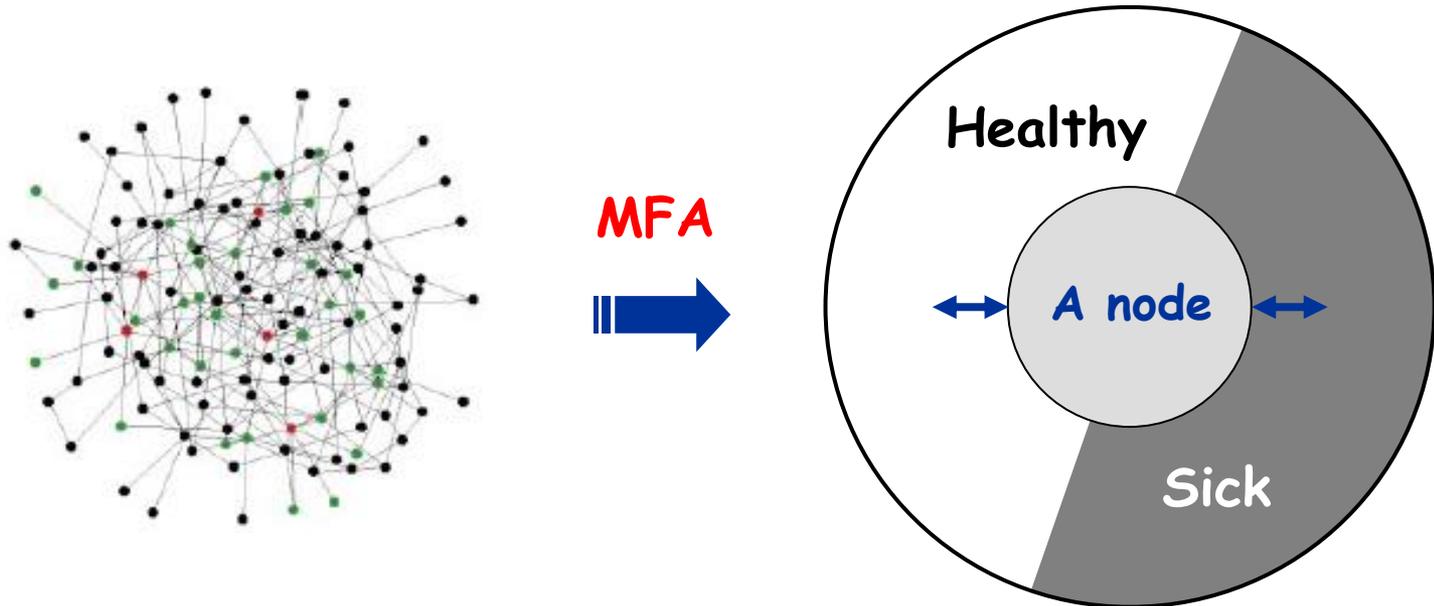
1. Make an approximated description about how one node changes its state through the interaction with **the average of all the rest** (= mean field)
2. Assume that 1. uniformly applies to all the nodes, and analyze **how the mean field itself behaves**

Mathematical description of MFA (difference equations)

- Original equations:

$$x^i_t = F^i(\{ x^i_{t-1} \})$$

- Approximate equations with MFA:

$$x^i_t = F'^i(x^i_{t-1}, <x>_{t-1})$$

$$<x>_t = \Sigma_i \, x^i_{t-1} \, / \, n$$

Each state-transition function
takes only two arguments:
its own state and the "mean field"

Example: SIS on a random network

- **Infection probability p_i**
- **Recovery probability p_r**
- **Edge probability p_e**

- **Write down a difference equation that describes how the probability of infected nodes, q_t (mean field), changes over time**

Example: SIS on a random network

Current state	Next state	Probability of this transition
0 (susceptible)	0 (susceptible)	$(1-q)(1-p_e q p_i)^{n-1}$
0 (susceptible)	1 (infected)	$(1-q)\left(1-(1-p_e q p_i)^{n-1}\right)$
1 (infected)	0 (susceptible)	$q p_r$
1 (infected)	1 (infected)	$q(1-p_r)$

- **Find equilibrium states**
- **Study the stability of those equilibrium points**
  - **When does the equilibrium q = 0 become unstable (i.e., epidemic occurs)?**

Example: SIS on a SF network

- **Infection probability** p_i
- **Recovery probability** p_r
- **Degree distribution** $P(k)$

- **Write down a difference equation that describes how the probability of infected nodes with degree k, $q_t(k)$ (many mean fields), changes over time**

