Using Cooccurrance Networks

Jim Brunner

Los Alamos National Laboratory

Coincidence Network

Constructing a coincidence network. I map the abundances according to

$$a(r_{ji}) = \begin{cases} \left\lfloor \left(\frac{r_{ji}}{\max_{s_k}(r_{jk})} \right) n \right\rfloor + 1 & \frac{r_{ji}}{\max_{s_k}(r_{jk})} \ge m \\ 0 & \frac{r_{ji}}{\max_{s_k}(r_{jk})} < m \end{cases}$$

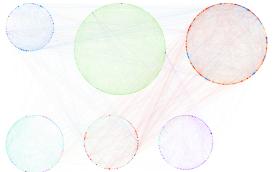
into "bins" relative to the maximum that taxa appears. Then count

$$w_{jk}^1 = \frac{\|\{i : a(r_{ji}) = a(r_{ki}) \neq 0\}\|}{S}$$

how often two organisms appear in the same bin.

Cooccurrance Network

Same idea but now edges weights are compared to a random graph (null model). So we only keep edges that have a higher than "random" weight.



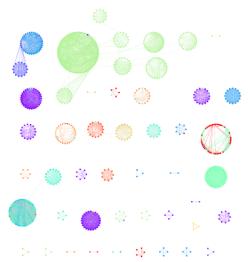
Cooccurrance Network - Pearson Correlation

We can also compute the Pearson correlation coefficient between taxa across the samples.

$$\rho_{xy} = \frac{1}{N} \frac{(\boldsymbol{x} - \mu_x \mathbf{1}) \cdot (\boldsymbol{y} - \mu_y \mathbf{1})}{\sigma_x \sigma_y}$$

Then, we keep an edge if $\rho > 0.8$ and p < 0.05, where p is the chance of correlation higher than ρ_{xy} in a random model. The random model assigns abundances as a binomial with parameters determined by sample and taxa. The p values are calculated using a Monte Carlo simulation with 1000 trials. The species level network using this method had $\sim 1/2$ as many edges.

Cooccurrance Network - Pearson Correlation





Brunner

Clustering

We can cluster the network to attempt to determine or evaluate meaningful groups of taxa.

- Community clustering
 - Minimize a function based on "edge betweeness". Determines edges that are between clusters.
- Spectral clustering
 - Performs a random walk on the network.

Analyzing a sample

- Filter GOTTCHA results try to determine probability of seeing groups of organisms Random Markov Field
- Diffusion on graph

$$\frac{\partial}{\partial t}u(v,t) = -Lu(v,t)$$

where v takes values in the vertex set of the graph. Then, we can encode "known" information in three ways: initial values, boundary values, or a forcing vector.

Analyzing a sample - Diffusion Process

$$\frac{\partial}{\partial t}u(v,t) = -Lu(v,t)$$

where v takes values in the vertex set of the graph. Then, we can encode sample information in three ways: initial values, boundary values, or a forcing vector.

Related to spectral clustering - spectral clustering groups by "distance" in firsk k eigenmodes of diffusion process. This process gives "distance" in weighted sum of eigenmodes of diffusion process.

Highest ranked nodes are "closest" to the sample data

□ ► ←□ ► ←□ ► ←□ ► ←□ ←□ 8/23

Initial Values

Initial Value Problem

Let $u_i(t)$ be the solution at node v_i to the discrete diffusion problem

$$\frac{d}{dt}\boldsymbol{u}(t) = -L\boldsymbol{u}$$

where L is the graph laplacian with initial conditions determined by sample information.

Then, if K is the information "known" from the sample and the values of v_k and v_l are unknown,

$$\int_0^\infty u_k(t)dt - \int_0^\infty u_l(t)dt > 0 \Rightarrow P(v_k = 1|\mathbf{K}) > P(v_l = 1|\mathbf{K})$$

Boundary Values

Boundary Value Problem

Let $u_i(t)$ be the solution at node v_i to the discrete diffusion problem

$$\frac{d}{dt}\boldsymbol{u}(t) = -L\boldsymbol{u}$$

where L is the graph laplacian with fixed values (which can be regarded as boundary values) $u_i = 1$ if node v_i is known to be "on", $u_i = 0$ if v_i is known to be "off".

Then, if **K** is the information "known" and the values of v_k and v_l are unknown, and $\tilde{\boldsymbol{u}}$ is the equilibrium solution to the diffusion problem,

$$\tilde{u}_k dt > \tilde{u}_l \Leftrightarrow P(v_k = 1 | \mathbf{K}) > P(v_l = 1 | \mathbf{K})$$

□ ► ←□ ► ←□ ► ←□ ► ←□ ←□ 10/23

Forcing Function

Forced Problem

Let $u_i(t)$ be the solution at node v_i to the discrete diffusion problem

$$\frac{d}{dt}\boldsymbol{u}(t) = -L\boldsymbol{u} + f$$

where L is the graph laplacian and f a forcing vector with $f_i = \alpha_{cc}$ if node v_i is known to be "on", $f_i = -\beta_{cc}$ if v_i is known to be "off", where cc denotes a connected component of the graph. We choose α_{cc} and β_{cc} so that on any connected component cc, $\sum \alpha_{cc} = \sum \beta_{cc} = 1$. Then, if **K** is the information "known" and the values of v_k and v_l are unknown, and \tilde{u} is the equilibrium solution to the diffusion problem,

$$\tilde{u}_k dt > \tilde{u}_l \Leftrightarrow P(v_k = 1 | \mathbf{K}) > P(v_l = 1 | \mathbf{K})$$

Small Network Examples

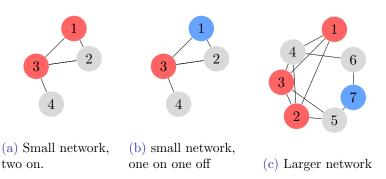


Figure: Test networks. Gray nodes were "unknown", blue nodes "off", and red "on".

