Estimating Time-Varying Networks

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Acknowledgments


E. Xing


L. Song


A. Ahmed

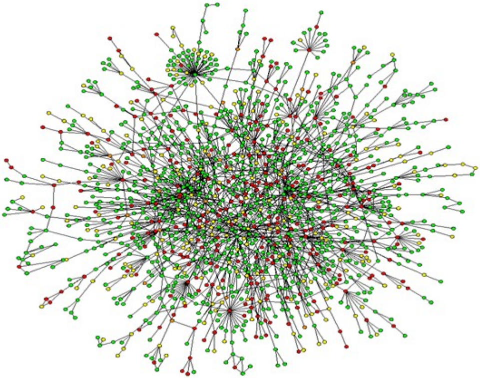

A. Parikh

Networks are mathematical abstractions of complex systems

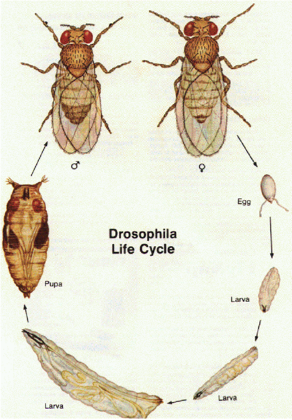
Networks are useful for

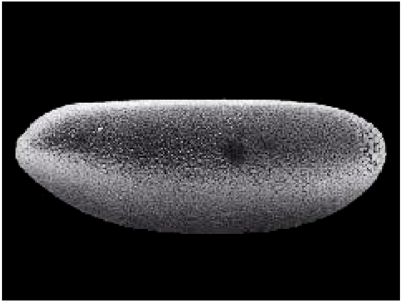
- visualization
- discovery of regularity patterns
- exploratory analysis
- ...

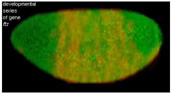
of complex systems.

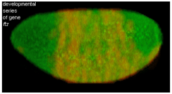


Interactions between variables are not always observable









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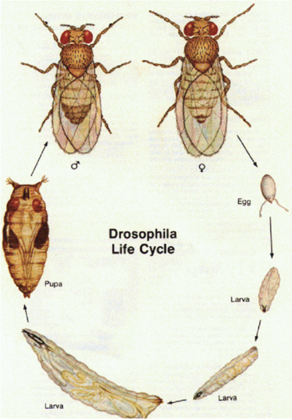
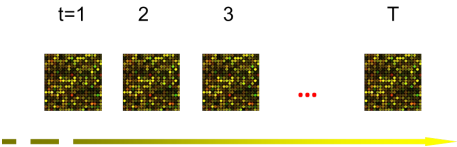
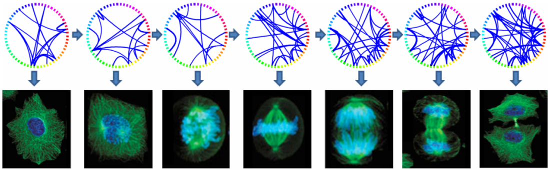
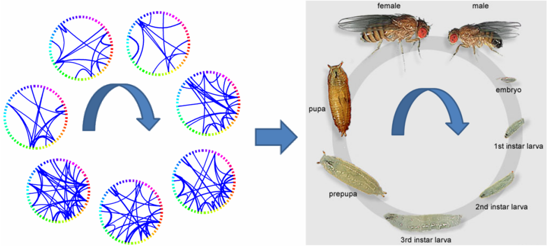


Data collected over a period of time is easily accessible



Estimating time-varying networks





Talk Objective

How to recover *changing* interactions between objects from data *collected over time*?

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Challenges:

- Number of samples small
- Large number of objects
- Noisy data
- Data may contain missing values
- ...

