

Essays on Bioinformatics and Social Network Analysis

Statistical and Computational Methods for Complex Systems

George G Vega Yon

University of Southern California, Department of Preventive Medicine

June 22, 2020

Keck School of
Medicine of USC

Committee

Paul Marjoram (chair), Kayla de la Haye,

Paul D Thomas, Duncan C Thomas, Emilio Ferrara

On the Prediction of Gene Functions Using Phylogenetic Trees (Ch. 2 & 4)

Exponential Random Graph Models for Small Networks (Ch. 5)

Goodness-of-fit for Small Networks (Ch. 3 & 6)

Connecting the Dots: Phylogenetic Modeling with ERGMs (Ch. 4)

Next Steps (Ch. 7)

On the Prediction of Gene Functions Using Phylogenetic Trees

Joint with: Paul D Thomas, Paul Marjoram, Huaiyu Mi, Duncan Thomas, and John Morrison
(Chapters 2 and 4)



- ▶ The GO project has $\sim 44,400$ validated terms ► more, $\sim 7.9M$ annotations on $\sim 4,600$ species.

source: Statistics from <http://pantherdb.org> and <http://geneontology.org>



- ▶ The GO project has $\sim 44,400$ validated terms ► more, $\sim 7.9M$ annotations on $\sim 4,600$ species.
- ▶ About $\sim 550,000$ are on human genes.

source: Statistics from <http://pantherdb.org> and <http://geneontology.org>



- ▶ The GO project has $\sim 44,400$ validated terms ► more, $\sim 7.9M$ annotations on $\sim 4,600$ species.
- ▶ About $\sim 550,000$ are on human genes.
- ▶ Yet, less than 10% of those annotations are based on experimental evidence.

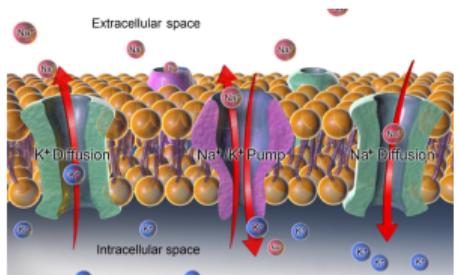
source: Statistics from <http://pantherdb.org> and <http://geneontology.org>

Gene functions can be classified in three types:

Gene functions can be classified in three types:

Molecular function

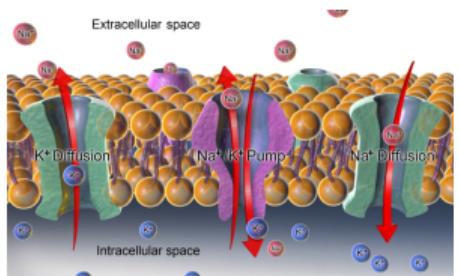
Active transport GO:0005215



Gene functions can be classified in three types:

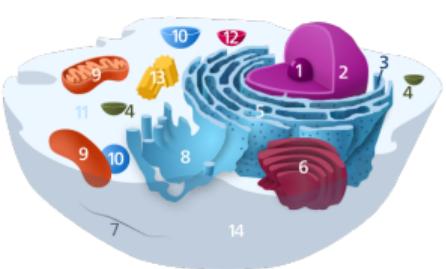
Molecular function

Active transport GO:0005215



Cellular component

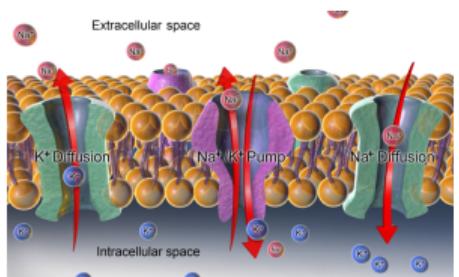
Mitochondria GO:0004016



Gene functions can be classified in three types:

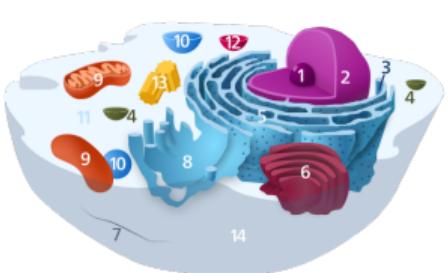
Molecular function

Active transport GO:0005215



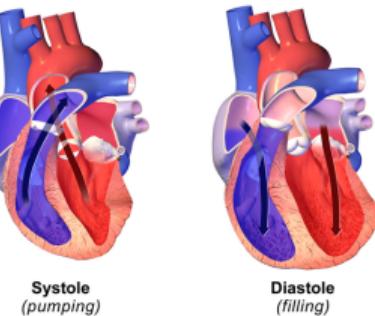
Cellular component

Mitochondria GO:0004016



Biological process

Heart contraction GO:0060047



GO Annotations and Phylogenetic Trees

Family: PTHR11258

see a bad one



Node type

- Duplication
- Other

GO Annotations and Phylogenetic Trees

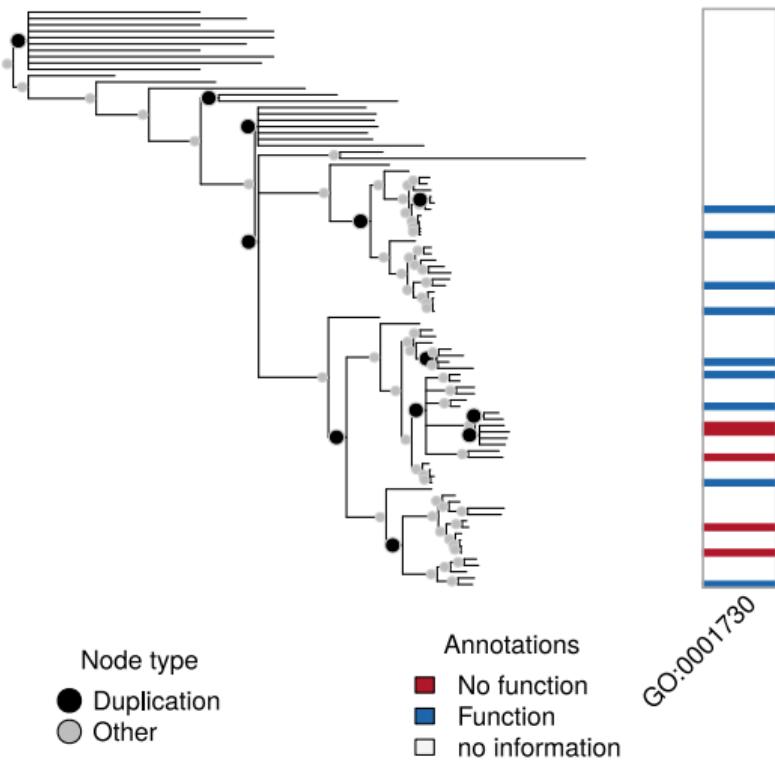
Family: PTHR11258

Type: Molecular Function

Name: 2'-5'-oligoadenylate synthetase activity

Desc: GO:0001730 involved in the process of cellular antiviral activity (wiki on [interferon](#)).

see a bad one



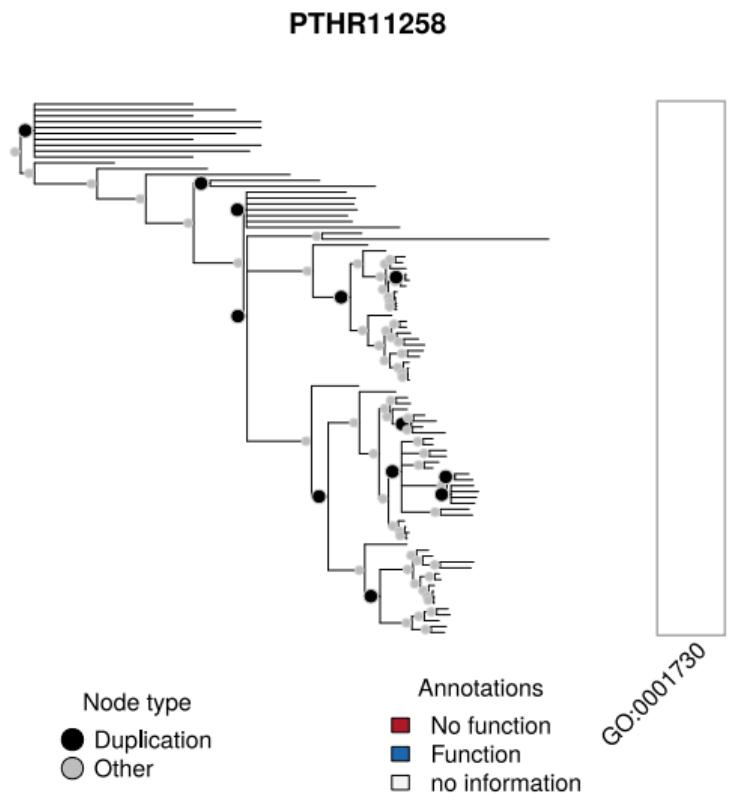
An evolutionary model of gene functions

Image a relay race...

