Learning (from) Networks

Fundamental Limits, Algorithms, and Applications

Soheil Feizi

Computer Science and Artificial Intelligence laboratory (CSAIL)
Research Laboratory of Electronics (RLE)
Broad institute of MIT and Harvard (Broad)

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Large-scale Data-driven Problems

Biological Sciences

>20,000 genes, proteins
Million SNPs, neurons

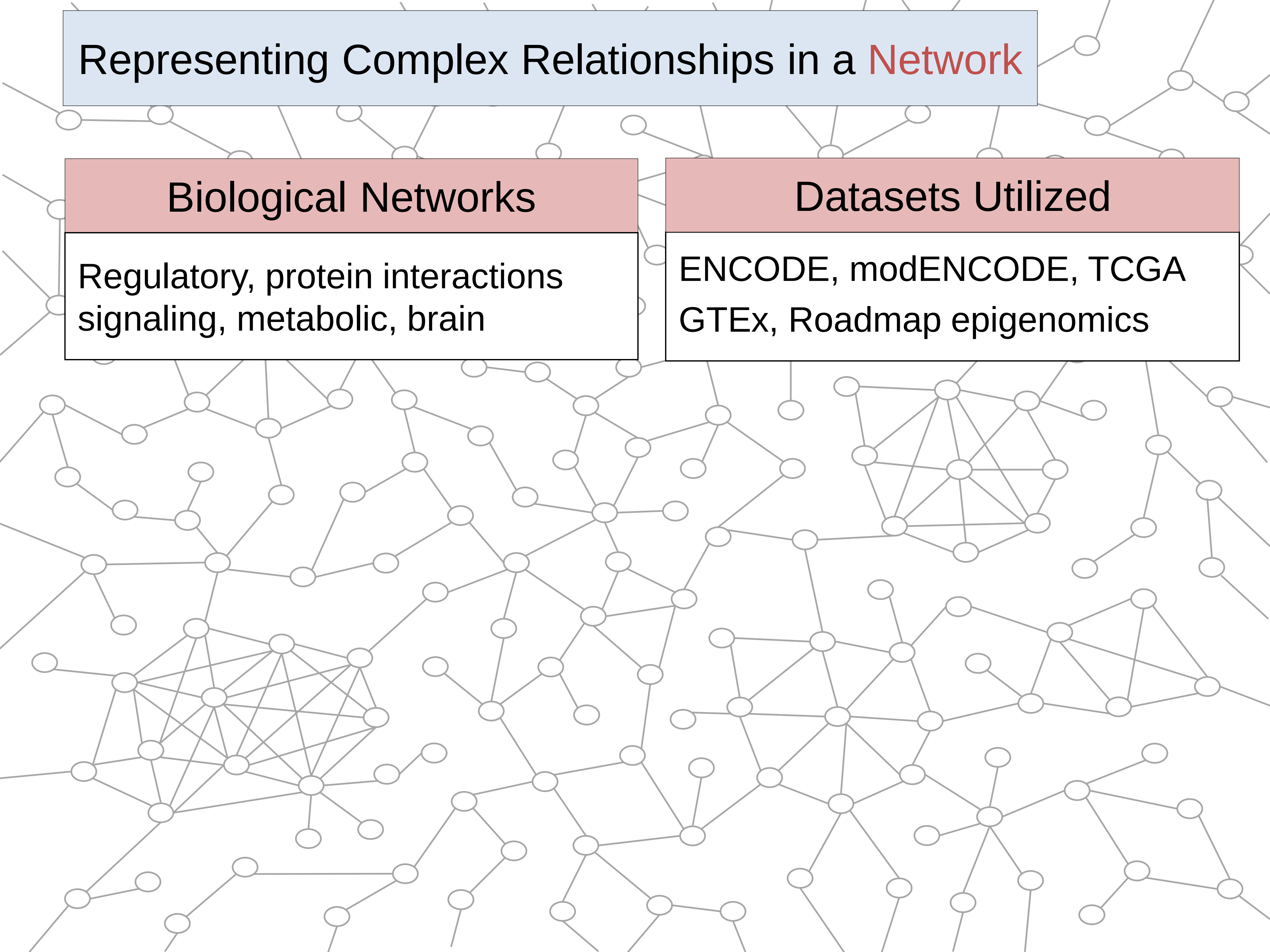
Social Sciences

Millions of people, firms
finances, services

Extracting Information from Data

Developing scalable algorithms
with theoretical guarantees
and significant applications

Representing Complex Relationships in a Network



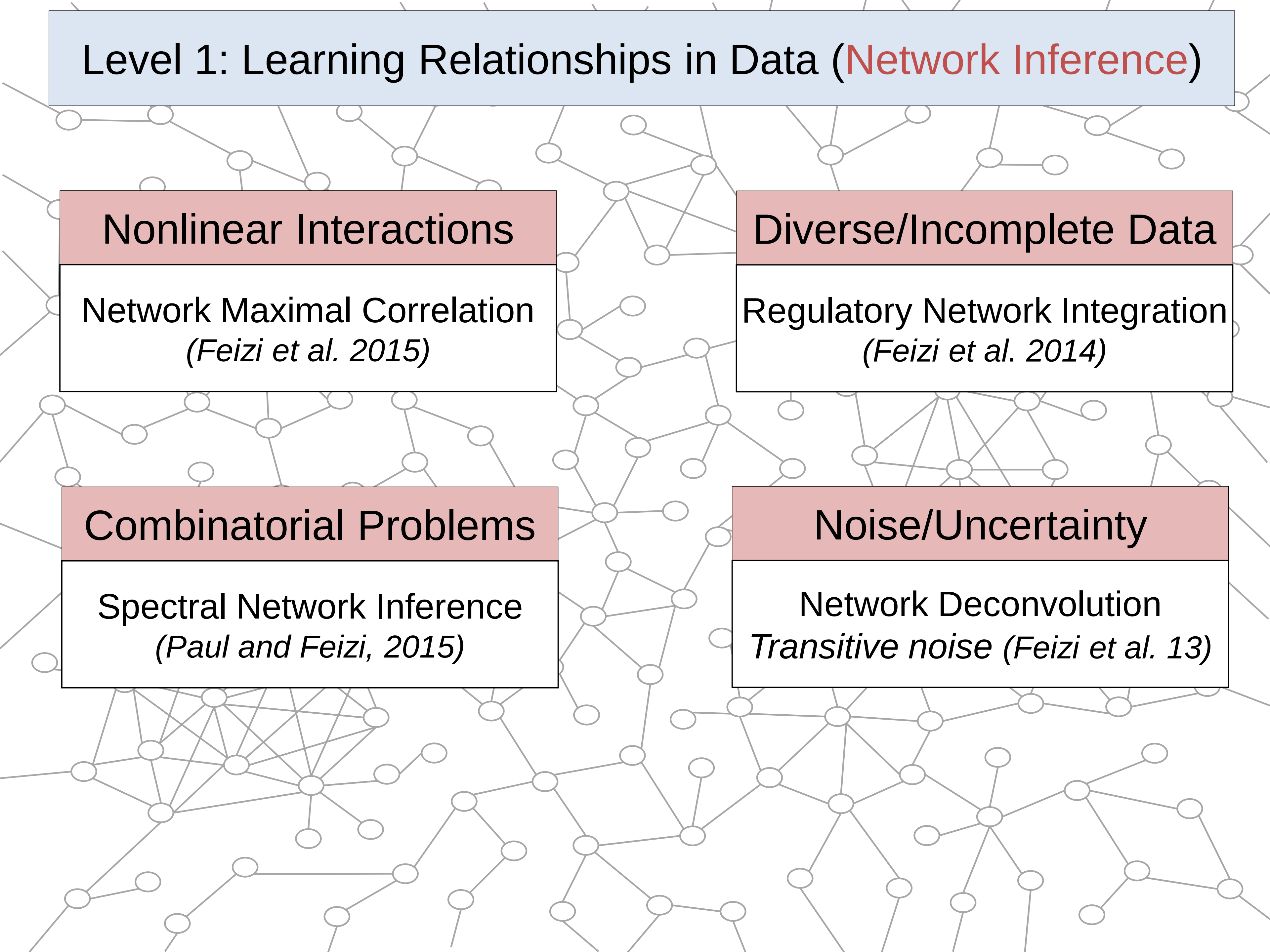
Biological Networks

Regulatory, protein interactions
signaling, metabolic, brain

Datasets Utilized

ENCODE, modENCODE, TCGA
GTEx, Roadmap epigenomics

Level 1: Learning Relationships in Data (Network Inference)



Nonlinear Interactions

Network Maximal Correlation
(Feizi et al. 2015)

Diverse/Incomplete Data

Regulatory Network Integration
(Feizi et al. 2014)

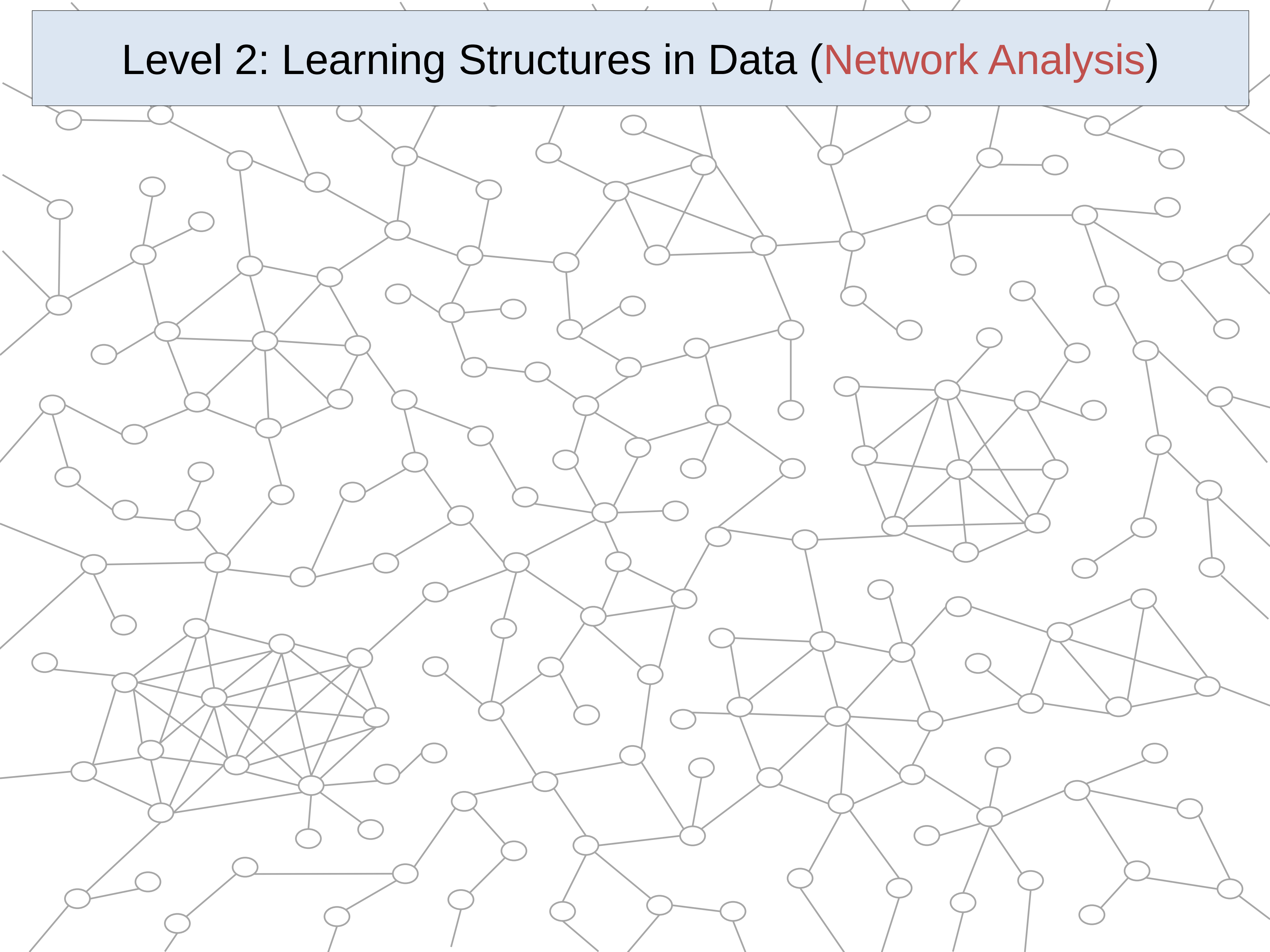
Combinatorial Problems

Spectral Network Inference
(Paul and Feizi, 2015)