Outline

1. Estimating Conditional Independence Relationships
    - Representation – Markov Networks
    - Estimating Graph Structure

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Outline

Markov Networks

Random vector $\mathbf{X} = (X_1, \ldots, X_p)'$

Graph $G = (V, E)$ with p nodes

- represents conditional independence relationships between nodes

Useful for exploring associations between measured variables

$$(a,b) \notin E \Longleftrightarrow X_a \perp X_b \mid X_{\overline{ab}} \qquad \left(\overline{ab} := V \backslash \{a,b\} \right)$$

$$\mathbb{P}[X_a \mid X_b, X_{\overline{ab}}] = \mathbb{P}[X_a \mid X_{\overline{ab}}]$$

(Koller and Friedman, 2009)

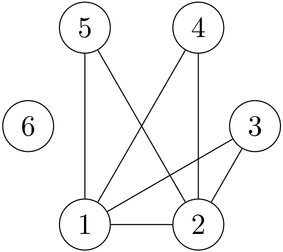
Two Common Markov Networks

Gaussian Markov Network: $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

$$p(\mathbf{x}) \propto \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})\right)$$

The precision matrix $\boldsymbol{\Omega} = \boldsymbol{\Sigma}^{-1}$ encodes both parameters and the graph structure

$$\begin{pmatrix} * & * & * & * & * & 0 \\ * & * & * & * & * & 0 \\ * & * & * & 0 & 0 & 0 \\ * & * & 0 & * & 0 & 0 \\ * & * & 0 & 0 & * & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$



(Koller and Friedman, 2009; Lauritzen, 1996)

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Discrete Markov network: $\mathbf{X} \in \{-1, 1\}^p$ (Ising model)

$$p(\mathbf{x}; \boldsymbol{\Theta}) \propto \exp\left(\sum_{a \in V} x_a \theta_{aa} + \sum_{a,b \in V \times V} x_a x_b \theta_{ab}\right)$$

$\boldsymbol{\Theta} = (\theta_{ab})_{ab}$ encodes the conditional independence relationships

(Koller and Friedman, 2009; Lauritzen, 1996)

Structure Learning Problem

Given an *i.i.d.* sample $\mathcal{D}_n = \{\mathbf{x}_i\}_{i=1}^n$ from a distribution $\mathbb{P} \in \mathcal{P}$

Learn the set of conditional independence relationships

$$\widehat{G} = \widehat{G}(\mathcal{D}_n)$$

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Gaussian Markov Networks (Drton and Perlman, 2007)

- Form the maximum likelihood estimator for the covariance matrix
- Test for zeros in the precision matrix

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Gaussian Markov Networks (Drton and Perlman, 2007)

- Form the maximum likelihood estimator for the covariance matrix
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Discrete Markov Networks (Chickering, 1996)

- Hard to learn structure, since the log partition function cannot be evaluated efficiently

Structure Learning in High-Dimensions

Penalized Pseudo-Likelihood Estimation

- Neighborhood Selection
- Useful for learning the structure of Gaussian and discrete Markov Networks

$$\widehat{\boldsymbol{\theta}}_a = \arg\max_{\boldsymbol{\theta}_a \in \mathbb{R}^p} \sum_{i \in [n]} \gamma(\boldsymbol{\theta}_a; \mathbf{x}_i) - \lambda ||\boldsymbol{\theta}_a||_1$$

Conditional likelihood: $\gamma(\boldsymbol{\theta}_a; \mathbf{x}_i) = \log \mathbb{P}[x_{i,a} \mid \mathbf{x}_{i,\overline{a}}; \boldsymbol{\theta}_a]$

(Meinshausen and Bühlmann, 2006)
(Ravikumar, Wainwright, and Lafferty, 2009)

Neighborhood Selection

Local structure estimation

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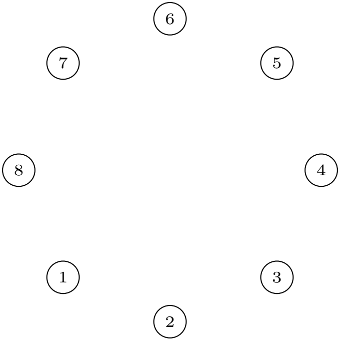

Estimated neighborhood

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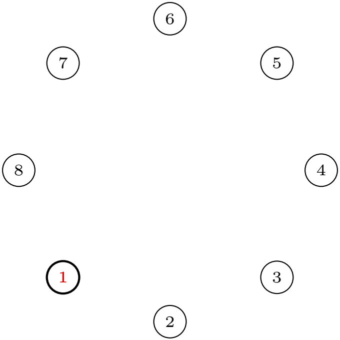