Small Network Examples

Configuration	Method	Ranking	Ties
(a) Small Network, two on.	IVP	2, 4	none
	BVP	4, 2	4, 2
	Forcing	2, 4	none
(b) Small Network, one on one off	IVP	4, 2	none
	BVP	4, 2	none
	Forcing	4, 2	none
(c) Larger network	IVP	4, 5, 6	none
	BVP	4, 5, 6	none
	Forcing	4, 5, 6	none

LANL

Brunner
Using Cooccurrance Networks

Network Examples

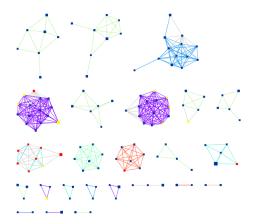


Figure: The "known" set - blue is off and red is on, while yellow is unknown. ◆ロ → ◆母 → ◆ き → を ● り へ ○

Brunner

Network Examples

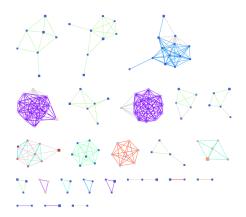


Figure: Result of initial value problem, with all nodes analyzed.

Hotter colors indicate higher likelihood.

Brunner
Using Cooccurrance Networks

Network Examples

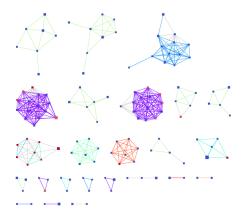


Figure: Result of boundary value problem. Hotter colors indicate higher likelihood, with red indicating assumed "on".

Brunner

Given a sample, we get ranking from a network N_j . Let $r^j(s)$ be the ranking given by diffusion on network j. Then,

$$F_j(s) = F(s, r^j(s)) = \sum_{i=1}^n c^{r_i^j} \frac{s_i}{\|s\|_1}$$

and we can attempt to optimize over the networks we have (if there's only a few that's easy). The conjecture is then

Conjecture

Assume that $F_j(s) > F_k(s)$. Then $P(s|N_j) > P(s|N_k)$.

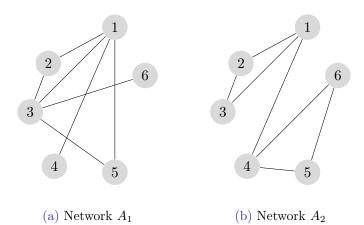
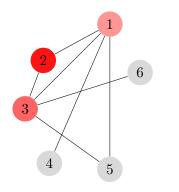
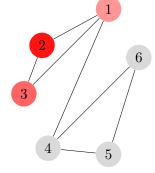


Figure: Test Networks

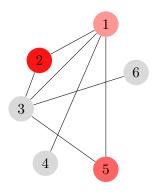


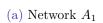


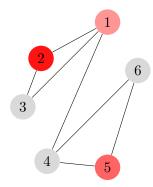
(a) Network A_1

(b) Network A_2

Figure: "Sample" $u_1 = (1/6, 1/2, 1/3, 0, 0, 0)$



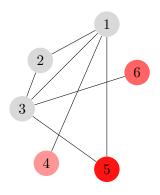


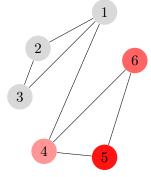


(b) Network A_2

Figure: "Sample" $u_2 = (1/6, 1/2, 0, 0, 1/3, 0)$

◆□ ► ◆□ ► ◆□ ► □ ● ◆○ ○ 20/23



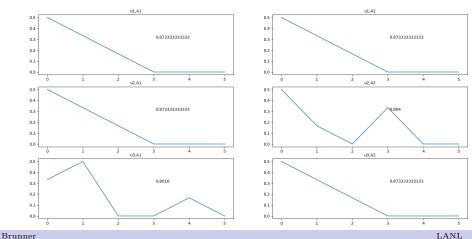


(a) Network A_1

(b) Network A_2

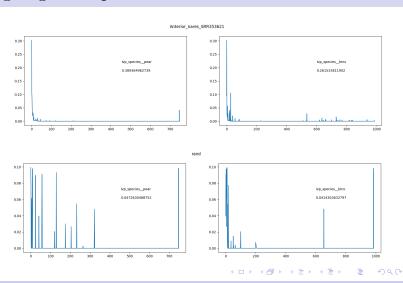
Figure: "Sample" $u_3 = (0, 0, 0, \frac{1}{6}, \frac{1}{2}, \frac{1}{3})$

Abundance v Rank



Using Cooccurrance Networks

LANL



Brunner

LANL