Noise/Uncertainty

Network Deconvolution
Transitive noise (Feizi et al. 13)

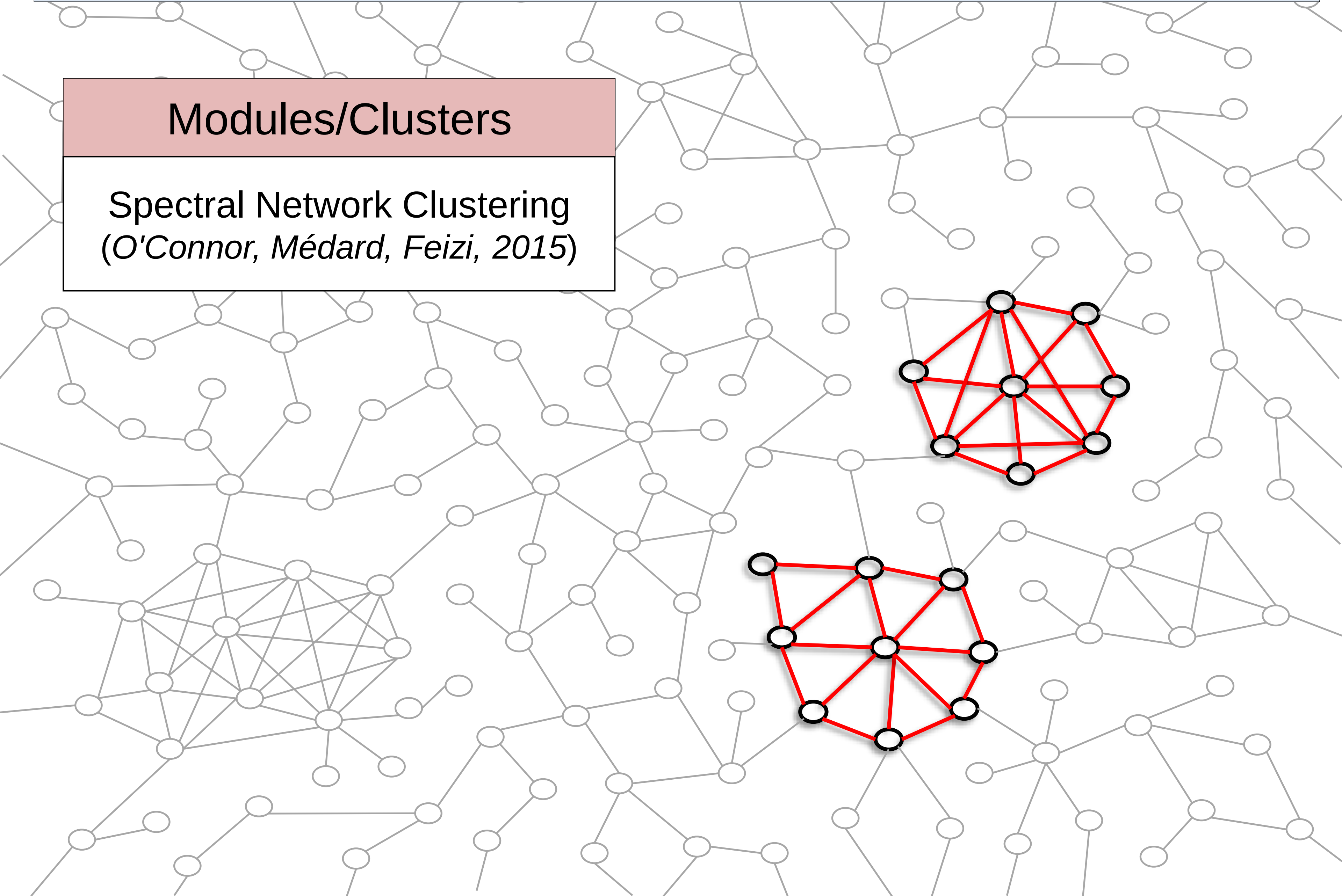
Level 2: Learning Structures in Data (Network Analysis)



Level 2: Learning Structures in Data (Network Analysis)

Modules/Clusters

Spectral Network Clustering
(*O'Connor, Médard, Feizi, 2015*)



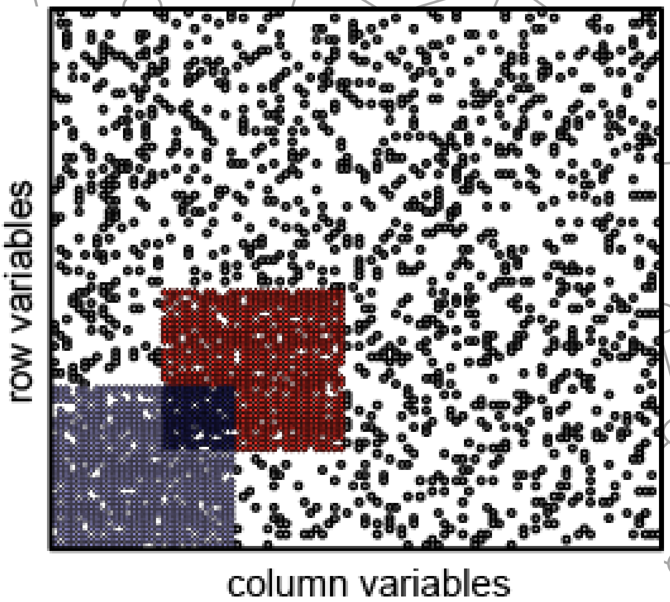
Level 2: Learning Structures in Data (Network Analysis)

Modules/Clusters

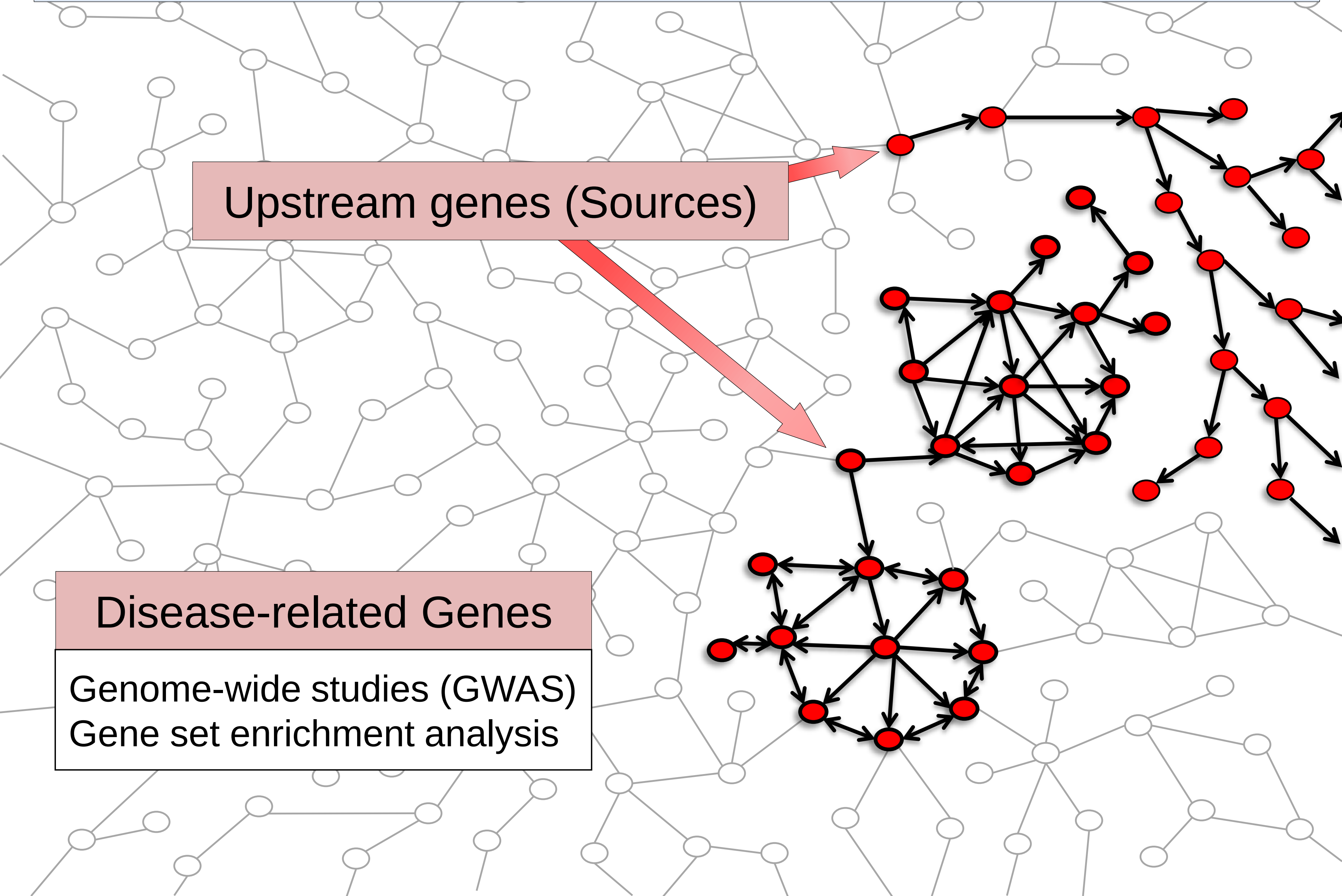
Spectral Network Clustering
(*O'Connor, Médard, Feizi, 2015*)

Bipartite Graph Clustering

Biclustering using Mess. Pass.
(O'Connor and Feizi, 2014)



Level 2: Learning Structures in Data (Network Analysis)

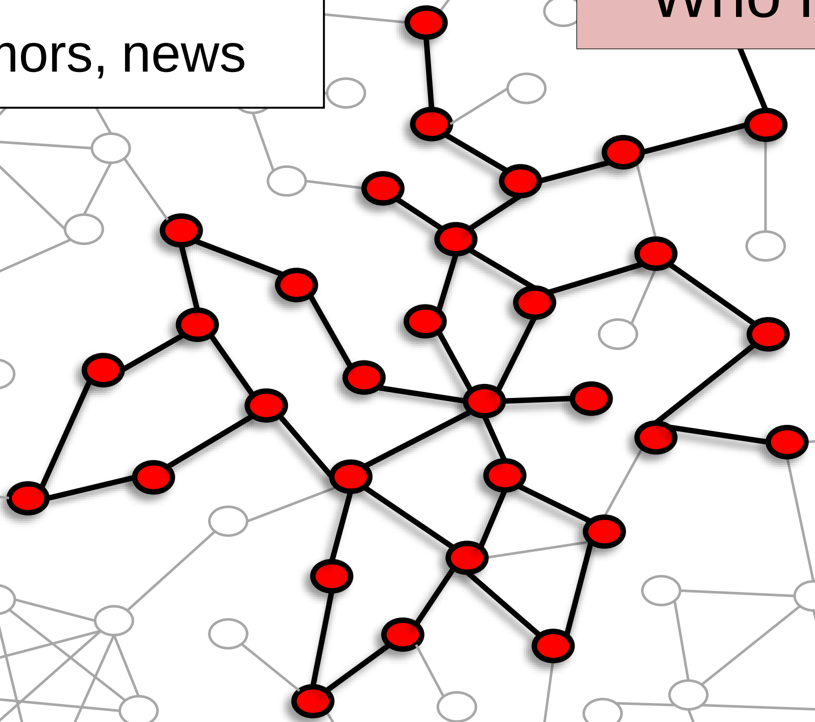


Upstream genes (Sources)

Disease-related Genes

Genome-wide studies (GWAS)
Gene set enrichment analysis

Level 2: Learning Structures in Data (Network Analysis)