Degree-dependent infection

- **Probability for a node with degree k to get infected from its neighbor:**

$$\sum_{k'} P_n(k'|k)q(k')p_i$$

Pn : neighbor degree probability distribution
If the network is nonassortative:

$$P_n(k') = \frac{k'}{\langle k \rangle}P(k')$$

FYI: Friendship paradox

- "Your friends have more friends than you do, on average"

$$\sum_{k'} k' P_n(k') = \sum_{k'} \frac{k'^2 P(k')}{\langle k \rangle} = \frac{\langle k^2 \rangle}{\langle k \rangle}$$

$$= \frac{\langle k \rangle^2 + \sigma(k)^2}{\langle k \rangle} = \langle k \rangle + \frac{\sigma(k)^2}{\langle k \rangle}$$

Calculation...

Current state	Next state	Probability of this transition
0 (susceptible)	0 (susceptible)	$(1 - q(k)) \left(1 - \sum_{k'} \frac{k'}{\langle k \rangle} P(k') q(k') p_i \right)^k$
0 (susceptible)	1 (infected)	$(1 - q(k)) \left(1 - \left(1 - \sum_{k'} \frac{k'}{\langle k \rangle} P(k') q(k') p_i \right)^k \right)$
1 (infected)	0 (susceptible)	$q(k) p_r$
1 (infected)	1 (infected)	$q(k)(1 - p_r)$

$$q_{t+1}(k) = (1 - q(k)) \left(1 - \left(1 - \sum_{k'} \frac{k'}{\langle k \rangle} P(k') q(k') p_i \right)^k \right) + q(k)(1 - p_r)$$

$$= (1 - q(k)) \left(1 - (1 - q_n p_i)^k \right) + q(k)(1 - p_r),$$

$$q_n = \frac{\sum_{k'} k' P(k') q(k')}{\langle k \rangle}$$

Calculation...

$$q_{t+1}(k) = (1 - q(k))\left(1 - (1 - kq_np_i)\right) + q(k)(1 - p_r)$$
$$= (1 - q(k))kq_np_i + q(k) - q(k)p_r = f(q(k))$$

$$q_{\text{eq}}(k) = \frac{kq_np_i}{kq_np_i + p_r}$$

With this:

$$q_n = \frac{1}{\langle k \rangle} \sum_{k'} k'P(k')\frac{k'q_np_i}{k'q_np_i + p_r}$$

Calculation...

$$q_n = \frac{1}{\langle k \rangle} \sum_{k'} k' P(k') \frac{k' q_n p_i}{k' q_n p_i + p_r}$$

- For BA SF networks, this becomes:

$$q_n = \frac{1}{2m} \sum_{k'=m}^{\infty} k' \cdot 2m^2 k'^{-3} \frac{k' q_n p_i}{k' q_n p_i + p_r},$$

$$1 = m p_i \sum_{k'=m}^{\infty} \frac{1}{k'(k' q_n p_i + p_r)}.$$

$$q_n \approx \frac{p_r}{(e^{\frac{p_r}{m p_i}} - 1) m p_i}$$

Calculation…

- Final stability analysis:

$$\frac{df(q(k))}{dq(k)}\bigg|_{q(k)=\frac{kq_np_i}{kq_np_i+p_r}} = -kq_np_i + \frac{p_r}{kq_np_i+p_r}\frac{k^2P(k)p_i}{\langle k\rangle} + 1 - p_r = r(k)$$

$$r(k) = -k\frac{p_r}{(e^{\frac{p_r}{mp_i}}-1)mp_i}p_i + \frac{p_r}{k\frac{p_r}{(e^{\frac{p_r}{mp_i}}-1)mp_i}p_i + p_r}\frac{k^2 \cdot 2m^2k^{-3}p_i}{2m} + 1 - p_r$$

$$= -\frac{kp_r}{(e^{\frac{p_r}{mp_i}}-1)m} + \frac{mp_i}{\frac{k^2}{(e^{\frac{p_r}{mp_i}}-1)m}+k} + 1 - p_r$$

Conclusion

- **If $p_i \to 0$:**

$$\lim_{p_i \to 0} r(k) = -\frac{kp_r}{\left(\left[e^{\frac{p_r}{mp_i}} \to \infty\right] - 1\right)m} + \frac{m\left[p_i \to 0\right]}{\frac{k^2}{\left(\left[e^{\frac{p_r}{mp_i}} \to \infty\right] - 1\right)m} + k} + 1 - p_r$$

$$= 1 - p_r$$

- **Since 0 < 1 − p_r < 1, the non-zero equilibrium state (i.e., epidemic) is still stable even if $p_i \to 0$ on scale-free networks!!**

Take-home lesson

- **Dynamics on networks can be influenced significantly by network topology**