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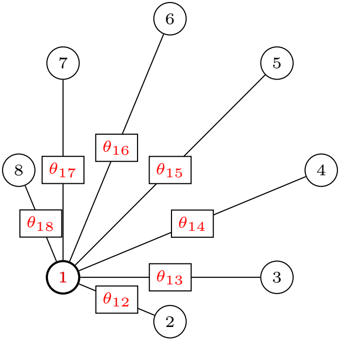

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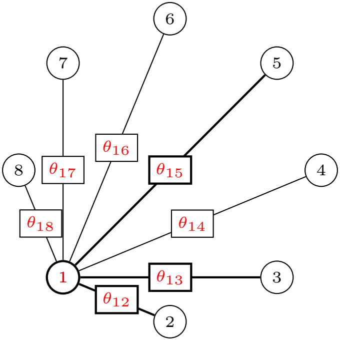

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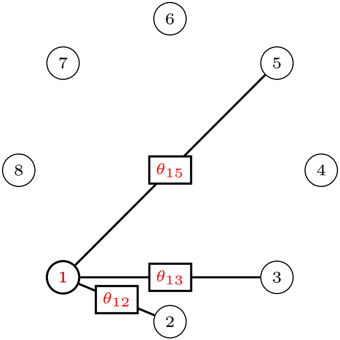
$$\widehat{\mathbf{N}}_a = \{2, 3, 5\}$$



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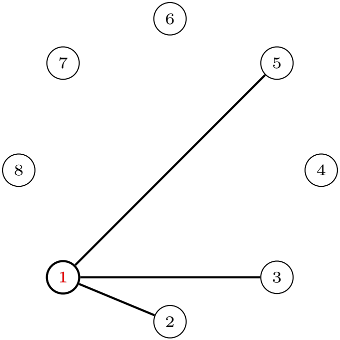

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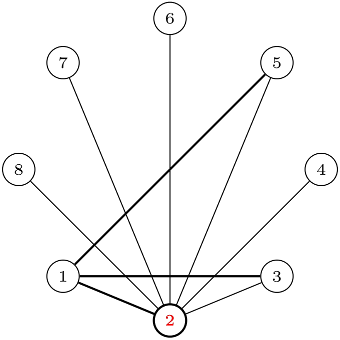

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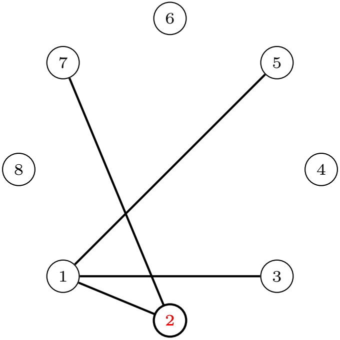

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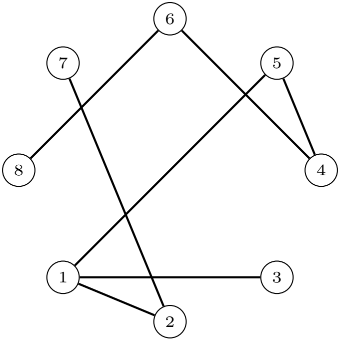

Properties of Neighborhood Selection

Graph structure can be recovered consistently

- provable guarantees in a high-dimensional setting
- Meinshausen and Bühlmann (2006); Ravikumar, Wainwright, and Lafferty (2009) Peng, Wang, Zhou, and Zhu (2009)

Fast estimation procedures

- efficient solvers for ℓ_1 penalized problems
- Beck and Teboulle (2009); Friedman, Hastie, and Tibshirani (2008)

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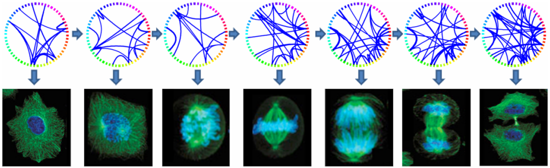
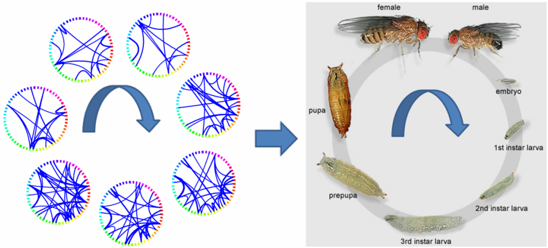
Estimating Time-Varying Networks