Spread of Information

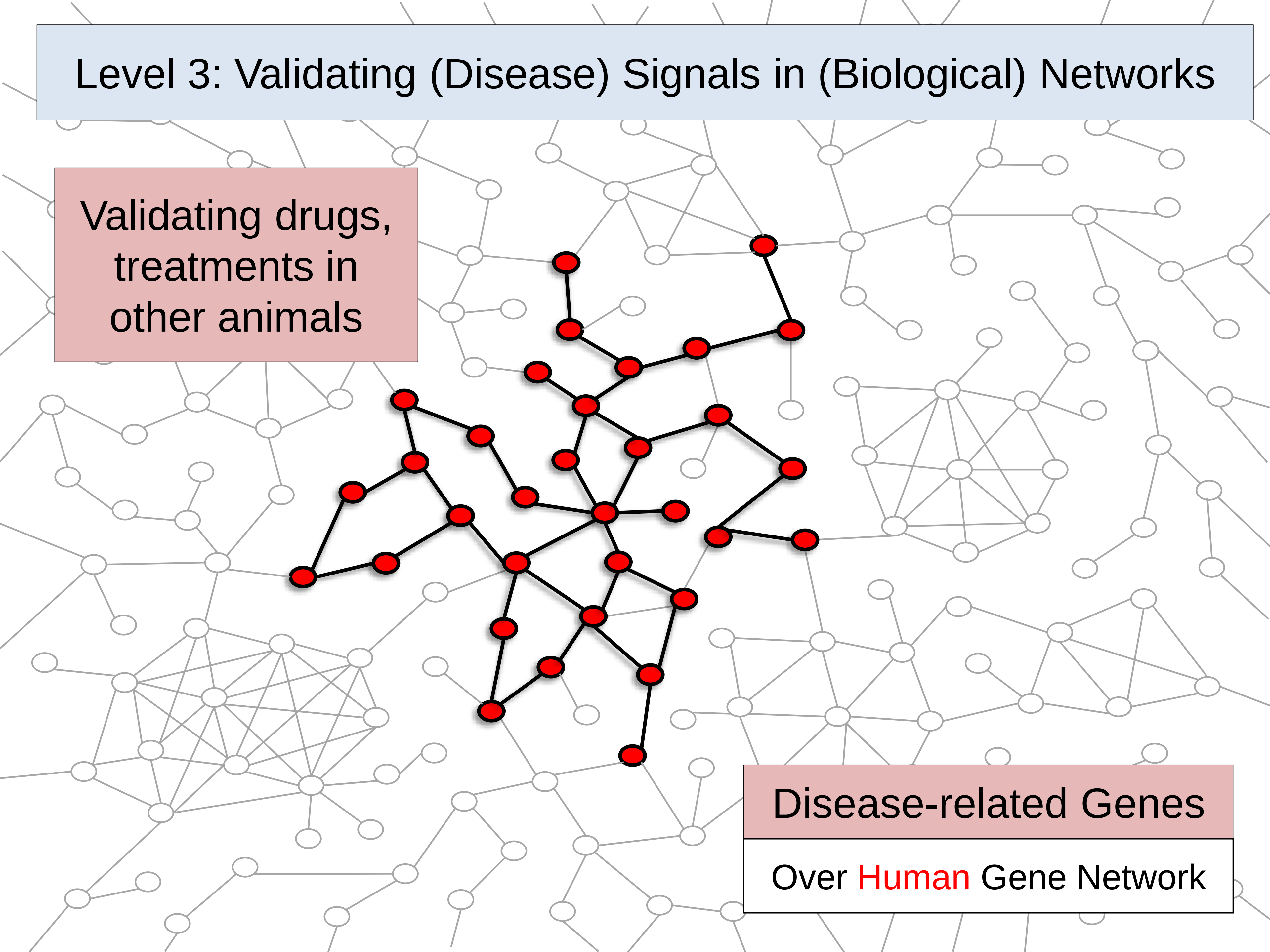
Viruses, rumors, news

Who is the source(s)?

Source Inference in Networks

Network Infusion *(Feizi et al. 2014)*

Level 3: Validating (Disease) Signals in (Biological) Networks

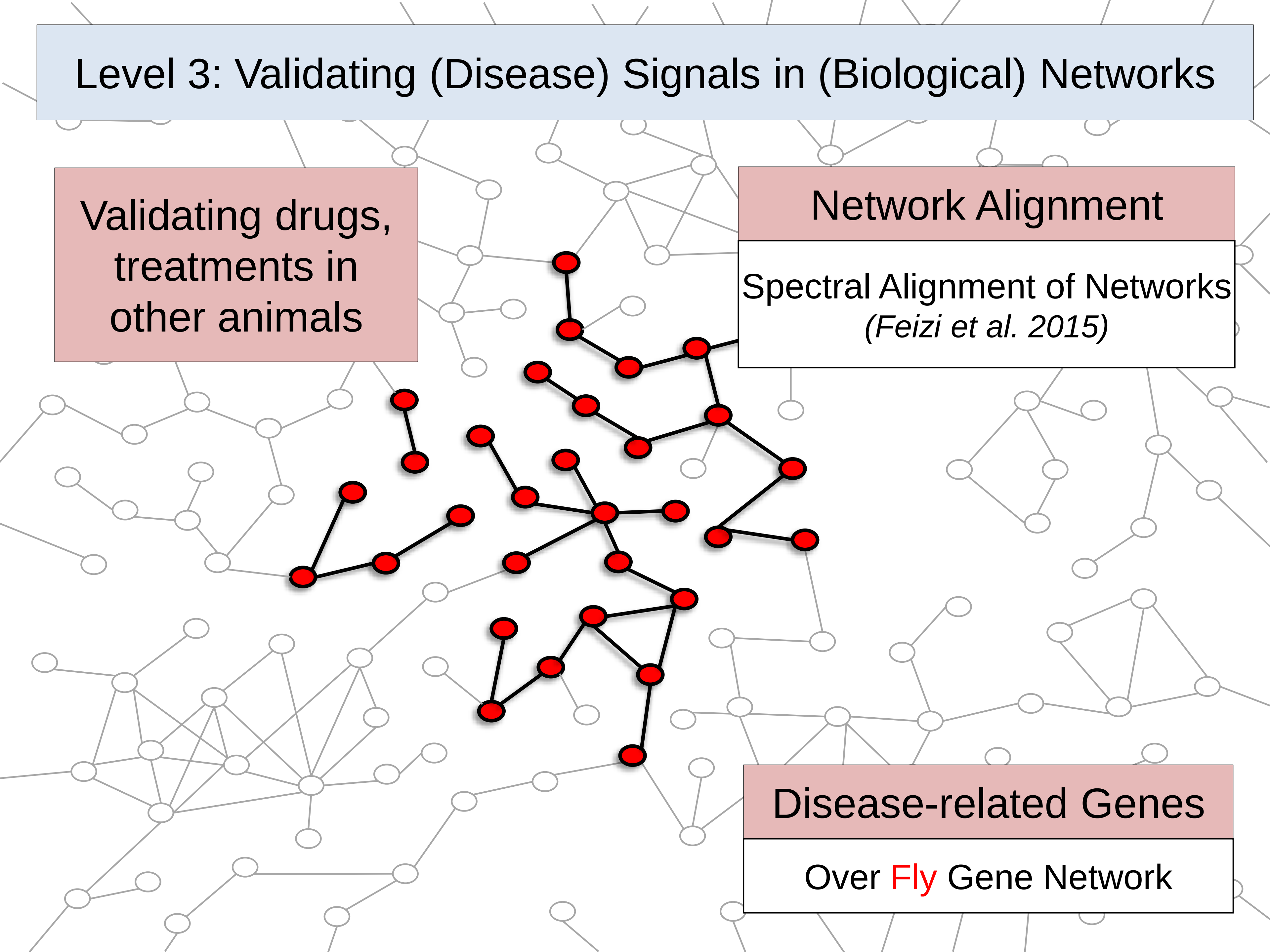


Validating drugs, treatments in other animals

Disease-related Genes

Over Human Gene Network

Level 3: Validating (Disease) Signals in (Biological) Networks



Validating drugs, treatments in other animals

Network Alignment

Spectral Alignment of Networks
(Feizi et al. 2015)

Disease-related Genes

Over Fly Gene Network

Network Inference:

- Network Integration *(Feizi et al., 2014)*
- Network Deconvolution *(Feizi et al., 2013)*
- Network Maximal Correlation (*Feizi et al., 2015*)
- Spectral DAG Inference (*Paul and Feizi 2015*)

0. Data

1. Inference

2. Analysis

3. Validation

Joint work with A. Makhdoumi, K. Duffy, M. Kellis, and M. Médard

Pairwise Association Measures

Linear correlation (Pearson 1880)

- Does not capture nonlinear associations

$$cor(X_1, X_2) = \mathbb{E}\left[X_1 \; X_2\right]$$

Mutual Information (Shannon 1948)

- Provides association strength, not functions

$$I(X_1; X_2) = \mathbb{E}\left[\log\left(\frac{P_{X_1,X_2}}{P_{X_1} \; P_{X_2}}\right)\right]$$

Maximal Correlation
(Hirschfeld 1935, Gebelein 1941)

$$\rho(X_1, X_2) = \sup_{\phi_1,\phi_2} \mathbb{E}[\phi_1(X_1) \; \phi_2(X_2)]$$

- Finding transformations with maximum correlation
- Provides association strength and functions

$$\mathbb{E}[\phi_i(X_i)] = 0, \quad i = 1, 2$$

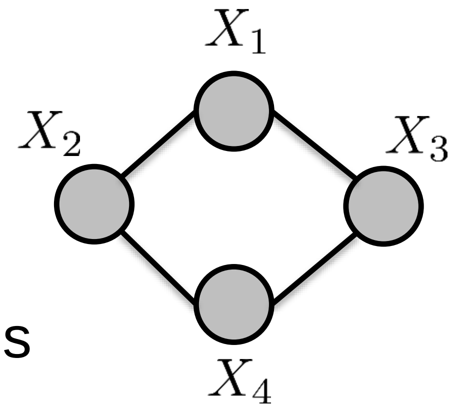
$$\mathbb{E}[\phi_i(X_i)^2] = 1, \quad i = 1, 2$$

- Properties, computation, convergence (Rényi 1959, Sarmonov 1962, Greenacre 1984, Courtade 2003, Raginsky 2014, etc)

A unifying framework based on projections on Hilbert spaces

Network Maximal Correlation

Network Maximal Correlation (NMC)



Variables connected over a given network

- Extensions for graphical models, relevance graphs

Multiple MC over edges leads to *2*|*E*| functions

- Each variable assigned to multiple transformations
- Difficult to interpret, over-fitting issues

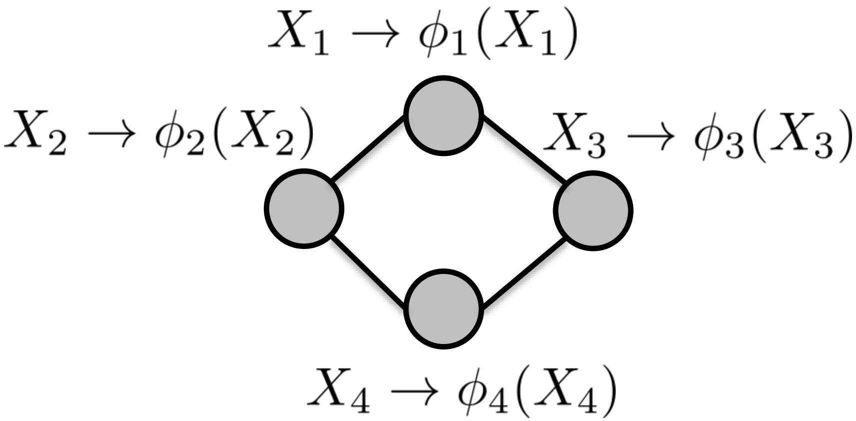
Idea: assigning single function to each variable maximizing total correlation

Network Maximal Correlation (NMC)

$$\max_{\phi_1,\ldots,\phi_n} \sum_{(i,j)\in E} \mathbb{E}[\phi_i(X_i)\ \phi_j(X_j)]$$

$$\mathbb{E}[\phi_i(X_i)^2] = 1, \quad 1 \le i \le n$$

$$\mathbb{E}[\phi_i(X_i)] = 0, \quad 1 \le i \le n$$



Basis expansion over Hilbert spaces

Optimization over functions → Optimization over real vectors

$$\phi_i(X_i) = \sum_{j=1}^{\infty} a_{i,j}\ \psi_{i,j}(X_i)$$

coefficients

orthonormal basis

If Hilbert spaces are compact, optimal solution exists

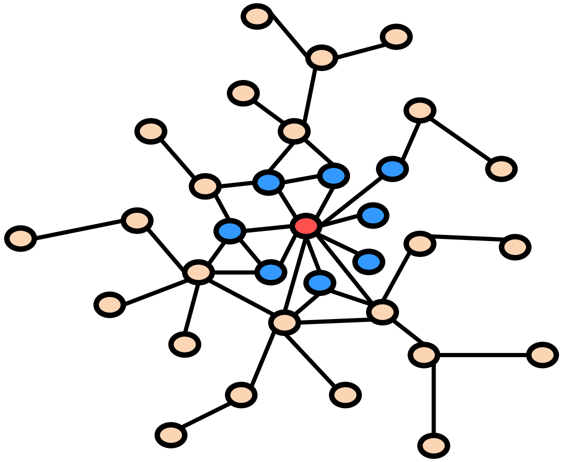
Inference of graphical models for unknown functions of Gaussian variables

