Spectral method for finding dominant graph structures: from undirected to directed graphs

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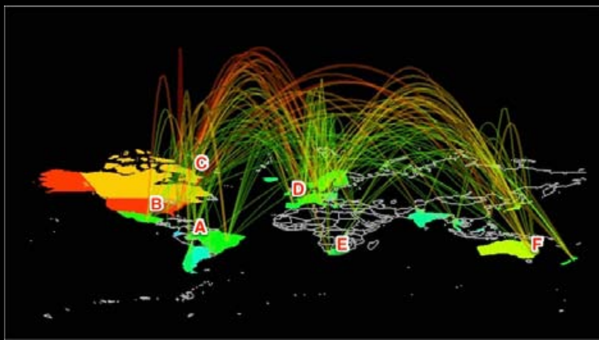
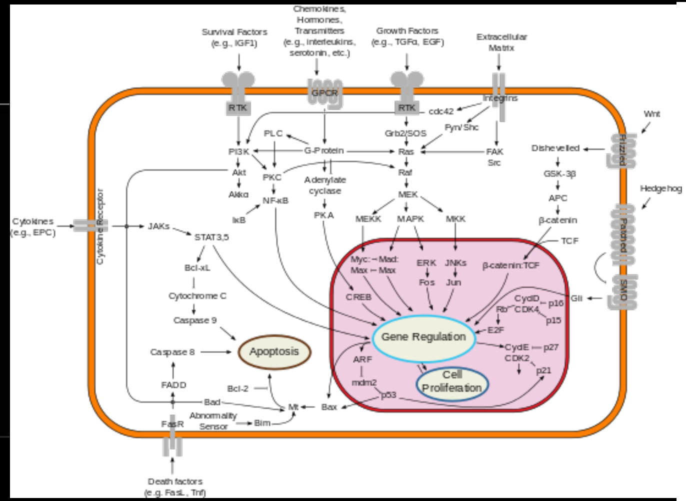
joint work with Marcus Weber and Christof Schütte

Spectra of graphs and applications 2016

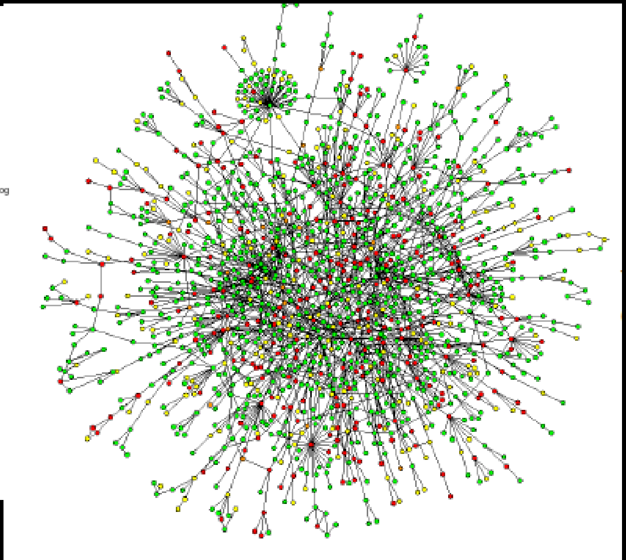
20.05.2016 Belgrade



Internet (www.cellbiol.com)



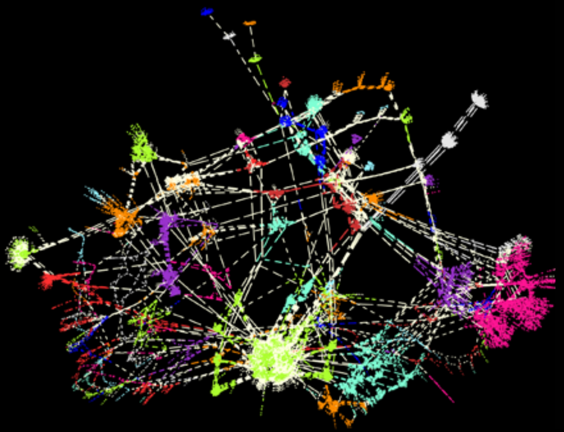
Metabolic network
www.wikipedia.com



Map of yeast protein-protein interactions,
by Hawoong Jeong

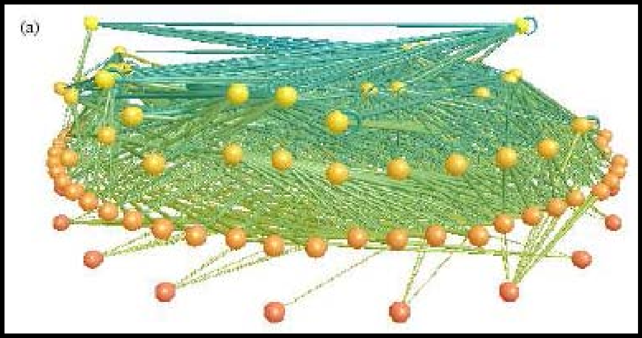
Networks describe a wide range of complex systems in various fields. Understanding the behavior of complex systems starts with understanding the topology of corresponding networks.