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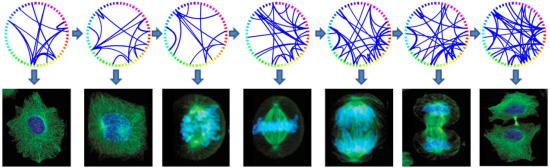
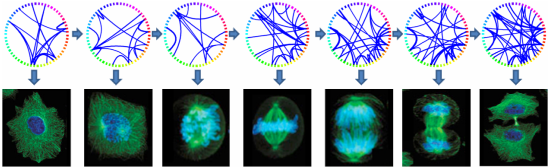


$$\mathbf{x}^t \sim \mathbb{P}(\boldsymbol{\theta}^t; G^t)$$

Estimating Time-Varying Networks



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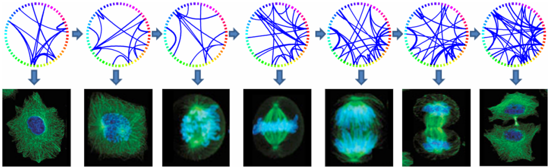
Nodal observations

Estimating Time-Varying Networks



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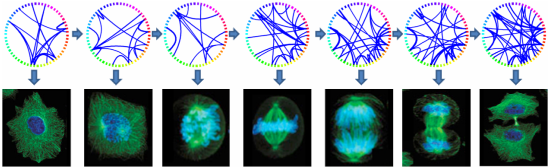

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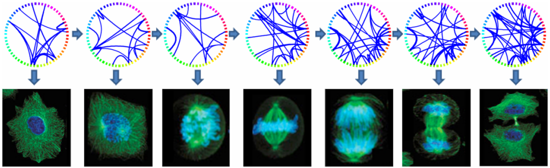

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Varying Structure

$$E^t = \{(a,b) \in V \times V \mid \theta^t_{ab} \neq 0\}$$

General Estimation Framework

Data: $\mathcal{D}_n = \{\mathbf{x}^t \mid \mathbf{x}^t \sim \mathbb{P}(\boldsymbol{\theta}^t; G^t)\}_{t \in \mathcal{T}_n}, \quad \mathcal{T}_n = \{1/n, 2/n, \ldots, 1\}$

$$\arg\max \; \ell(\mathcal{D}_n, \{\boldsymbol{\theta}^t\}) - \text{pen}\left(\{\boldsymbol{\theta}^t\}\right)$$

Loss: $\ell(\mathcal{D}_n, \{\boldsymbol{\theta}^t\})$

- measures the fit of model to data

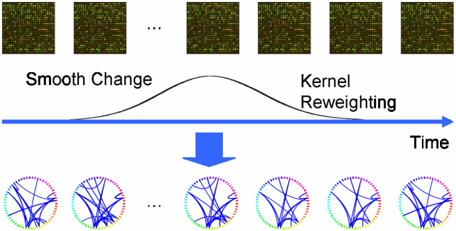
Penalty: $\text{pen}\left(\{\boldsymbol{\theta}^t\}\right)$

- balances the complexity of model and the fit to data
- encodes structural assumptions about model class

Two scenarios

Two scenarios

1. Smooth Networks



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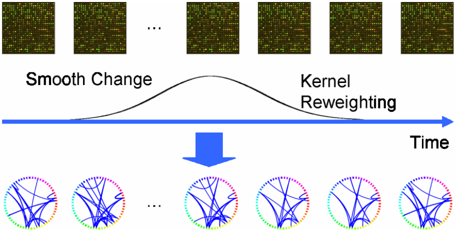
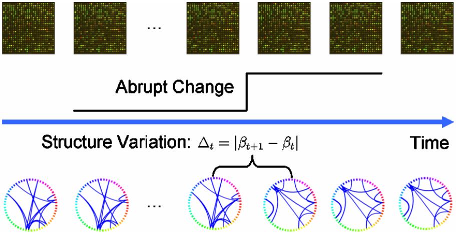
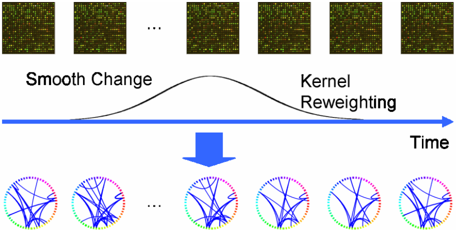