Graphical Model Inference

Graphical models: crucial in modern statistics

- Characterize conditional independency
- Succinct representation of data
- Efficient computation of marginals, mode
- Example: Bayesian networks, Markov Random Fields

$$P(X_1, X_2, \ldots, X_n) = \frac{1}{Z} \prod_{i \in V} \underset{\substack{\uparrow \\ \text{node} \\ \text{potential}}}{\Phi(X_i)} \prod_{\underset{\substack{\uparrow \\ \text{network} \\ \text{edges}}}{(i,j) \in E}} \underset{\substack{\uparrow \\ \text{edge} \\ \text{potential}}}{\Psi(X_i, X_j)}$$

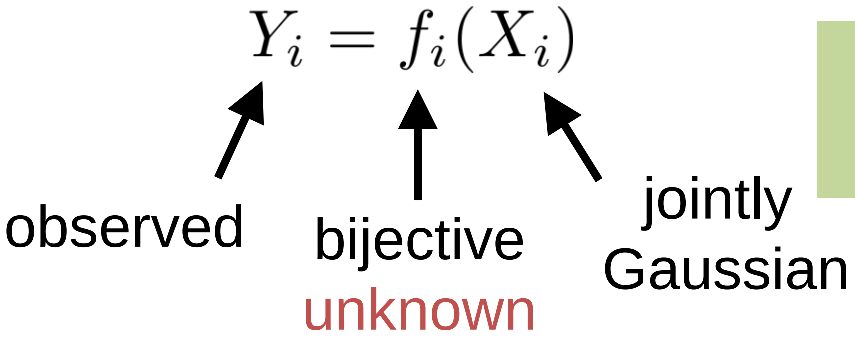


Existing methods for binary variables (Bresler 2015), Gaussian variables, exponential variables (Wainwright-Jordan 2008), Semiparametric Copula, monotone functions (Liu et al. 2012), Kernel embedding (Song et al 2010)

graphical models for nonlinear functions of Gaussians

Graphical Model Inference

Setup:



$$Y_i = f_i(X_i)$$

observed

bijective

unknown

jointly Gaussian

$$\sum_{i'\neq i} \rho_{i,i'} \geq \sum_{i'\neq i} \rho^2_{i,i'}, \quad \forall 1 \leq i \leq n$$

NMC Opt.

$$\max \quad \sum_{(i,i')} \mathbb{E}[g_i(Y_i)\; g_{i'}(Y_{i'})],$$

$$\mathbb{E}[g_i(Y_i)] = 0, \quad 1 \leq i \leq n,$$

$$\mathbb{E}[g_i^2(Y_i)] = 1, \quad 1 \leq i \leq n$$

Covariance matrix

$$\Lambda_{nmc}(i,j) = \mathbb{E}[g_i^*(Y_i) g_j^*(Y_j)]$$

$$J_{nmc} = \Lambda_{nmc}^{-1}$$

Precision matrix (E_{nmc})

Theorem:

If $(i,j) \notin E_{nmc} \;\Rightarrow\; Y_i \perp Y_j | \{Y_k, k \neq i,j\}$

$$X_i = g_i^*(Y_i)$$

Proof Sketch of Graphical Model Inference Theorem+ Intuition

$$\begin{aligned} \max \quad & \sum_{(i,i')} \mathbb{E}[g_i(Y_i)\; g_{i'}(Y_{i'})], \\ & \mathbb{E}[g_i(Y_i)] = 0, \quad 1 \le i \le n, \\ & \mathbb{E}[g_i^2(Y_i)] = 1, \quad 1 \le i \le n \end{aligned}$$

Replace in the NMC optimization $Y_i = f_i(X_i)$

Define: $\phi_i(X_i) = g_i(f_i(X_i))$

Proof Sketch of Graphical Model Inference Theorem+ Intuition

$$\max \sum_{(i,i')} \mathbb{E}[\phi_i(X_i)\ \phi_{i'}(X_{i'})]$$
$$\mathbb{E}[\phi_i(X_i)^2] = 1, \quad 1 \le i \le n$$
$$\mathbb{E}[\phi_i(X_i)] = 0, \quad 1 \le i \le n$$

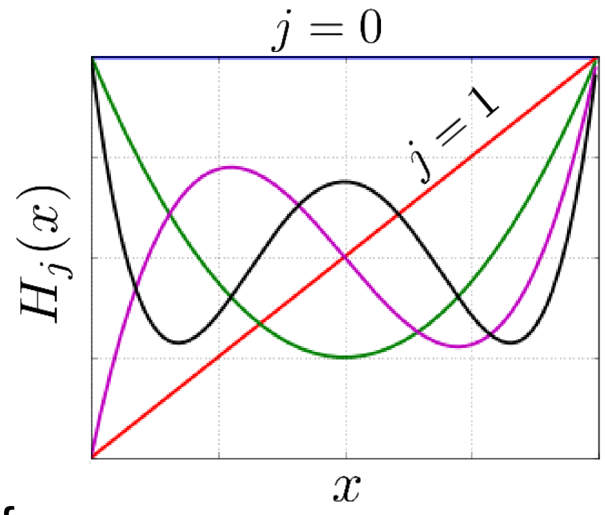
Basis expansion over Hilbert spaces

$$\phi_i(X_i) = \sum_{j=1}^{\infty} a_{i,j}\ \psi_{i,j}(X_i)$$

coefficients

orthonormal basis

Hermitte-Chebychev polynomials



Key property:

$$\int_{-\infty}^{\infty} H_j(x_1)H_{j'}(x_2)h(x_1,x_2)dx_1dx_2 = \rho^j \mathbf{1}_{j=j'}$$

Gaussian density

Correlation coef.

Proof Sketch of Graphical Model Inference Theorem+ Intuition

$$\max \quad \sum_{(i,i')} \sum_{j=1}^{\infty} a_{i,j} a_{i',j} \; \rho_{i,i'}^{j}$$

$$\sum_{j=1}^{\infty} (a_{i,j})^2 = 1, \quad 1 \leq i \leq n$$

correlation coefficient

Proof Sketch of Graphical Model Inference Theorem+ Intuition

$$\max \quad \sum_{(i,i')} \sum_{j=1}^{\infty} a_{i,j} a_{i',j} \ \rho_{i,i'}^{j}$$

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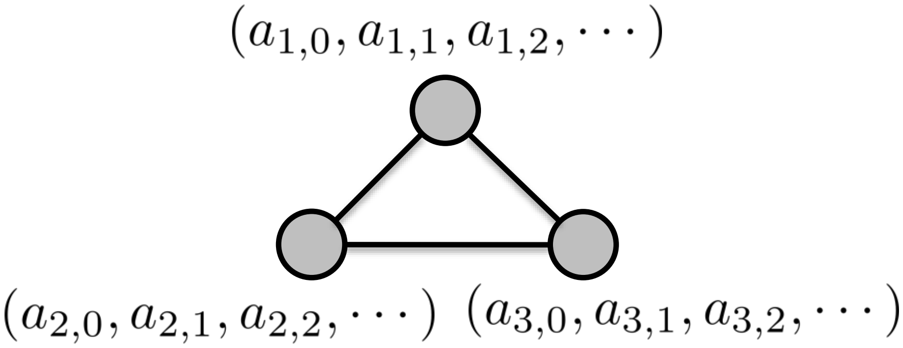

Proof Sketch of Graphical Model Inference Theorem+ Intuition

$$\max \quad \sum_{(i,i')} \sum_{j=1}^{\infty} a_{i,j} a_{i',j} \; \rho^{j}_{i,i'}$$

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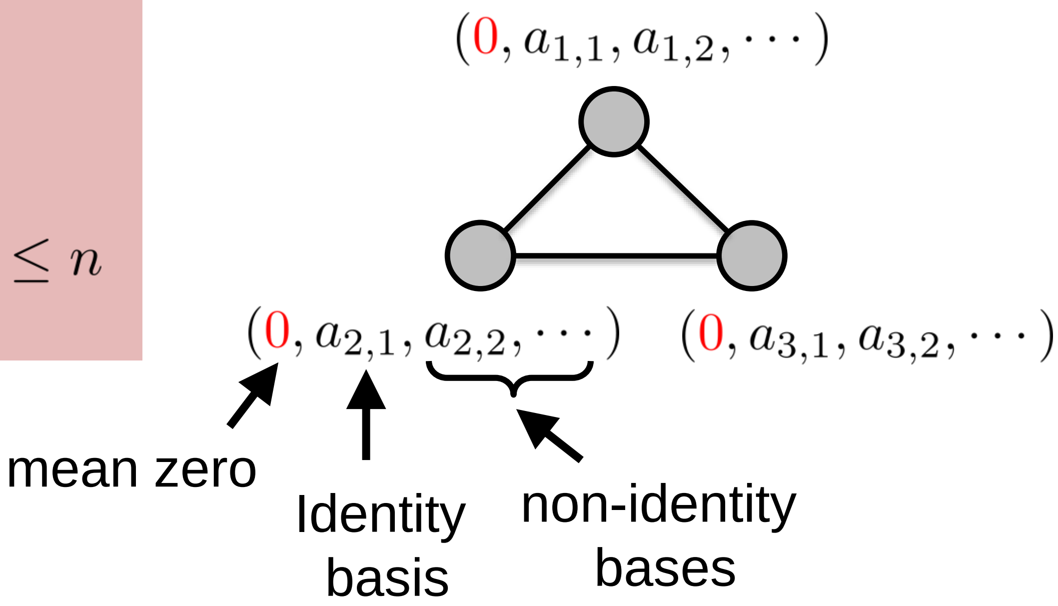


$(0, a_{1,1}, a_{1,2}, \cdots)$

$(0, a_{2,1}, \underbrace{a_{2,2}, \cdots}\,)$ $(0, a_{3,1}, a_{3,2}, \cdots)$

mean zero

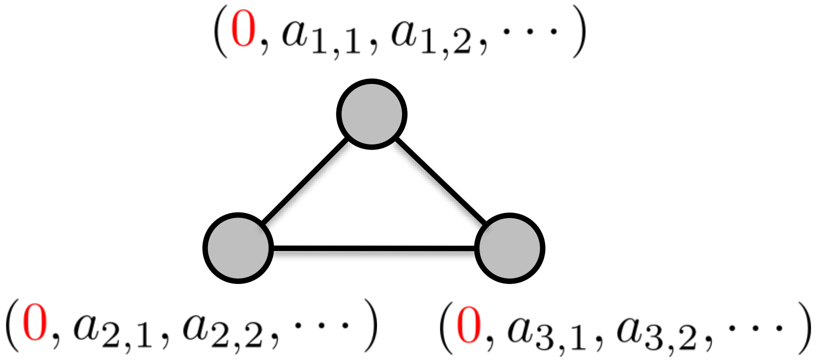
Identity basis

non-identity bases

Proof Sketch of Graphical Model Inference Theorem+ Intuition

$$\max \sum_{(i,i')} \sum_{j=1}^{\infty} a_{i,j} a_{i',j}\ \rho^{j}_{i,i'}$$

$$\sum_{j=1}^{\infty} (a_{i,j})^2 = 1, \quad 1 \leq i \leq n$$



Lemma:

$$\sum_{i' \neq i} \rho_{i,i'} \geq \sum_{i' \neq i} \rho^{2}_{i,i'}, \quad \forall 1 \leq i \leq n$$

Global optimum

$$a^*_{i,1} = 1 \qquad 1 \leq i \leq n$$
$$a^*_{i,j} = 0 \qquad j \geq 2$$

$$\phi^*_i(X_i) = g^*_i(Y_i) = X_i$$

transformations of observed variables

latent variables

Positively-Dominant (PD) correlation coefficients

Proof based on Lagrange multiplier condition (Jeyakumar et al. 2007) and Gerschgorin's circle theorem

Statistical Properties of NMC

Sample NMC converges exponentially fast to NMC

$$m \geq c\left(\frac{|E|^2 D^3}{\epsilon^2 \delta^2}\right)\log\left(\frac{\max\{|V|,|E|\}}{\eta}\right) \Rightarrow \mathbb{P}[|\rho_m(G) - \rho_G| > \epsilon] \leq \eta$$

number of samples

smallest marginal prob.