Social network
(http://www.facebook.com)



Transportation network

Human brain network
(www.sciencephoto.com)

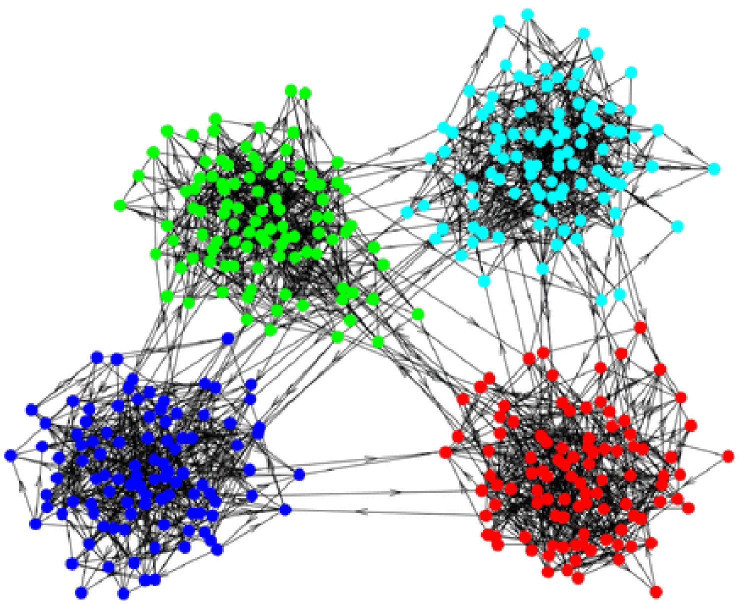


Food Web (http://www.foodwebs.org)

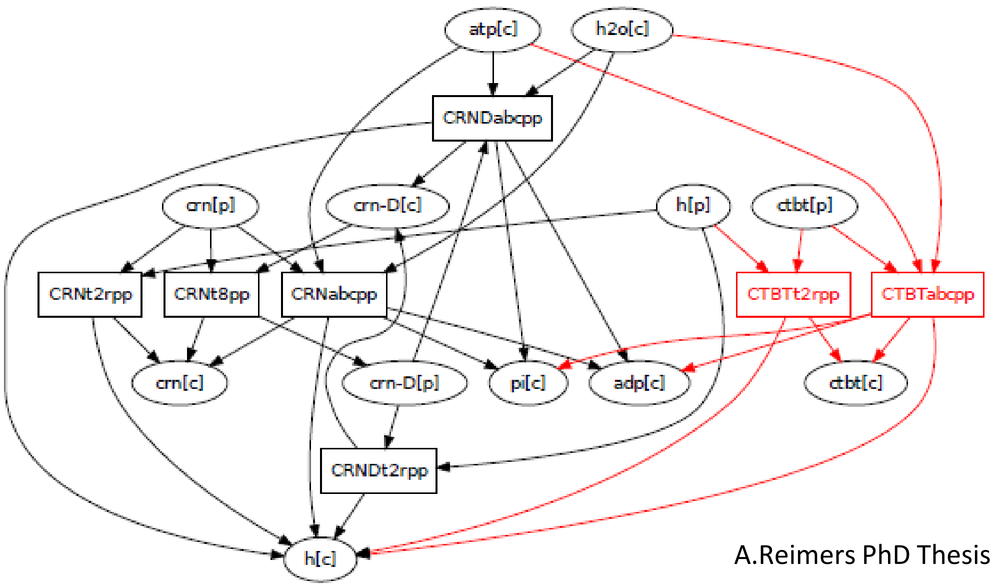
Finding dominant structures

<u>Graph theory:</u> **Modules (communities, clusters)** are densely connected subgraphs that are loosely interconnected with the rest of the network.

<u>Applications:</u> Groups of nodes which share common properties in the system.
→**Biological systems: functional units (protein complexes, biochemical pathways)**