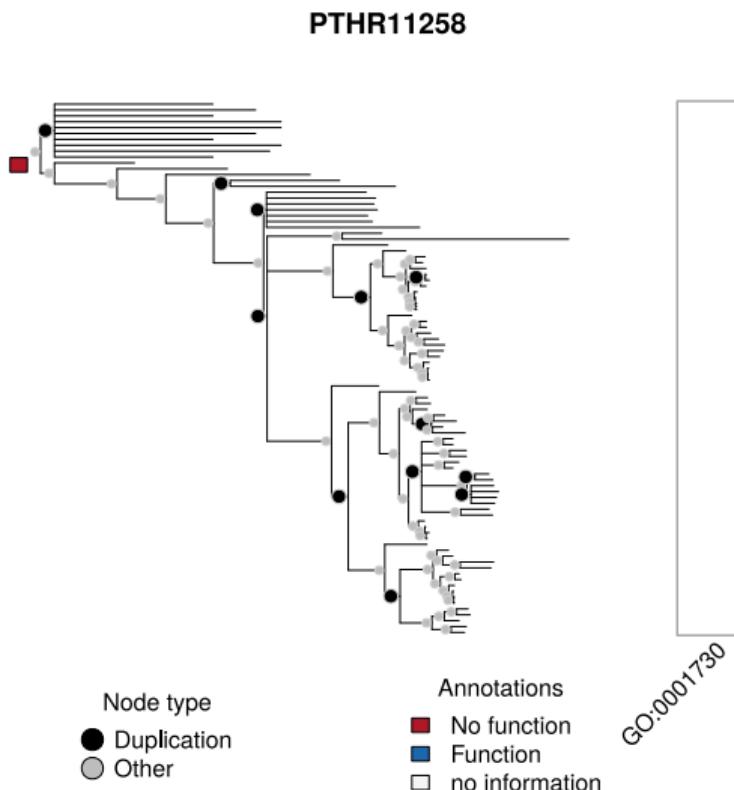


Figure 1 ISTAF 2019 4 × 100 m relay race (Martin Rulsch, wikimedia)

An evolutionary model of gene functions



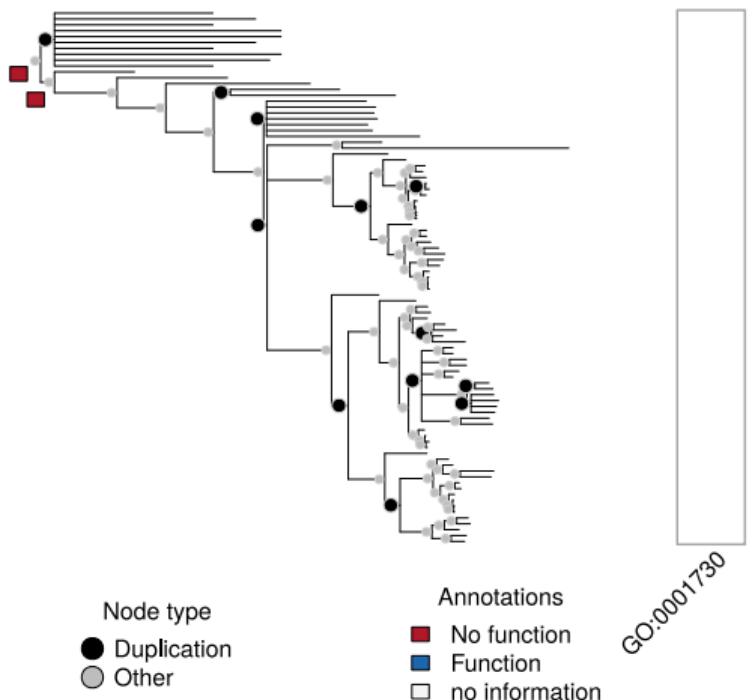
An evolutionary model of gene functions



- ▶ Starting with the root node (no function in this case).