Proof idea: convergence rate of empirical distributions (Devroye 1983, Berend and Kontorovich 2012)

NMC for discrete variables → Maximum Correlation Problem (Hotelling 1935), Multivariate Eigenvalue Problem (Chu et al. 1993)

Efficient algorithm to compute NMC based on Alternating Conditional Expectation (Breiman & Friedman 1985)

Distributed NMC computation based on graph partitioning

Inference of nonlinear interactions in cancer

Inferring Nonlinear Gene Modules in Cancer

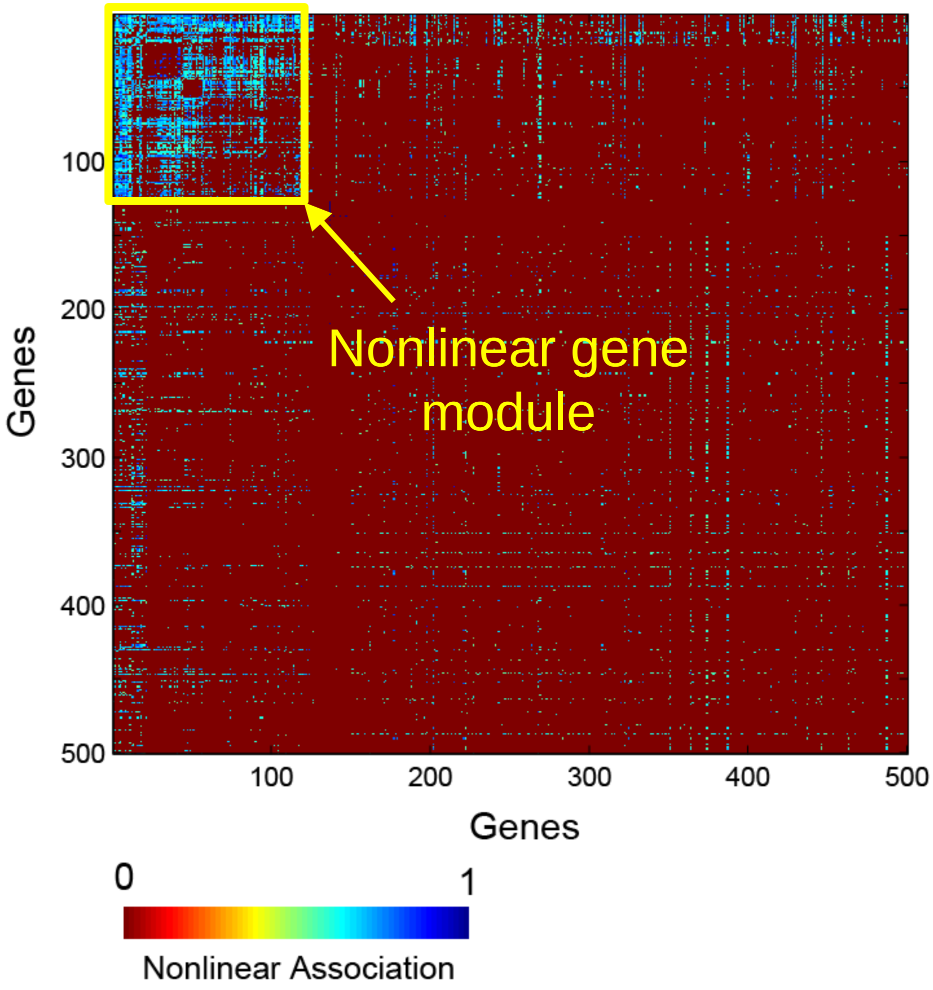
TCGA dataset: The Cancer Genome Atlas

RNA seq. counts for 24 cancer types: breast cancer, kidney cancer, liver cancer, etc

We identified gene interactions with the highest nonlinear associations

Nonlinear gene modules: present over NMC network, but not in linear network

Spectral network clustering
(O'Connor*, Médard, Feizi*, 2015)

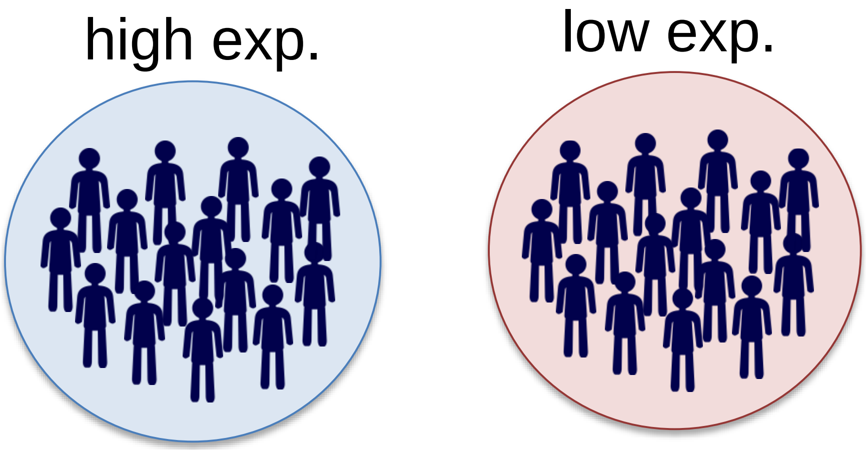


Glioma cancer

Nonlinear gene module

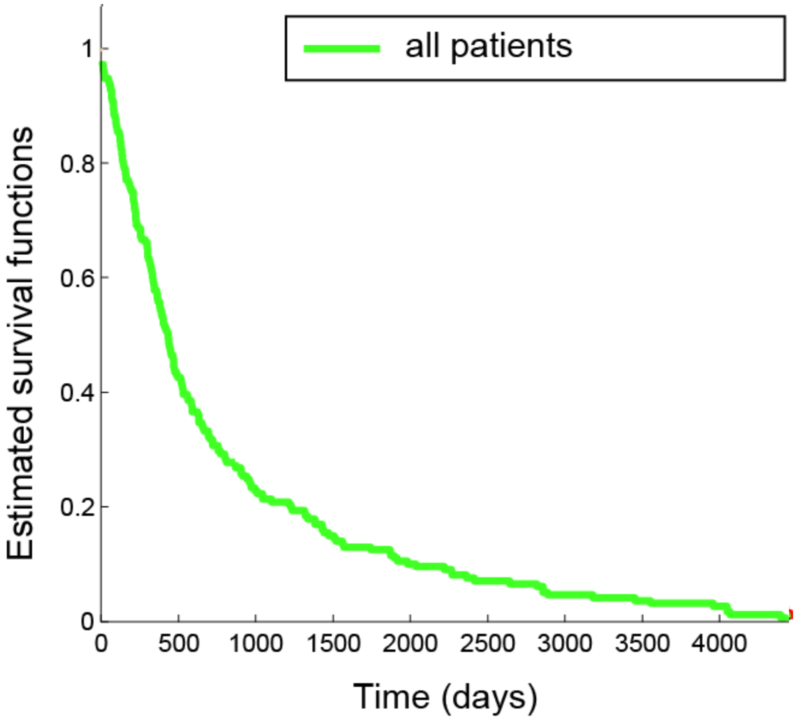
Validation Using Survival Time Analysis

Divide cancer patients to two equal-size groups based on average expression of gene module



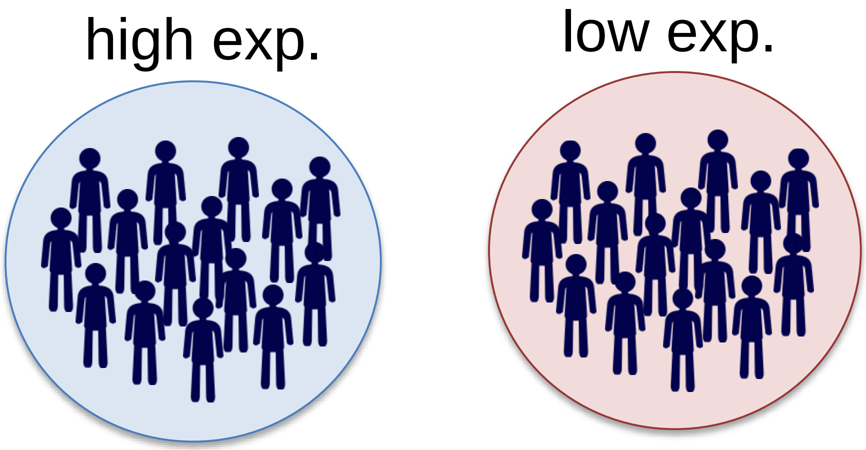
Question: do patient survival times in two groups differ significantly?

- Estimate survival function (Kaplan-Meier 1958)
- Log-rank p-value (Bland and Altman 2004)
- Multiple hypothesis correction (Benjamini and Hochberg 1995)



Validation Using Survival Time Analysis

Divide cancer patients to two equal-size groups based on average expression of gene module



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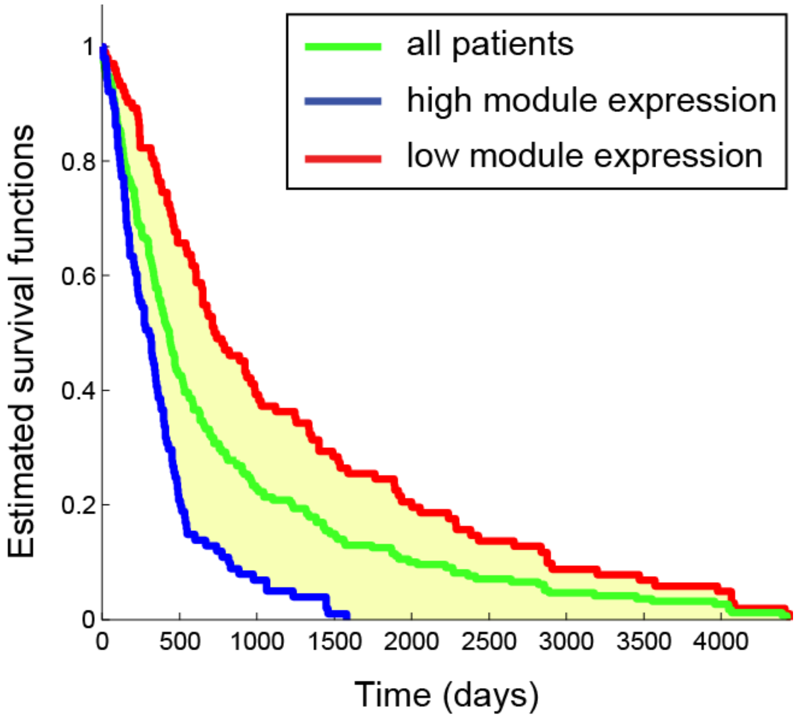


More than 80% of cancer patients with high expression of this gene module survive less than two years

Validation Using Survival Time Analysis

Divide cancer patients to two equal-

high exp.

low exp.