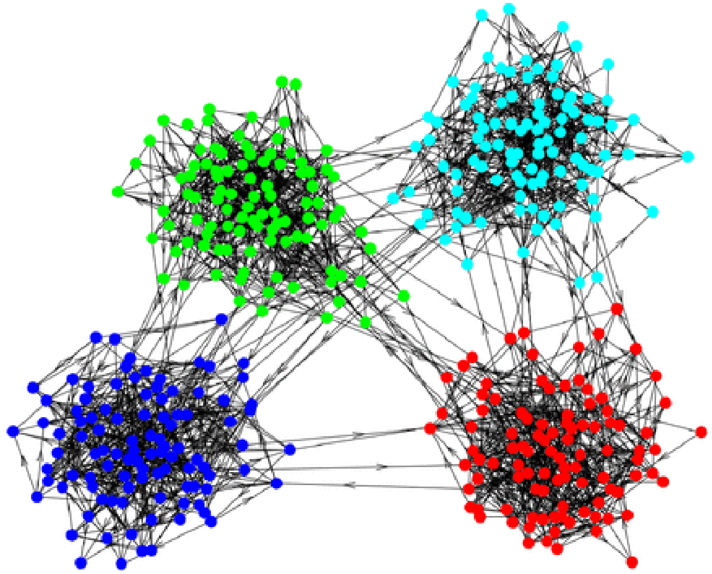
Beber et al. 2012 Interface



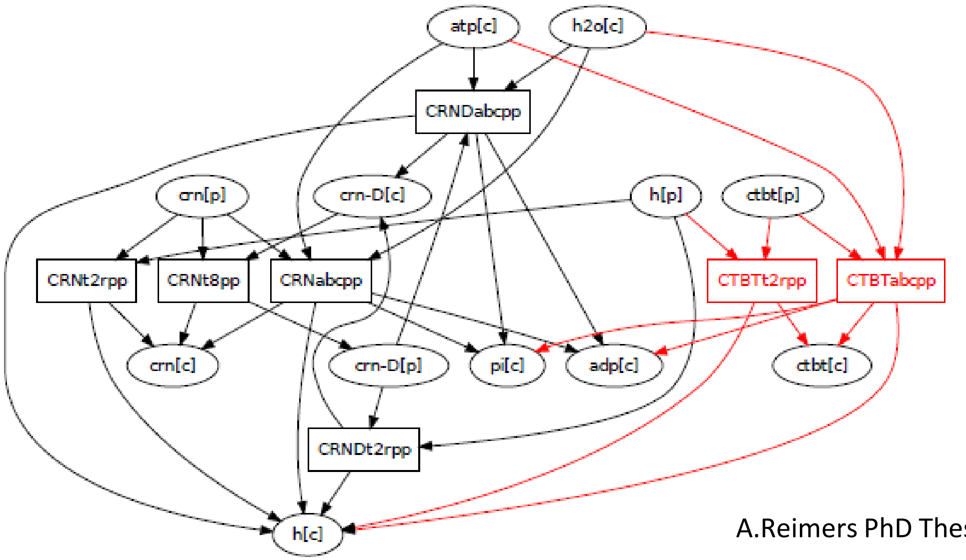
A.Reimers PhD Thesis

What are dominant graph structures?

- Modules
- Dominant (important) cycles/pathways



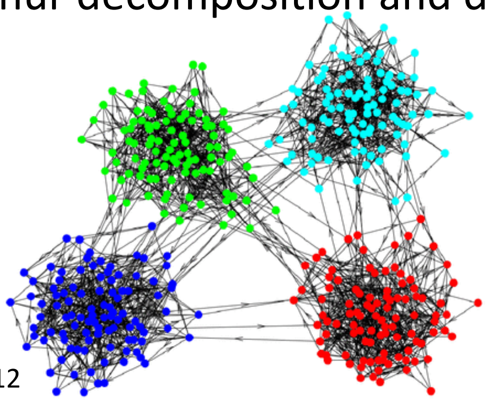
Beber et al. 2012 Interface



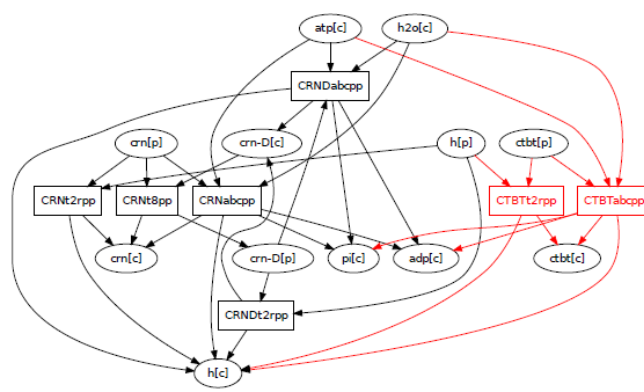
A.Reimers PhD Thesis

Outline:

- **What are dominant network structures?**
  - definition in terms of a random walk process
  - relations to spectral properties
- **How do dominant structures appear?**
  - Eigenvalue perturbation:
    - real to complex eigenvalues
    - 1- and 2-cycle perturbations
- **How can we find dominant network structures?**
  - Schur decomposition and dominant structures



Beber et al. 2012
Interface



A.Reimers PhD Thesis

Dominant network structures: random walk process

Graph $G = (V, E)$ is defined with:

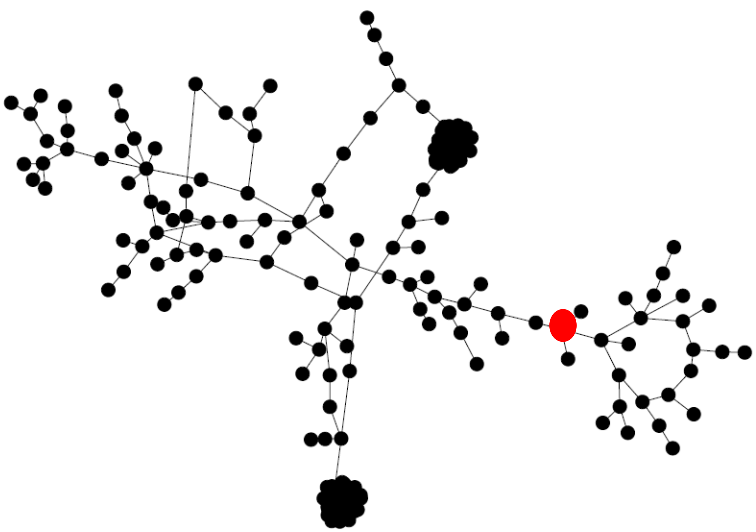
- a set of nodes (states) $V = \{1, \dots, n\}$,
- a set of edges $E \subset V \times V$.

Adjacency matrix A of a graph G is

$$A(x,y) = \begin{cases} > 0, & (x,y) \in E; \\ = 0, & (x,y) \notin E. \end{cases}$$

Introduce a random walk process (RW) on a graph G as a Markov chain $(X_n)_{n \in \mathbb{N}}$, with stochastic matrix P

$$P(x,y) = \frac{A(x,y)}{d(x)}, \quad d(x) = \sum_{y \in V} A(x,y).$$



Transition rule:

In every time-step, the process jumps to one of his neighbors with the same probability.

Dominant structures are metastable sets of a RW process.

Dominant network structures:

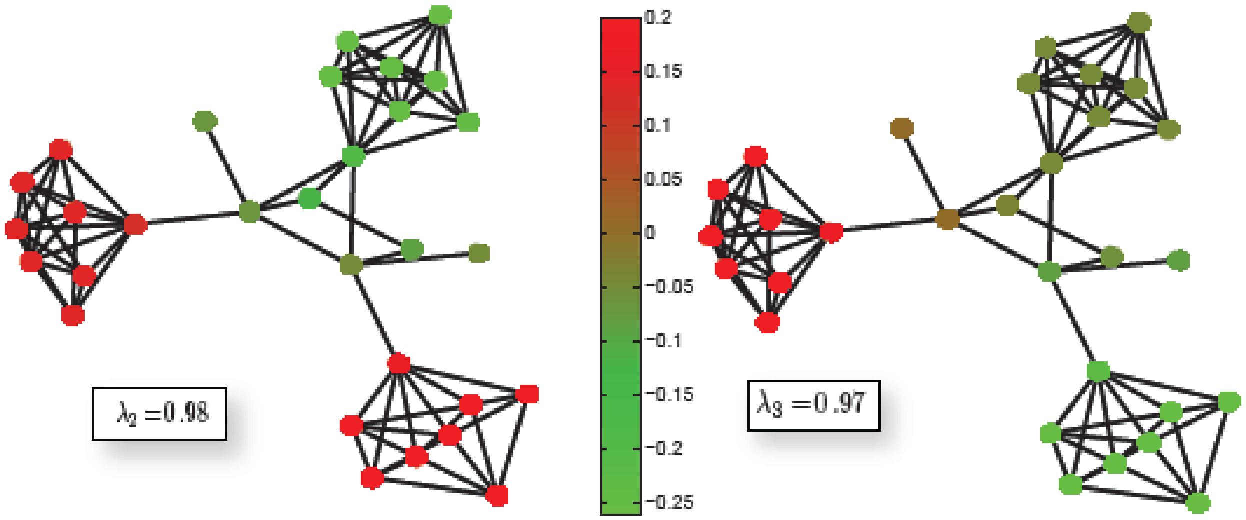
relations to spectral properties

- In terms of the random walk process on a graph, modules are metastable sets.

Undirected graphs:

- Use spectral clustering methods to identify modules: number of dominant eigenvalues of P represent number of modules; corresponding eigenvectors indicate the elements of modules.