An evolutionary model of gene functions

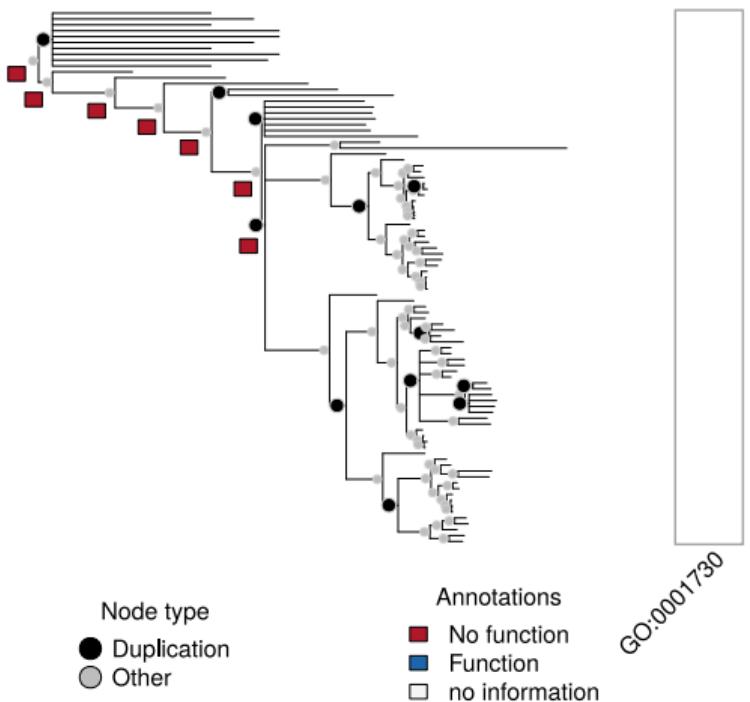
PTHR11258



- ▶ Starting with the root node (no function in this case).
- ▶ Passes the baton to its offspring.

An evolutionary model of gene functions

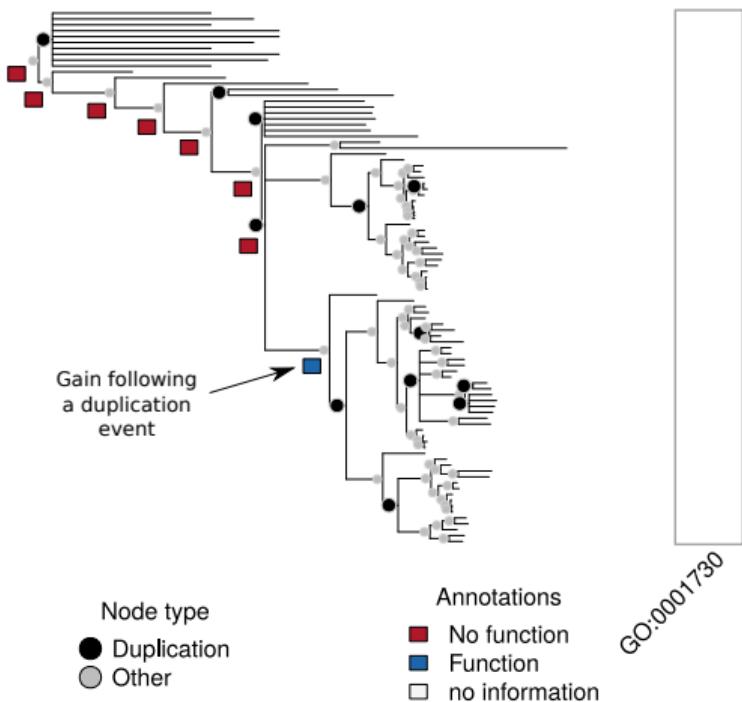
PTHR11258



- ▶ Starting with the root node (no function in this case).
- ▶ Passes the baton to its offspring.
- ▶ Possibly without change.

An evolutionary model of gene functions

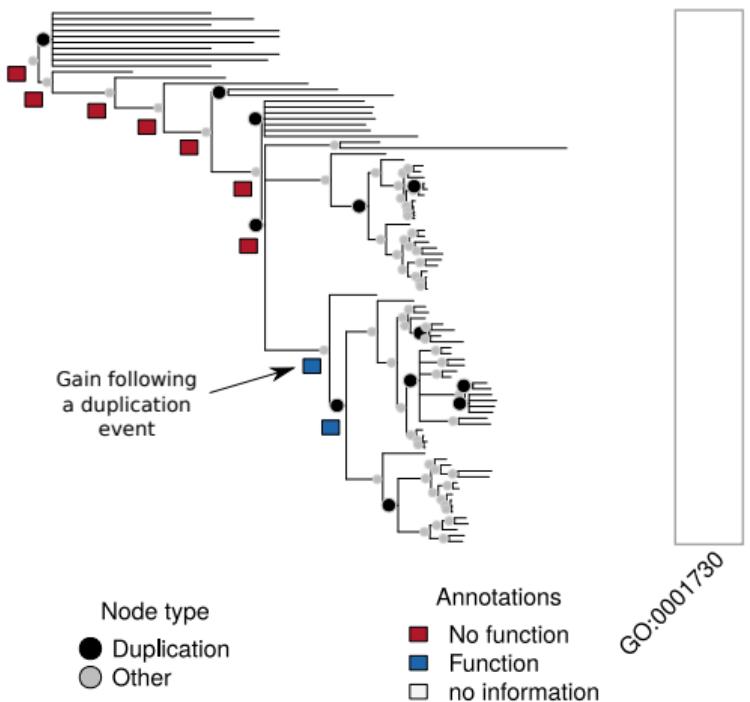
PTHR11258



- ▶ Starting with the root node (no function in this case).
- ▶ Passes the baton to its offspring.
- ▶ Possibly without change.
- ▶ Or, with some probability, gaining...

