TBT4165: Expressions / Formulae to know

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- Adjacency matrix $A = [a_{ij}]$, where

$$a_{ij} = \begin{cases} 1 & \text{if there's a link } \textit{from} \text{ node } i \text{ to } j \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

- The total number of links is determined as

$$M = \frac{1}{2} \sum_{i=1,j=1}^{N} a_{ij} \tag{2}$$

- The average number of links per node:

$$\langle k \rangle = \frac{2M}{N} \tag{3}$$

  with a maximum value of $\langle k \rangle = N - 1$.

- The degree of a node i.

$$k_i = \sum_{j=1}^{N} a_{ij} = \sum_{j=1}^{N} a_{ji}. \tag{4}$$

  This expression is valid for undirected (symmetric) network. Also understand how this changes when the network is directed.

- Degree distribution:

$$P(k) = \frac{n_k}{N} = \frac{1}{N} \sum_{i=1}^{N} \delta_{k_i,k}, \tag{5}$$

  where n_k is the number of nodes with degree k.

- The clustering coefficient C_i:

$$C_i = \frac{\text{number of actual connections between neighbors}}{\text{number of possible connections between neighbors}}$$

and also:

$$C_i \;=\; \frac{2\Delta_i}{k_i(k_i-1)} \;=\; \frac{1}{k_i(k_i-1)} \sum_{j=1,l=1}^{N} a_{ij} a_{jl} a_{li}, \tag{6}$$

where Δ_i is the number of triangles for which node i is part of.

- Neighborhood connectivity of a node, defined as:

$$k_{nn,i} = \frac{1}{k_i} \sum_j k_j a_{ij}, \tag{7}$$

where index nn denotes "nearest neighbor."

- Node strength s_i:

$$s_i \;=\; \sum_{j=1}^{N} a_{ij} |w_{ij}|, \tag{8}$$

where $|w_{ij}|$ is the absolute value of the strength (weight) of the link between nodes i and j.

- Average link weight $\langle w \rangle$:

$$\langle w \rangle \;=\; \frac{1}{2M} \sum_{ij} a_{ij} |w_{ij}| \tag{9}$$

- Weighted clustering coefficient:

$$c_i^w \;=\; \frac{1}{s_i(k_i-1)} \sum_{j,l=1}^{N} \frac{|w_{ij}| + |w_{il}|}{2} a_{ij} a_{jl} a_{li} \tag{10}$$

- Weighted neighborhood connectivity:

$$k_{nn,i}^w \;=\; \frac{1}{s_i} \sum_j \; a_{ij} |w_{ij}| k_j \tag{11}$$

- Binomial distribution:

$$P(k) \;=\; \binom{N-1}{k} p^k (1-p)^{N-1-k} \tag{12}$$

- Linear preferential attachment probability $\Pi(k_i)$:

$$\Pi(k_i) \;=\; \frac{k_i}{\sum_{j=1}^{N} k_j} \tag{13}$$

- Measure of network modularity Q:

$$Q = \frac{1}{2M} \sum_{ij} \left(a_{ij} - \frac{k_i k_j}{2M} \right) \delta_{g_i, g_j}, \tag{14}$$

where the group membership of node i is denoted by g_i, and the delta function is 1 only if nodes i and j belong to the same group, otherwise it is zero.

- SI-model:

$$\frac{ds}{dt} = -\beta\ s\ x, \tag{15}$$
$$\frac{dx}{dt} = \beta\ s\ x, \tag{16}$$

where $s = S/N$ the fraction of susceptible nodes, and $x = X/N$ the fraction of infected nodes.

- SIR-model:

$$\frac{ds}{dt} = -\beta\ s\ x, \tag{17}$$
$$\frac{dx}{dt} = \beta\ s\ x - \gamma x, \tag{18}$$
$$\frac{dr}{dt} = \gamma x, \tag{19}$$

with $r = R/N$ the fraction of recovered individuals.

- SIS-model:

$$\frac{ds}{dt} = \gamma x - \beta\ s\ x, \tag{20}$$
$$\frac{dx}{dt} = \beta\ s\ x - \gamma x. \tag{21}$$

with the conservation criterion that $s + x = 1$.

- TO - topological overlap - the fraction of nearest neighbor nodes *shared* by two nodes i and j:

$$w_{ij}^{TO} = \frac{\sum_k a_{ik} a_{kj} \ + \ a_{ij}}{\min(k_i, k_j) \ + \ 1 \ - \ |a_{ij}|} \tag{22}$$

Note that w_{ij}^{TO} takes values from zero to 1, and that the last two terms in the denominator ensures that $w_{ij}^{TO} = 1$ only when there is a direct link between nodes i and j. Also, any pair of nodes i and j with a distance $L(i,j) \geq 3$ will have $w_{ij}^{TO} = 0$.

- Weighted TO: For the case when links contain a strength value $w_{ij} \in [0, 1]$, we may generalize the expression to

$$w_{ij}^{wTO} \;=\; \frac{\sum_k w_{ik} w_{kj} a_{ik} a_{kj} \;+\; w_{ij} a_{ij}}{\min(s_i, s_j) \;+\; 1 \;-\; |w_{ij} a_{ij}|}. \tag{23}$$

- The change in a metabolite's concentration:

$$\frac{dM_i}{dt} \;=\; \sum_{j=1}^{n} S_{ij} \nu_j. \tag{24}$$

Here, ν_j corresponds to the metabolic flux through reaction j, and S is the stoichiometric matrix. Apply steady-state approximation, and it turns into:

$$\sum_{j=1}^{n} S_{ij} \nu_j \;=\; 0. \tag{25}$$

- Shadow price:

$$\pi_i \;=\; -\frac{\partial Z}{\partial b_i}, \tag{26}$$

where Z is the objective function and b_i is a bound value.

- PhPP analysis: We determine the phenotypic phase plane analysis (PhPP) and the properties of the different phases by calculating

$$\alpha \;=\; -\frac{\pi_x}{\pi_y}, \tag{27}$$

the ratio between the shadow prices associated with the two single source uptake fluxes x and y.