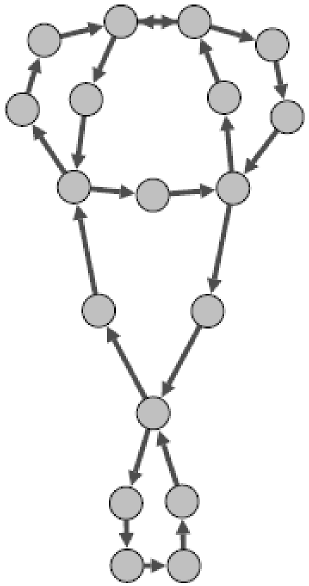
$$\lambda_1 = 1 \quad \lambda_2 = 0.98 \quad \lambda_3 = 0.97 \quad \lambda_4 = 0.76 \quad \lambda_5 = 0.41 \dots$$



Dominant network structures:
relations to spectral properties

Directed graphs:

However, for directed graphs P can have complex eigenvalues due to cycles that appear in the graph.
Metastability of non-reversible Markov processes is **NOT** very well understood.
Dominant spectrum is connected to modules and dominant cycles.



i	λ_i
1	1
2	0.7156 + 0.0053i
3	0.7156 - 0.0053i
4	0.3593 + 0.8579i
5	0.3593 - 0.8579i
6	0.3260 + 0.6374i
7	0.3260 - 0.6374i

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    - 1- ,2- and 3-cycle perturbations
- **How can we find dominant network structures?**
  - Schur decomposition and dominant structures

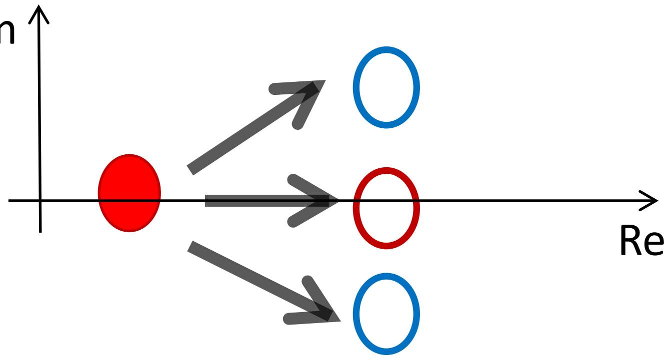
Eigenvalue perturbation:
real to complex eigenvalues

Consider the perturbation

$$P_\epsilon = P + \epsilon L$$

with a generator matrix L, $L_{i,j} \geq 0, i \neq j$ and $\sum_j L_{ij} = 0, \forall i \in V$.
We assume the following asymptotic expansions

$$\begin{aligned} \lambda_j^\epsilon &= \lambda_j + \epsilon \eta_j + \mathcal{O}(\epsilon^2) \\ u_j^\epsilon &= \tilde{u}_j + \epsilon v_j + \mathcal{O}(\epsilon^2). \end{aligned}$$



Then, one can show:

- simple eigenvalue λ_j: $\eta_j = \langle u_j, L u_j \rangle$ - a shift of λ_j along the real line.
- degenerate eigenvalue $\lambda_j = \lambda_{j+1}$: $\begin{cases} \text{remain two-fold;} \\ \text{split along real line;} \\ \textbf{split into complex plane.} \end{cases}$

Eigenvalue perturbation:
real to complex eigenvalues

For a two-fold eigenvalue $\lambda_j = \lambda_{j+1}$ and $\lambda_j^\epsilon = \lambda_j + \epsilon\eta_j + \mathcal{O}(\epsilon^2)$, η_j are given by the eigenvalues of the matrix

$$\hat{L} = \begin{pmatrix} \langle u_j, Lu_j \rangle & \langle u_j, Lu_{j+1} \rangle \\ \langle u_{j+1}, Lu_j \rangle & \langle u_{j+1}, Lu_{j+1} \rangle \end{pmatrix}.$$

Using the anti-symmetric part $\hat{L}^A = (\hat{L} - \hat{L}^T)/2$ of $\hat{L}$,

$$\hat{L}^A = \frac{1}{2}\begin{pmatrix} 0 & \delta \\ -\delta & 0 \end{pmatrix}, \delta = \hat{L}_{12} - \hat{L}_{21}.$$

we can show that the perturbation drives the two-fold real eigenvalue into the complex plane iff the deviation from symmetry of $\hat{L}$ is strong enough

$$\delta^2 > \frac{1}{2}(\hat{L}_{11} - \hat{L}_{22})^2 + \hat{L}_{12}^2 + \hat{L}_{21}^2. \qquad (1)$$

Eigenvalue perturbation: real to complex eigenvalues

Consequence: perturbations of a single entry of P or of a 2-cycle can never move a double eigenvalue into the complex plane.

Example: Let us consider the reversible transition matrix

$$P = \begin{pmatrix} 0.8566 & 0.1195 & 0.0239 \\ 0.0566 & 0.9195 & 0.0239 \\ 0.0566 & 0.1195 & 0.8239 \end{pmatrix},$$

with eigenvalues $\lambda_1 = 1$ and $\lambda_2 = \lambda_3 = 0.8$.
Perturbation of P using the 2-cycle $\gamma = (1,2)$:

$$L_1 = \sigma_1 \begin{pmatrix} -1 & 1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \sigma_1 = 0.1242.$$