Network Maximal Correlation

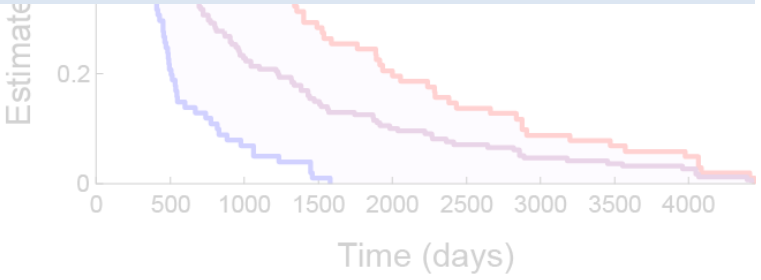
Key idea: computing optimal transformations to reveal nonlinear dependencies

Technique used: basis expansion over Hilbert spaces

Applications: graphical model inference, nonlinear gene modules in cancer

Thinking beyond linear models: nonlinear regression, nonlinear principle component analysis, …

More than 80% of cancer patients with high expression of this gene module survive less than two years



Network Analysis:

- Network Biclutering (*O'Connor and Feizi, 2014*)
- Network Clustering (*O'Connor et al., 2015*)
- Network Infusion (*Feizi et al., 2014*)

0. Data

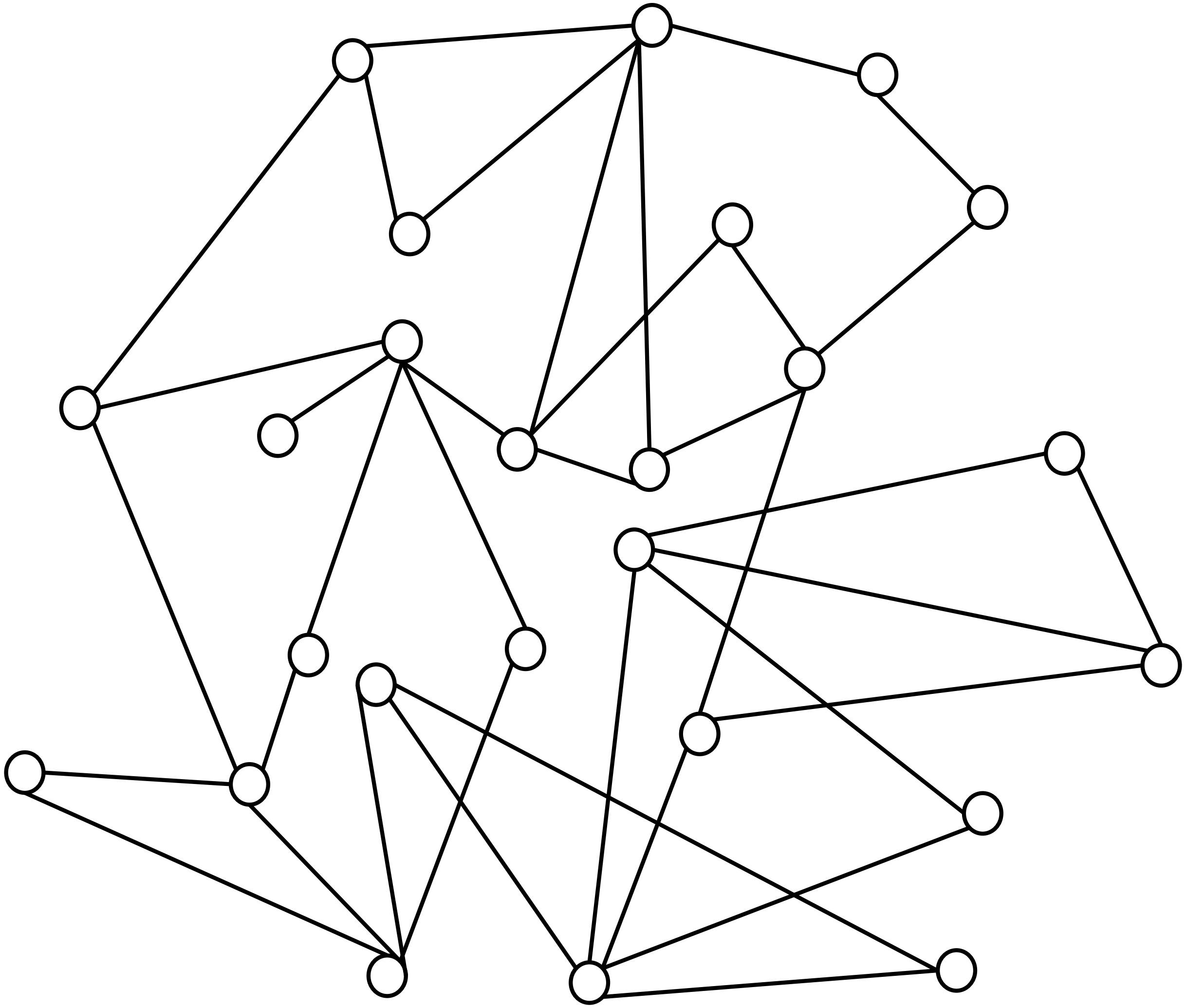
1. Inference

2. Analysis

3. Validation

Joint work with L. O’Connor and M. Médard

Network Clustering: finding nodes that are heavily interacting with each other but not with others



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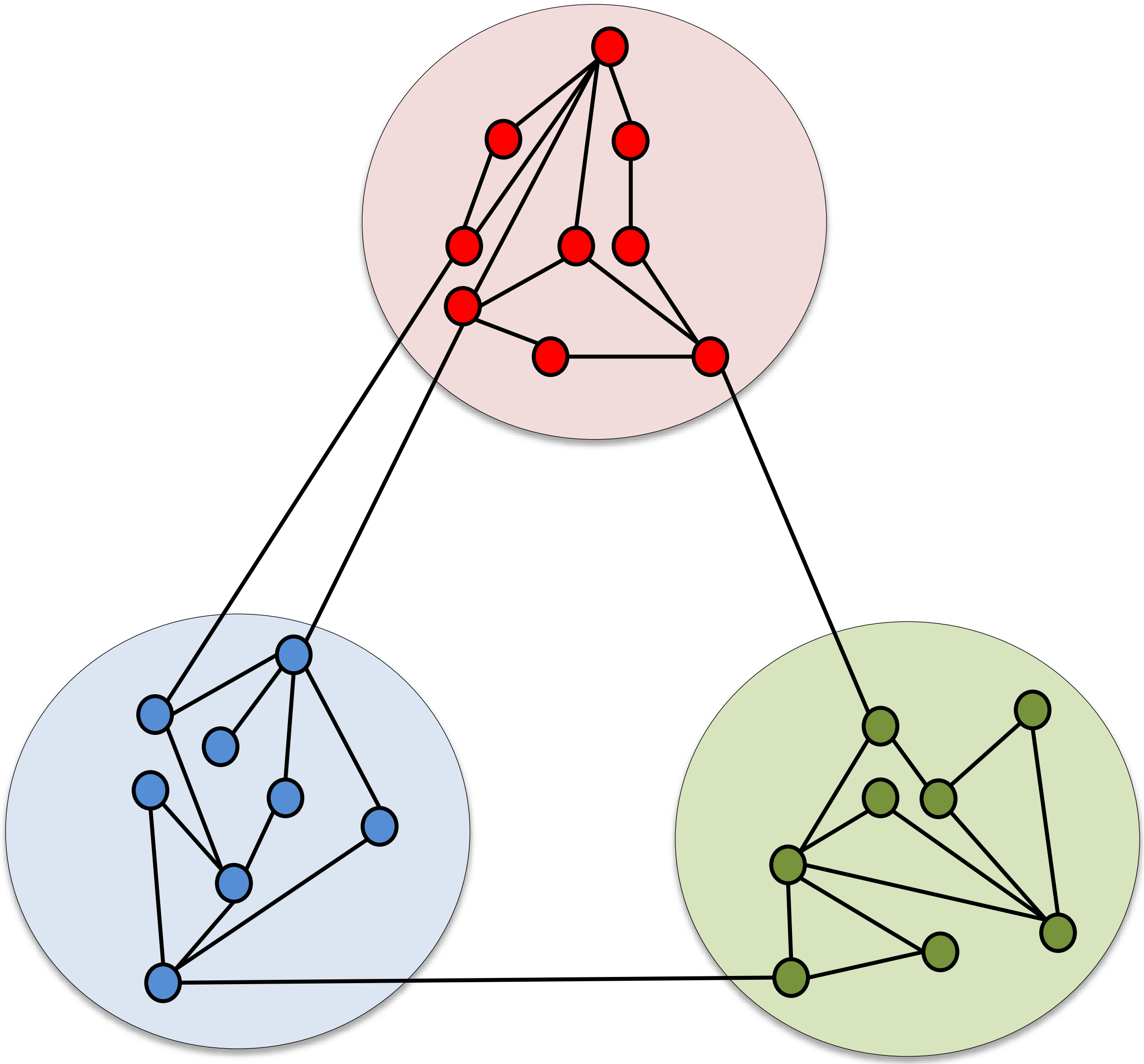
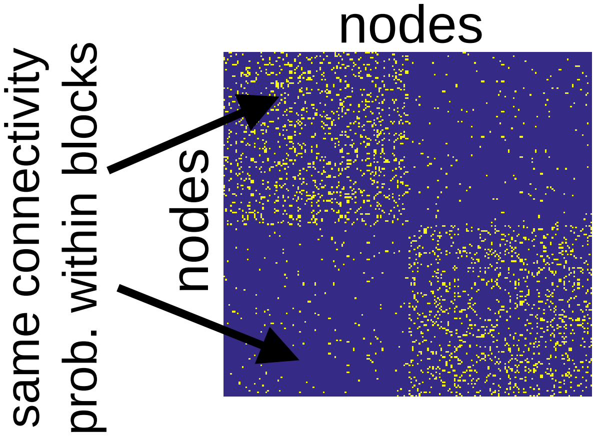


Prior Work on Network Clustering

Stochastic Block Models (SBMs)

Missing heterogeneity within blocks: degree-dependent structures

Sensitivity with respect to network clustering setup



Network Clustering Methods: Modularity (Newman 2006), Laplacian (Moher at al. 1991), normalized Laplacian (Chung 1997), Beth Hessian (Saade et al. 2014), SDP-based methods (Amini et al 2014, Hajek et al. 2015), Degree-Corrected (Qin and Rohe, 2013)

Performance characterizations (Decelle 11, Sussman et al. 12, Abbe at al 14, Zhang et al 14, Chen and Hero 15, etc)

Random Dot Product Graphs

(Kraetzel et al 2005):

Link function is linear

Constraints to have valid probabilities

Some methods for ML inference (Young et al. 2007, Sussman et al. 12, Athreya et al. 2013)

$$p_{i,j} = l(< v_i, v_j >)$$

edge probability

link function

latent position vectors

Idea: logistic link function

Maximum Likelihood Inference

Logistic RDPG:

- Link function is a logistic function
- No constraints to have valid probabilities
- Includes most SBMs and linear RDPGs

$$l(x) = \frac{1}{1+e^{-(x-\mu)}}$$

offset parameter

Under some conditions, ML inference of latent vectors can be solved asymptotically exactly using spectral clustering

Proof Sketch: ML inference using logistic link function:

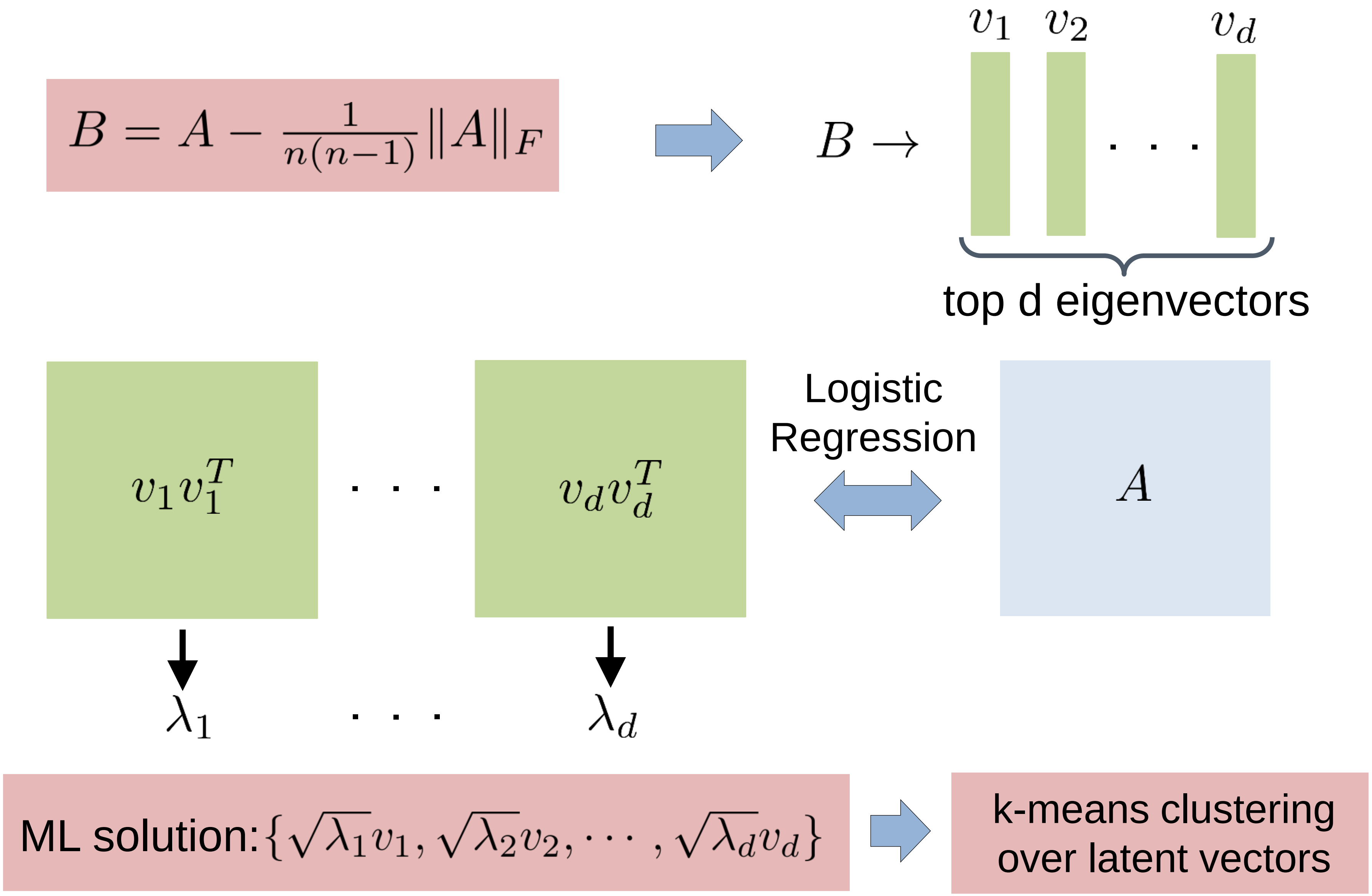
$$\max_{X} \quad Tr(AX) + \sum_{i,j} \log(1 - \frac{1}{1+e^{-(X_{ij}-\mu)}}),$$