2. Networks With Jumps



Two scenarios

1. **Smooth Networks**
   (Song et al., 2009)
   (Kolar et al., 2010)
   (Kolar and Xing, 2011)
   (Kolar and Xing, 2012c)



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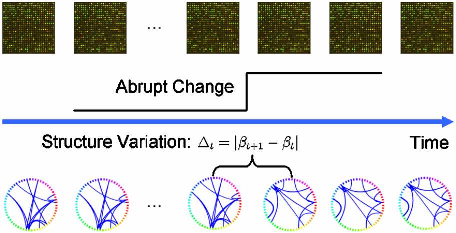
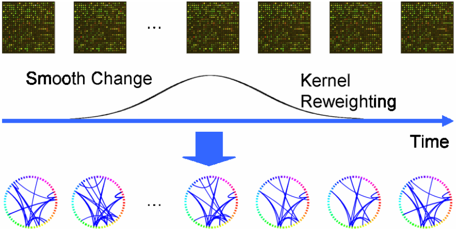


Smoothly Evolving Networks

$$\gamma(\boldsymbol{\theta}; \mathbf{x}_t) = \log \mathbb{P}[x_{t,a} \mid \mathbf{x}_{t,\bar{a}}; \boldsymbol{\theta}]$$

$$w_\tau(t) = \frac{K_h(t-\tau)}{\sum_{t \in \mathcal{T}_n} K_h(t-\tau)}$$



$$\widehat{\boldsymbol{\theta}}_a(\tau) = \arg\max_{\theta} \sum_{t \in \mathcal{T}} w_\tau(t)\gamma(\boldsymbol{\theta}; \mathbf{x}_t) - \lambda ||\boldsymbol{\theta}||_1$$

Kolar, Song, Ahmed, and Xing (2010)

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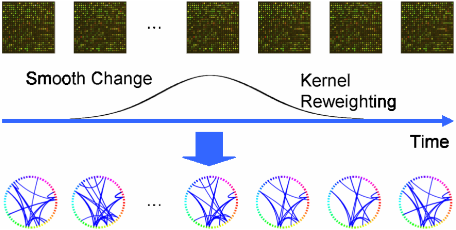

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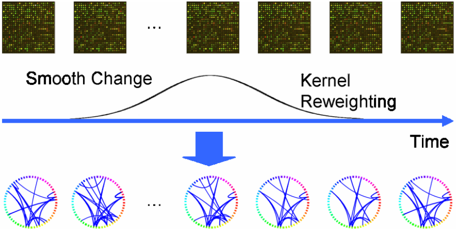

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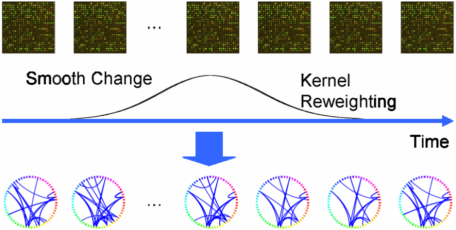

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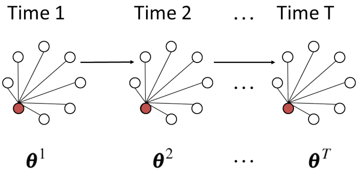

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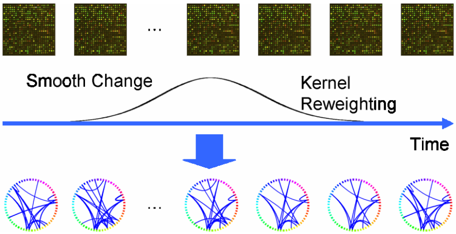
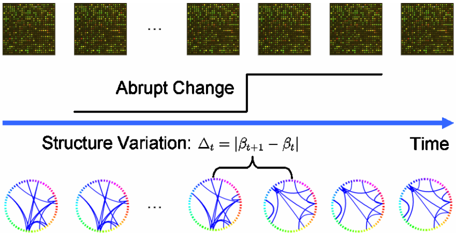
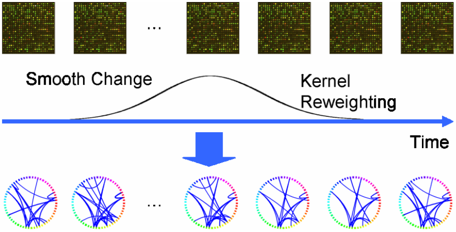