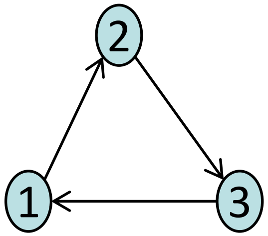
Then, eigenvalues of $P_\epsilon = P + \epsilon L_1$ are real-valued:

$$\lambda_1 = 1, \lambda_2 = 0.8, \lambda_3 \begin{cases} < 0.8 & \text{if } \epsilon > 0 \\ = 0.8 & \text{if } \epsilon = 0 \\ > 0.8 & \text{if } \epsilon < 0 \end{cases}$$

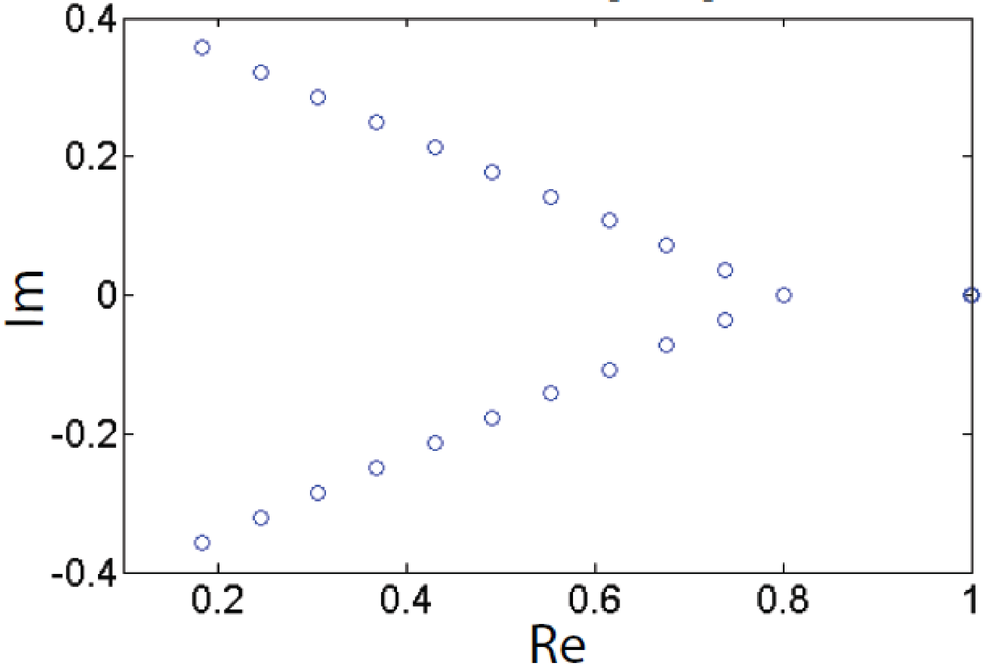
Eigenvalue perturbation:
real to complex eigenvalues

Perturbation of P using the 3-cycle $\gamma = (1,2,3)$:

$$L_2 = \sigma_2 \begin{pmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \\ 1 & 0 & -1 \end{pmatrix}, \quad \sigma_1 = 0.4119.$$



Then, eigenvalues of $P_\epsilon = P + \epsilon L_2, \epsilon \in [0,1]$ are



Eigenvalue perturbation:
real to complex eigenvalues

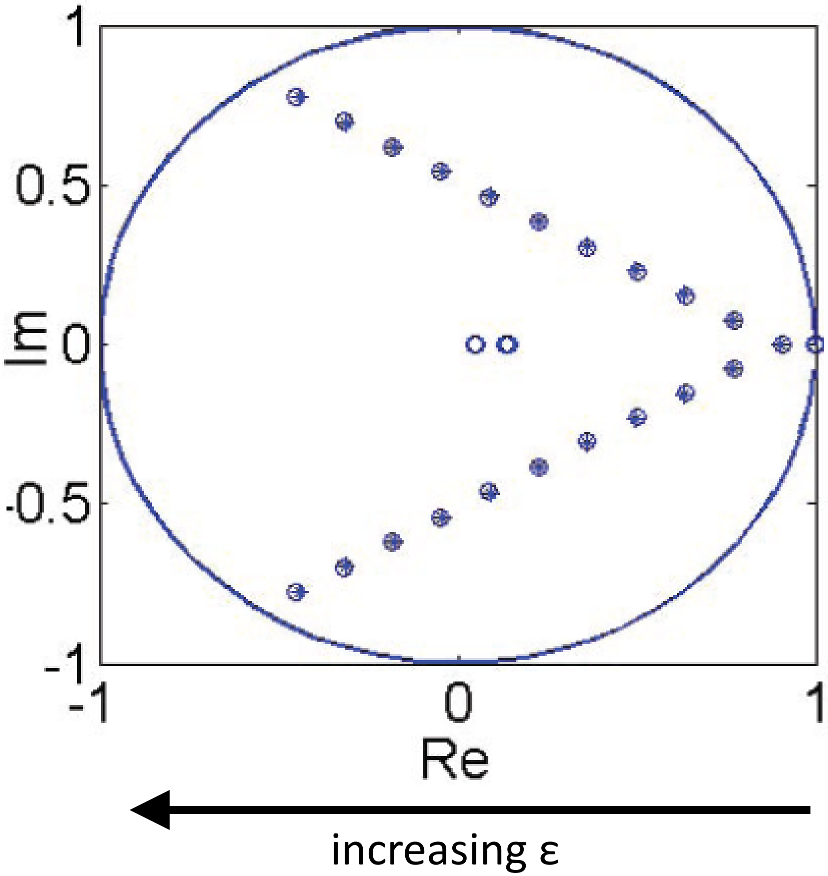
From metastable sets to dominant cycles: Let us consider the reversible transition matrix