Linear term

$$X = VV^T, \quad V \in \mathbb{R}^{n\times d}$$

Approximate the nonlinear term using the first and second order terms in its Taylor expansion

Spectral Inference Algorithm- Asym. Exact



$$B = A - \frac{1}{n(n-1)}\|A\|_F$$

$B \rightarrow$ v_1 v_2 $\cdots$ v_d

top d eigenvectors

$v_1 v_1^T$ $\cdots$ $v_d v_d^T$

Logistic Regression

A

λ_1 $\cdots$ λ_d

ML solution: $\{\sqrt{\lambda_1}v_1, \sqrt{\lambda_2}v_2, \cdots, \sqrt{\lambda_d}v_d\}$

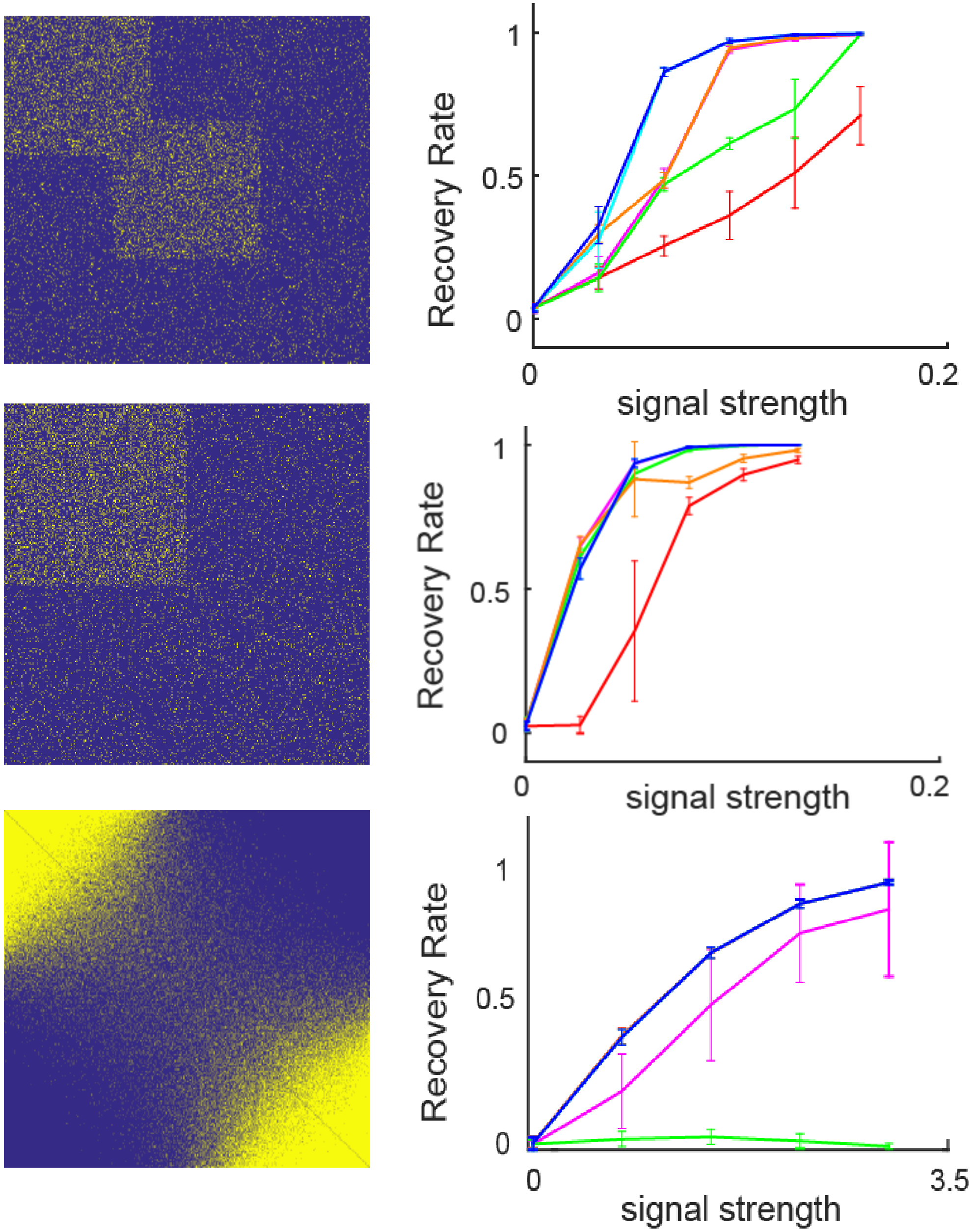
k-means clustering over latent vectors

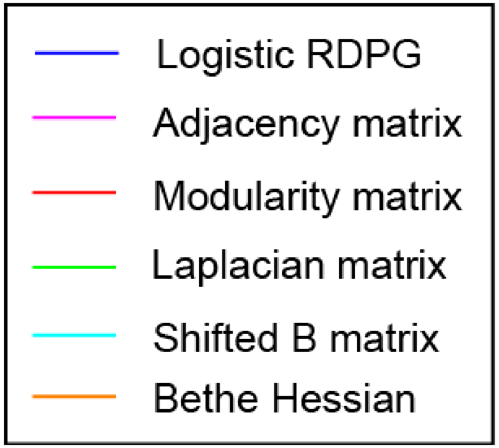
Performance Evaluations

Efficient computation even for large networks

Robust performance under various network clustering setups

Theoretical performance guarantees

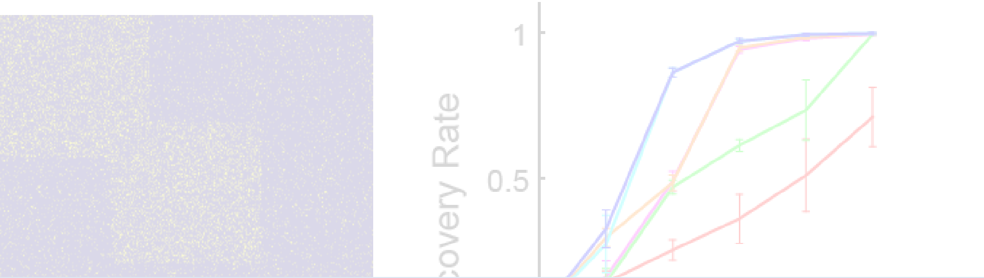




Performance Evaluations

Efficient computation even for large networks

Robust performance

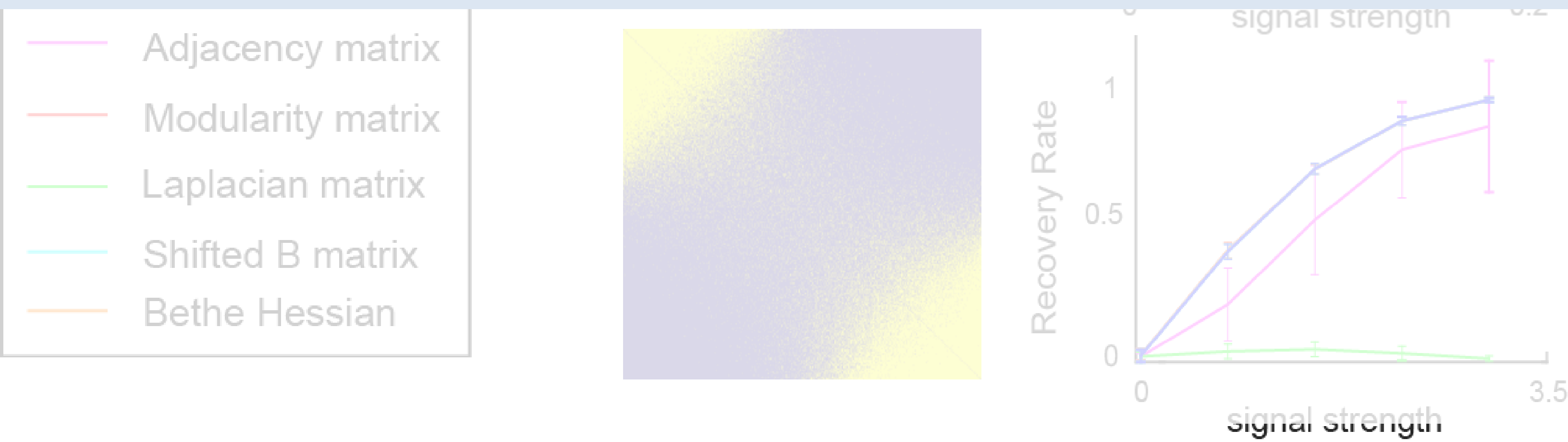


Inference of low dimensional latent vectors

Key idea: using logistic link function in RDPG model

Key technique: spectral method to solve ML inference

Application: network clustering



Network Alignment:

- Spectral Alignment of Networks *(Feizi et al. 2015)*

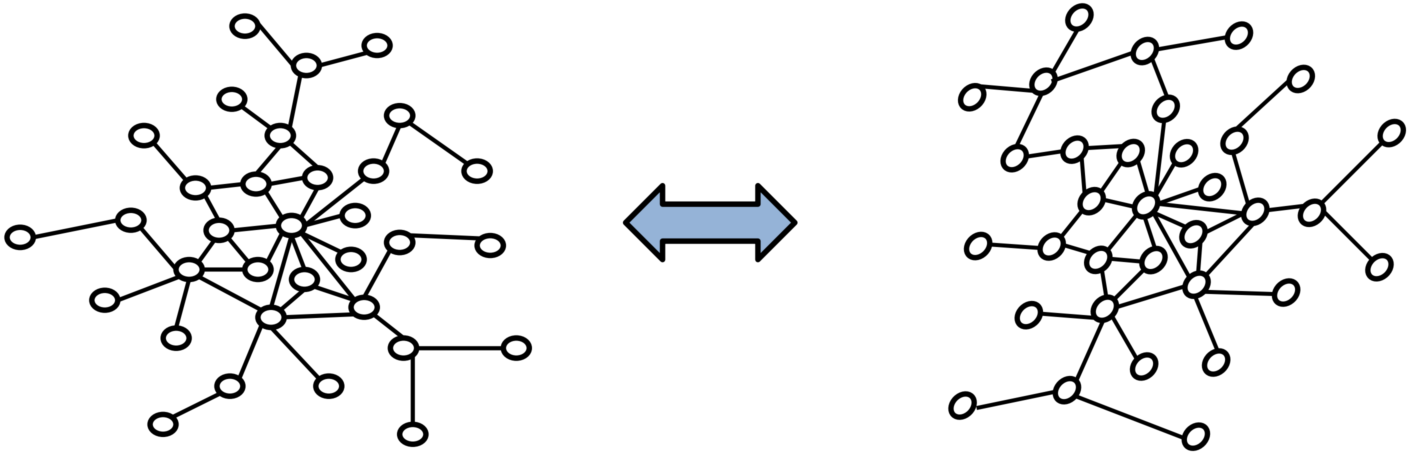
0. Data

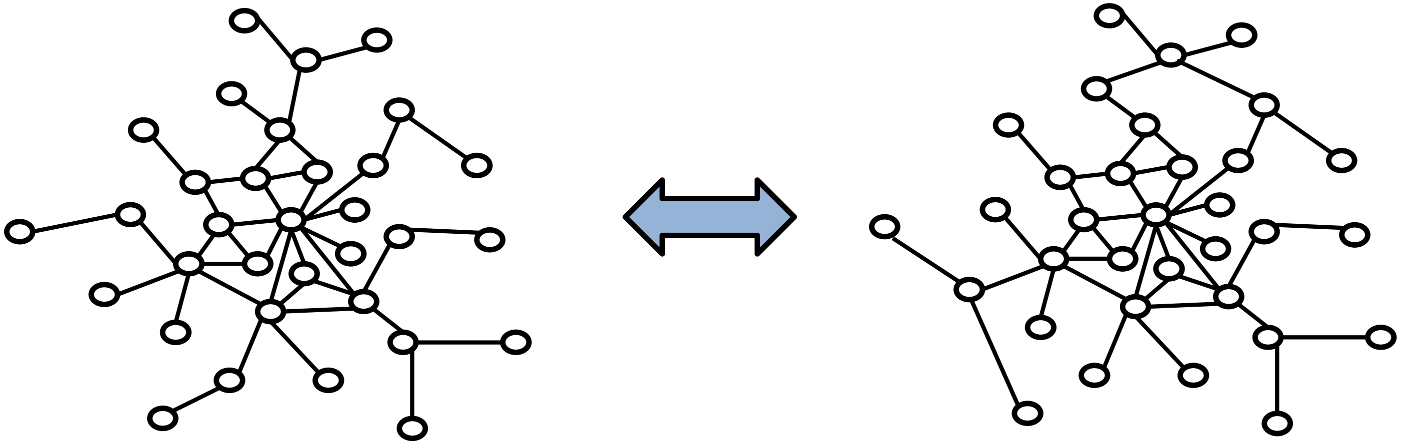
1. Inference

2. Analysis

3. Validation

Joint work with G. Quon, M. Médard, M. Kellis, and A. Jadbabaie





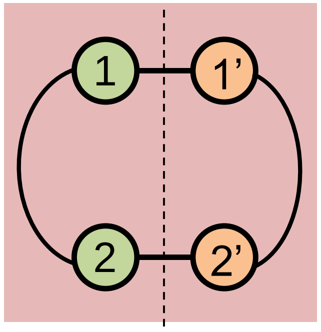
Applications of Network Alignment:

- Comparative analysis across species
- Validation of candidate human drugs in mouse and model organisms
- Data de-anonymization using dataset similarities

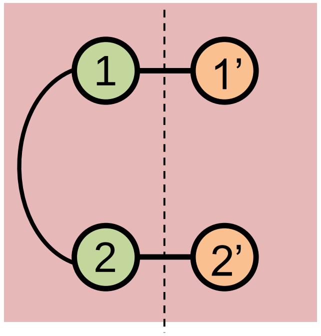
Network Alignment- Objective Function

Goal: Identifying mappings between nodes of two networks that preserve connectivity structures

match



mismatch



Existing practical network alignment methods: maximize # of matches

Mismatch effects have been ignored

- Many mismatched across biological networks

Idea #1:proposed objective

(# matches) - β (# mismatches) → Quadratic Assignment Problem

β: Relative match-mismatch importance

QAP is NP-hard (Makarychev et al. 2010)

Prior work on QAP

Exact search methods: based on branch-and-bound (Bazarra et al. 1983) and cutting plane (Bazarra et al. 1983)

Linearizations: transform QAP into a mixed integer linear program

- Lawlers linearization, Kaufmann and Broeckx linearization, Frieze and Yadegar linearization, Adams and Johnson linearization

Semidefinite/convex relaxations: intersection of orthogonal and stochastic matrices

- Orthogonal relaxations (Finke et al. 1987), projected eigenvalue bounds (Hadley et al. 1992), convex relaxations (Anstreicher et al. 2001, Zhao et al. 1998), and matrix splitting (Peng et al. 2010)

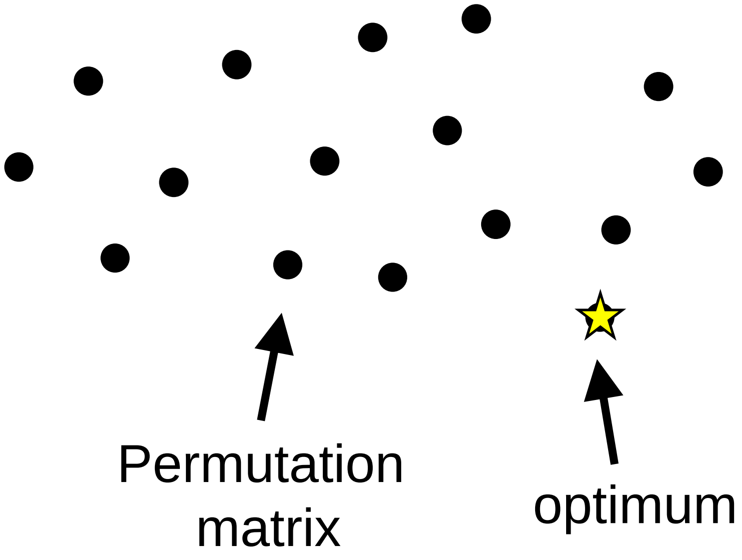
Other relaxations: Bayesian framework (Kolar et al. 2012), message passing (Bayati et al. 2013), spectral methods (Singh et al. 2008, Liao et al. 2009)

An efficient method with some theoretical guarantees and low computational complexity

Quadratic Assignment Problem (QAP)

$$\begin{aligned} \max \quad & Tr\left(G_1 X G_2 X^T\right) \\ & X \in \sqcap \end{aligned}$$

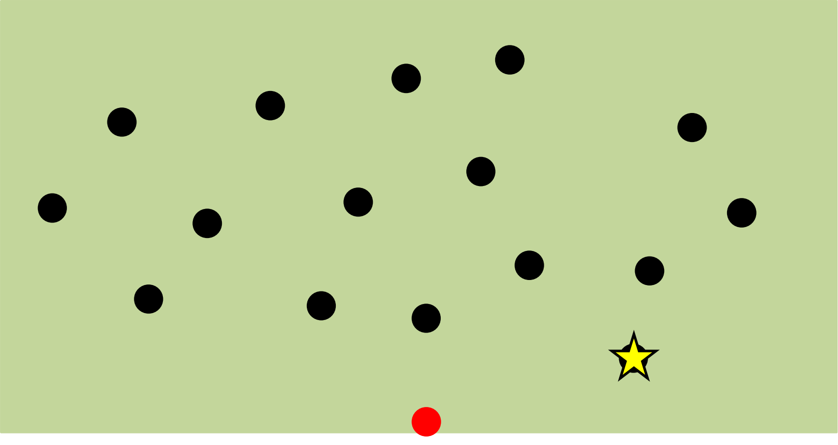
Set of all permutation matrices



Orthogonal Relaxation of QAP

$$\max \quad Tr\left(G_1 X G_2 X^T\right)$$
$$X \in \mathcal{O}$$

Set of all
orthogonal matrices



optimum
orthogonal matrix

Step 1: Relaxation over orthogonal matrices

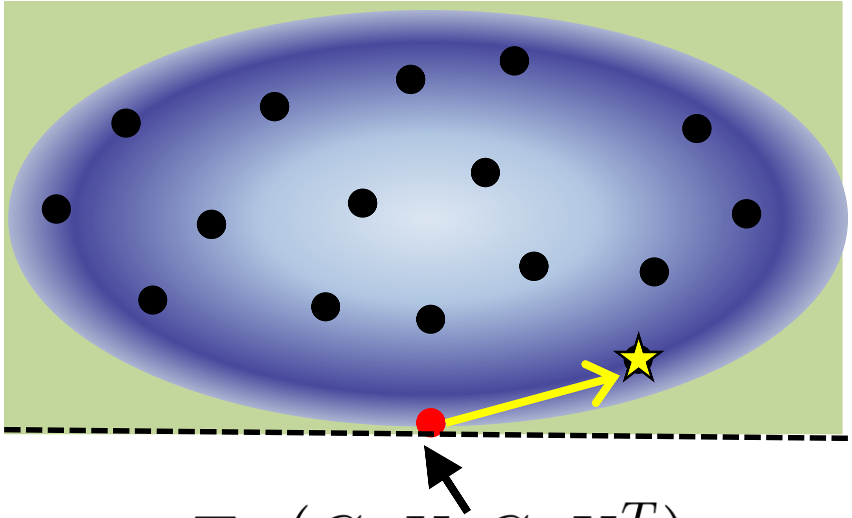
- Exact solution using spectral matrix decomposition Finke et al. 1987
- Optimum may not be a permutation

Ellipsoid Level Sets of QAP

$$\begin{aligned} \max \quad & Tr\left(G_1 X G_2 X^T\right) \\ & X \in \mathcal{O} \end{aligned}$$

↑

Set of all
orthogonal matrices



$$Tr\left(G_1 X_0 G_2 X^T\right)$$

Step 1: Relaxation over orthogonal matrices

- Exact solution using spectral matrix decomposition Finke et al. 1987
- Optimum may not be a permutation

Step 2: Projection tangent to level sets

- Efficient computation using maximum weight bipartite matching Linear Programming, Hungarian method Kuhn 1955, Greedy generalized Sharkey, Edwin Romeijn 2010

Spectral Alignment of Networks

Theorem:

$$\left| f(X^*) - \tilde{f}(X^*_{lin}) \right| \leq \epsilon^2 \sum_{i=1}^{n} \sigma_i(G_1)\sigma_i(G_2)$$

$$\|X^* - X_0\|_2 \leq \epsilon$$

singular values

Further results:

- Asymptotically exact for Erdös-Rényi graphs (under some conditions)
- Alignment of graphs with structures: modular networks (tighter bounds using SDP
- Validations on synthetic networks: power-law, regular, modular graphs
- Applied to Twitter subgraphs, user de-anonymization

Comparative gene network analysis across species

Alignment of Gene Regulatory Networks

Human network: 19,088 genes

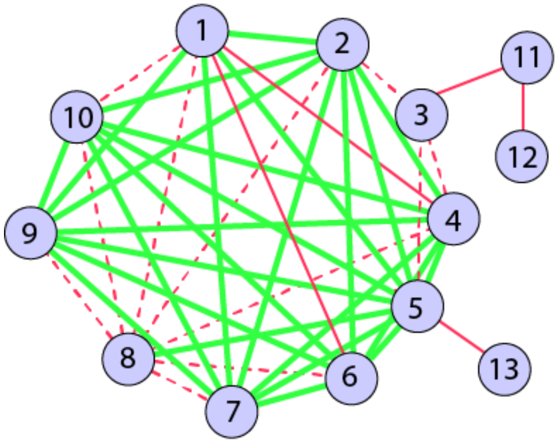
Fly network: 12,897 genes

Goal: inferring bijective mappings across two graphs (restricted to homolog genes)

Our spectral method leads to balanced # of matches and mismatches (fewest # mismatches, the 2nd highest # matches)

Strong conservation of centrality measures, and several biological processes

Conserved biological process across human and fly


regionalization (fly GO: 0003002)
negative reg. (human GO: 0010629)

ID	**Human/Fly gene**
1	TBX3/mid
2	HOXA7/Antp
3	CBX7/Pc
4	BMP4/dpp
5	GATA6/pnr
6	FOXG1/slp1
7	TFAP2A/TfAP-2
8	ZFPM2/ush
9	POU2F1/vvl
10	SMAD7/Dad
11	HINFP/CTCF
12	SMARCC2/mor
13	SMARCA2/brm

🟩 interactions exist in both human and fly
🟥 interactions exist in fly but not in human
- - - interactions exist in human but not in fly

Spectral Alignment of Networks

Asymptotically exact for Erdös-Rényi graphs (under some

Spectral Alignment of Networks

Key ideas: matches and mismatches+ spectral relaxation of QAP

Key technique: spectral decomposition + maximum weight bipartite matching

Applications: comparative analysis of gene networks, Twitter subgraphs

Thinking beyond edges: representing graphs using eigenvectors and eigenvalues

- Applied to Twitter subgraphs, user de-anonymization

Network Inference:

- Network Integration
- Network Deconvolution
- ✓ Network Maximal Correlation
- Spectral DAG Inference

Network Analysis/Validation:

- ✓ Network Alignment
- Network Biclutering
- ✓ Network Clustering
- Network Infusion

0. Data

1. Inference

2. Analysis

3. Validation

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Current/past (co-)advisees

- Luke O'Connor, PhD at Harvard
- Allison Paul, high school student
- Michael Colavita, high school student
- Aritro Biswas, undergrad at MIT
- Eric Mazumdar, undergrad at MIT
- Anna Matilde Tanga, high school student
- Amy Zhang, master at MIT
- Muriel L. Rambeloarison, master at MIT
- Liz Deny, undergrad at MIT
- Sebastian Palacios, undergrad at MIT
- Orhan Tunc Celiker, undergrad at MIT
- Eric Soderstrom, undergrad at MIT