2. Networks With Jumps



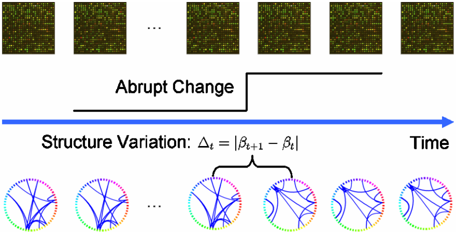
Two scenarios

1. Smooth Networks

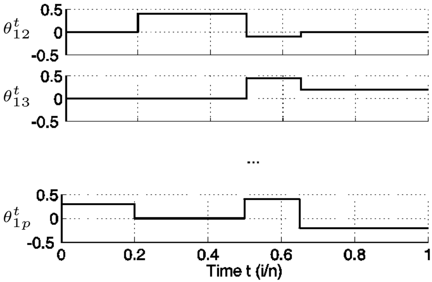


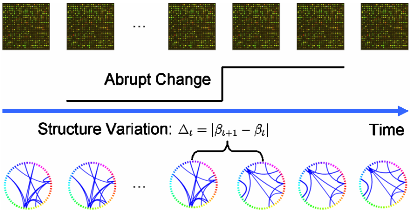
2. **Networks With Jumps**

   (Kolar et al., 2010)
   (Kolar, Song, and Xing, 2009)
   (Kolar and Xing, 2012a)



Networks With Jumps

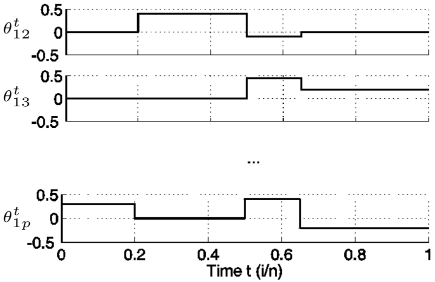


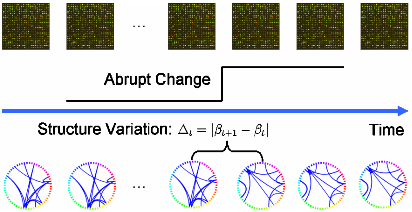


$$\max_{\{\boldsymbol{\theta}^t\}_{t \in \mathcal{T}_n}} \sum_t \gamma(\boldsymbol{\theta}^t; \mathbf{x}^t) - \lambda_1 \sum_t ||\boldsymbol{\theta}^t||_1$$
$$- \lambda_2 \sum_t ||\boldsymbol{\theta}^t - \boldsymbol{\theta}^{t-1}||_2$$

Kolar, Song, Ahmed, and Xing (2010)

Networks With Jumps





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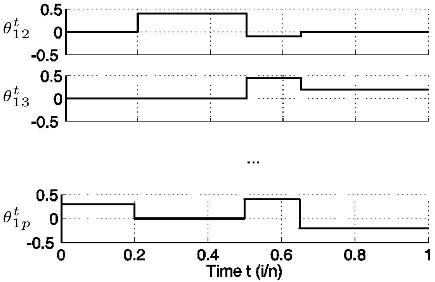
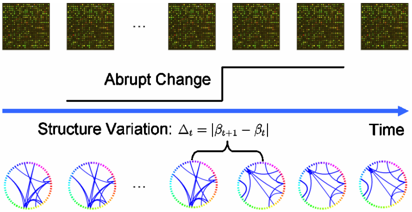
Sparsity

Kolar, Song, Ahmed, and Xing (2010)

Networks With Jumps





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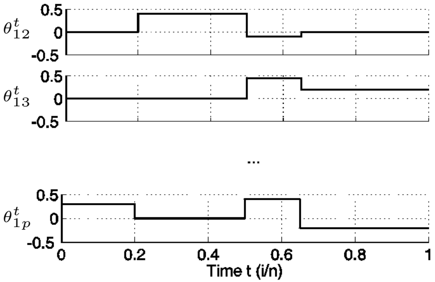
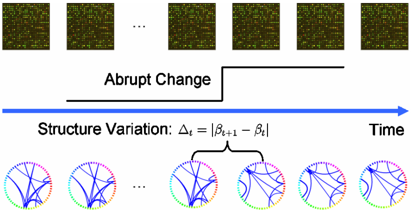
Sparsity