$$P = \begin{pmatrix} 0.1437 & 0.0401 & 0.3494 & 0.4344 & 0.0323 \\ 0.0189 & 0.0740 & 0.2585 & 0.4861 & 0.1625 \\ 0.0074 & 0.0115 & 0.9385 & 0.0184 & 0.0242 \\ 0.0130 & 0.0307 & 0.0261 & 0.9094 & 0.0209 \\ 0.0010 & 0.0109 & 0.0365 & 0.0223 & 0.9292 \end{pmatrix},$$

with eigenvalues $\lambda = 1,\ 0.9048,\ 0.9048,\ 0.1353,\ 0.0498.$

Eigenvalue perturbation:
real to complex eigenvalues

After the perturbation of a 3-cycle $\gamma = (3,4,5)$: $L = \sigma(C_\gamma - I_\gamma)$, $\sigma = 0.9$. the eigenvalues of $P_\epsilon = P + \epsilon L, \epsilon \in [0,1]$ are



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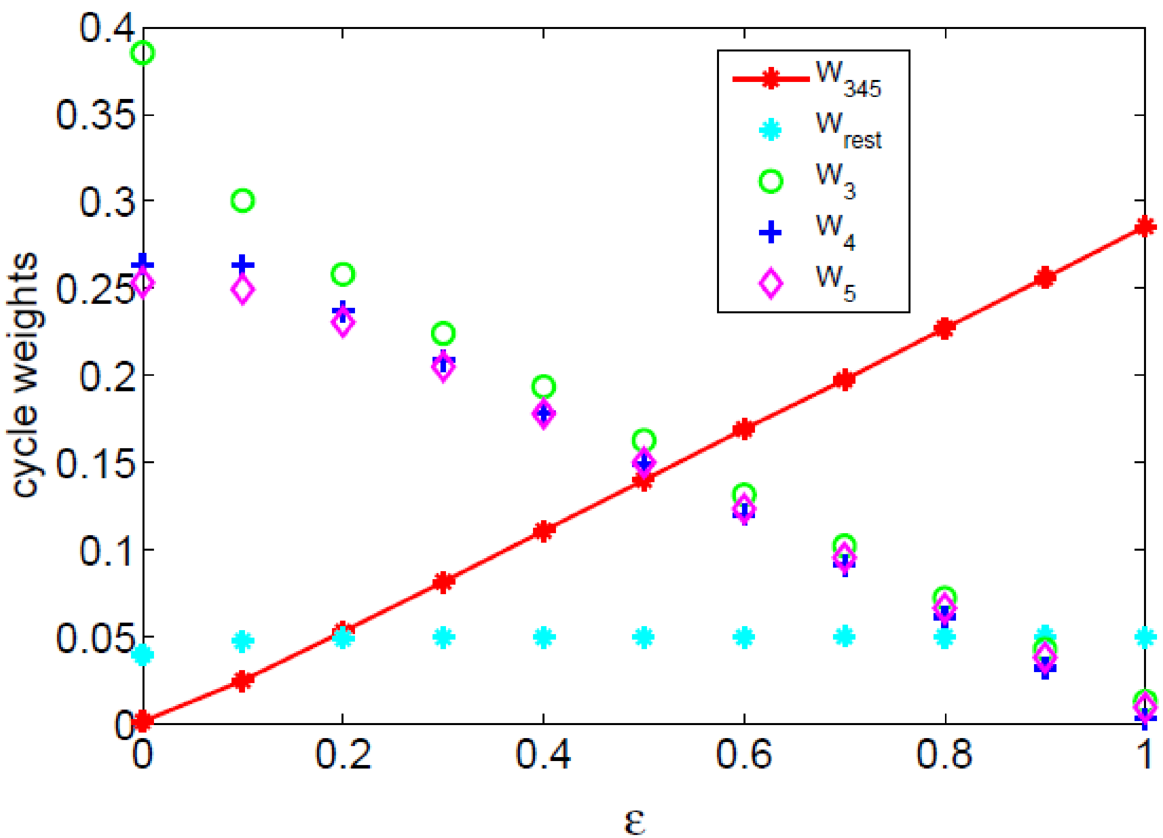
Eigenvalue perturbation:

real to complex eigenvalues

The change of dominant structures from **three metastable sets (for $\epsilon = 0$) to a dominant cycle $(3, 4, 5)$ (for $\epsilon = 1$)** can be observed by following changes of cycle weights (induced by visits of the RW).