Structural Changes

Kolar, Song, Ahmed, and Xing (2010)

Networks With Jumps





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Sparsity

Structural Changes

Fused Penalty (Tibshirani et al., 2005)

Kolar, Song, Ahmed, and Xing (2010)

Outline

1. Estimating Conditional Independence Relationships
   - Representation – Markov Networks
   - Estimating Graph Structure
2. Time-Varying Networks
   - Smoothly Varying Networks
   - Networks With Jumps
3. An Application
4. Some theoretical results

Outline

Drosophila Life Cycle

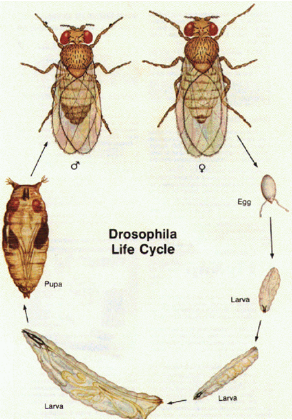
Data from Arbeitman et al. (2002)

66 microarray measurements across full life cycle

Four stages in the life cycle

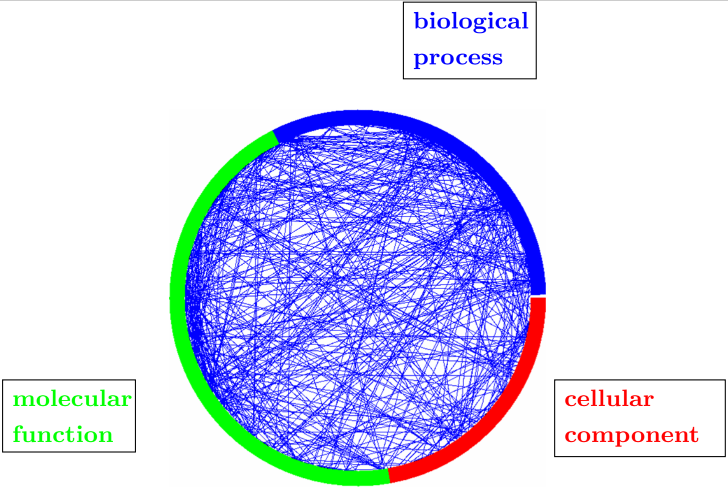
- embryo
- larva
- pupal
- adult

Analyze subset of 588 genes related to development

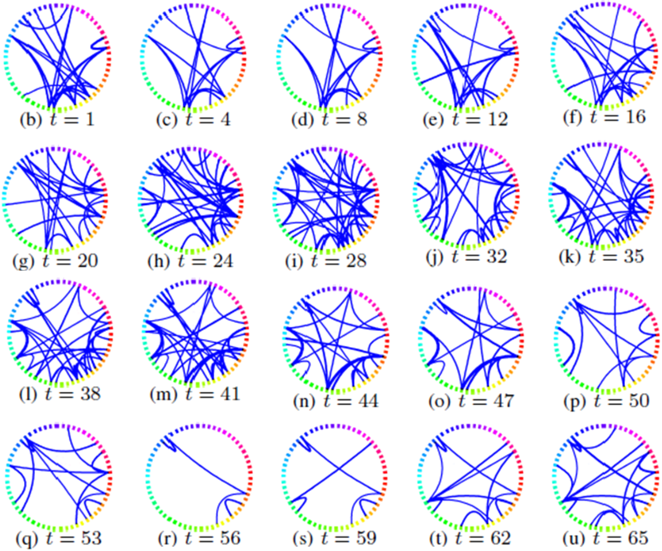


Kolar, Song, Ahmed, and Xing (2010)

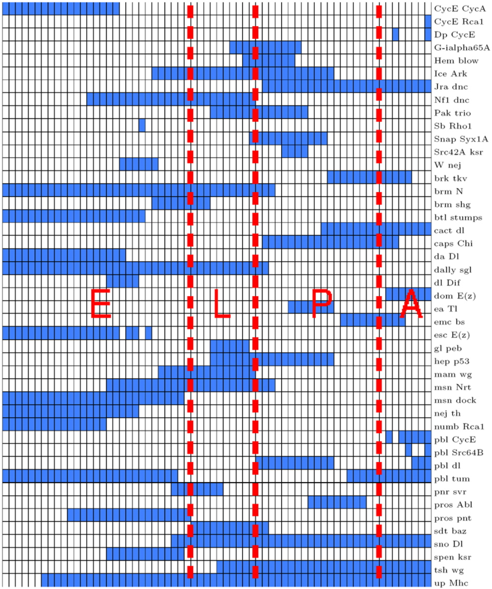
Estimated Dynamic Network



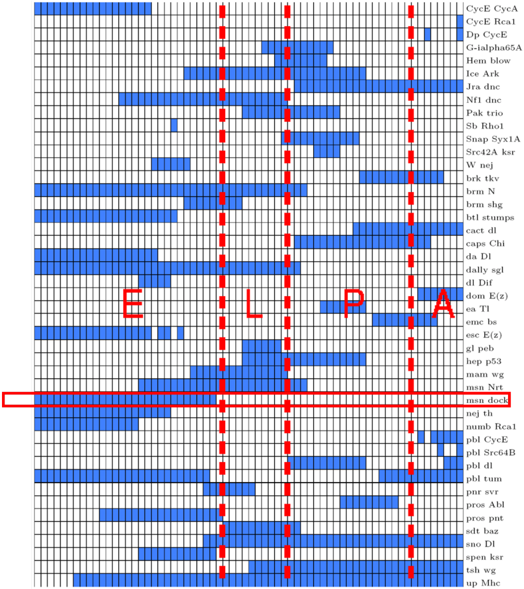
Transient Group Interactions



Known Gene Interactions



Known Gene Interactions



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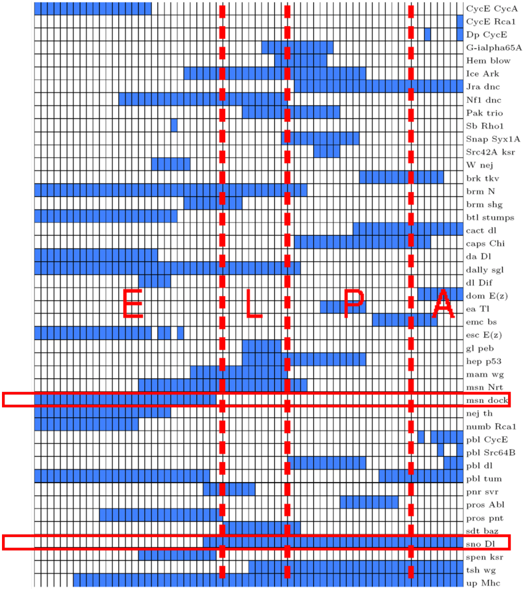

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Theoretical Properties

Theorem (Kolar and Xing (2012c))

Under suitable technical assumptions the graph G^τ is recovered with exponentially high probability for any fixed point $\tau \in [0,1]$.

Fisher information matrix:

$$\mathbf{Q}_a^\tau := \mathbb{E}[\nabla^2 \log \mathbb{P}_{\boldsymbol{\theta}_a^\tau}[X_a|\mathbf{X}_{\overline{a}}]], a \in V, \tau \in [0,1]$$

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Kernel satisfies regularity conditions

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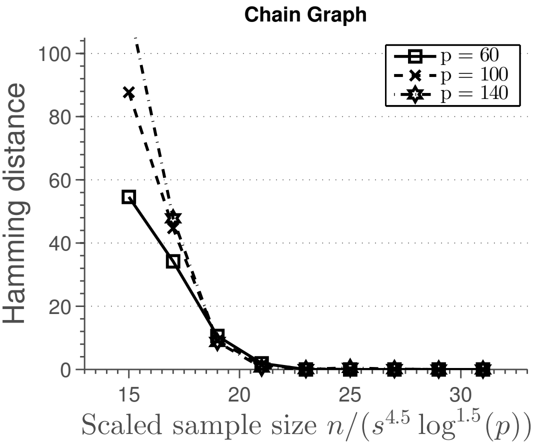
$$\mathbb{P}\left[\text{graph not recovered}\right] = \mathcal{O}\left(\exp\left(-C s^{-3} n h + C' \log p\right)\right) \xrightarrow{n,p\to\infty} 0$$

Simulation Results



Thank you!

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