We can observe module/cycle transitions using our cycle weight function

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Perturbation of the Schur decomposition

The Schur decomposition (X_ϵ, R_ϵ) of P_ϵ has the form

$$P_\epsilon X_\epsilon = X_\epsilon R_\epsilon, \quad \text{s.t.} \quad X_\epsilon^T D_\epsilon X_\epsilon = \mathrm{Id},$$

so that the columns of X_ϵ form an $\langle\cdot,\cdot\rangle$-orthonormal basis (as the eigenvectors did for reversible P_ϵ) and where R_ϵ has the following form

$$R_\epsilon = \begin{pmatrix} B_\epsilon & U_\epsilon \\ 0 & \tilde{\Lambda}_\epsilon \end{pmatrix}.$$

Theorem

Up to first order in ϵ the upper 2×2 block of the Schur form R_ϵ of P_ϵ is given by $\lambda \mathrm{Id}_{2\times 2} + \epsilon \hat{L}_s$ where $\hat{L}_s$ denotes the Schur form of $\hat{L}$ (and thus has the same eigenvalues). Thus, the Schur form $\hat{L}_s$ of the projection of L to the eigenspace of a double eigenvalue of the reversible matrix P is sufficient to see whether the perturbation leads to a complex conjugated pair of eigenvalues.

Perturbation of the Schur decomposition

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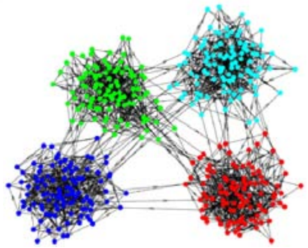
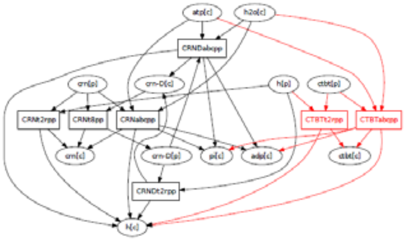
Our approach:

- Analysis: we can use Schur form R_ϵ to conclude whether the perturbation L forces a pair of eigenvalues into the complex plane.
- Algorithm: we use leading Schur vectors X_ϵ as membership functions in spectral clustering (PCCA+).

Summary:

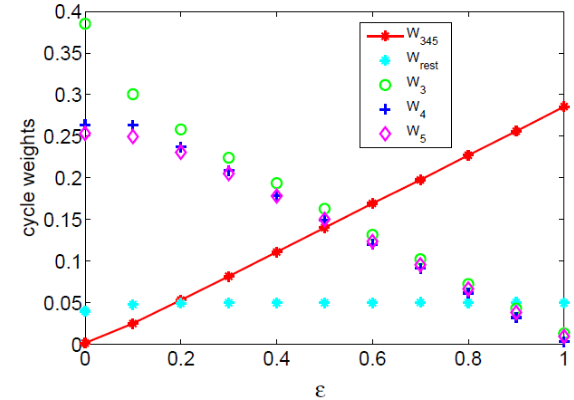
Applications:



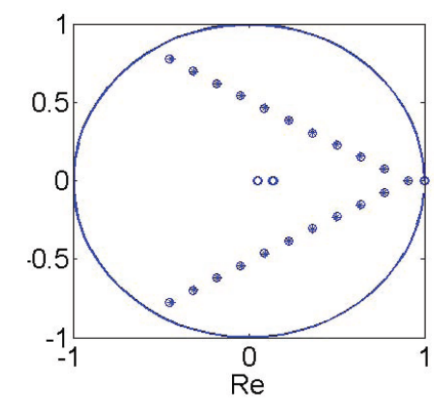


Dominant network structures can help us find important parts of complex systems (protein complexes, biochemical pathways)

Theory:



- Dominant network structures:
  - often visited by random walk process
  - relations to spectral properties: modules vs. dominant cycles
- Eigenvalue perturbation:
  - real to complex eigenvalues using cycle petrurbations
  - measure the importance of a structure by cycle weights
- Schur decomposition and dominant structures
  - alternative to the spectral decomposition
  - encodes important perturbation information



References:

- N. Djurdjevac Conrad, Marcus Weber and Ch. Schütte, ***Finding dominant structures of nonreversible Markov processes***, submitted 2015.
- R. Banisch and N. Djurdjevac Conrad, ***Cycle flow based module detection in directed recurrence networks****, EPL 2014.*
- Marcus Weber, Konstantin Fackeldey, ***G-PCCA: Spectral Clustering for Non-reversible Markov Chains***, submitted 2015.

Thank you

for your attention

Questions?

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