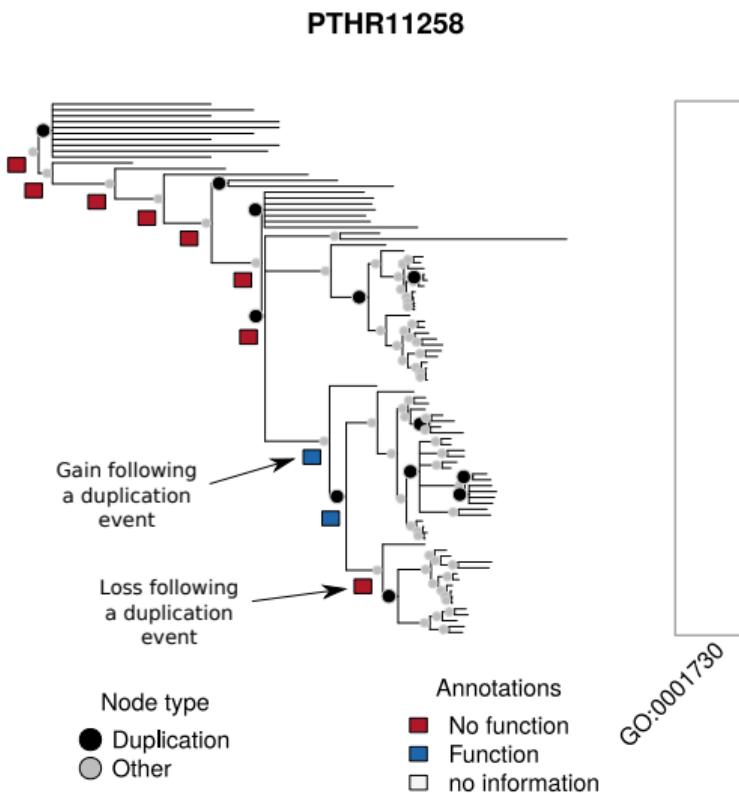
An evolutionary model of gene functions

PTHR11258



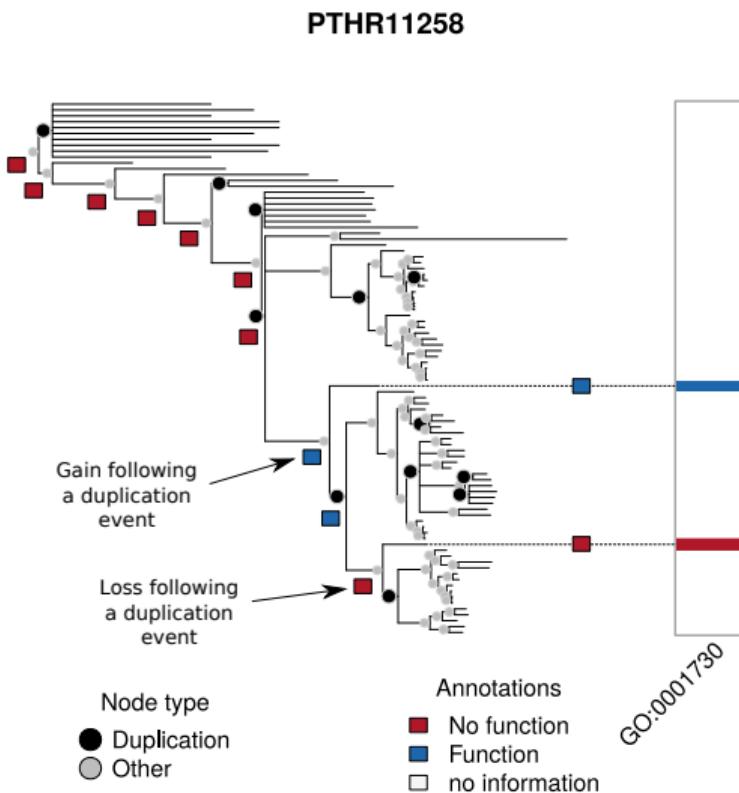
- ▶ Starting with the root node (no function in this case).
- ▶ Passes the baton to its offspring.
- ▶ Possibly without change.
- ▶ Or, with some probability, gaining...

An evolutionary model of gene functions



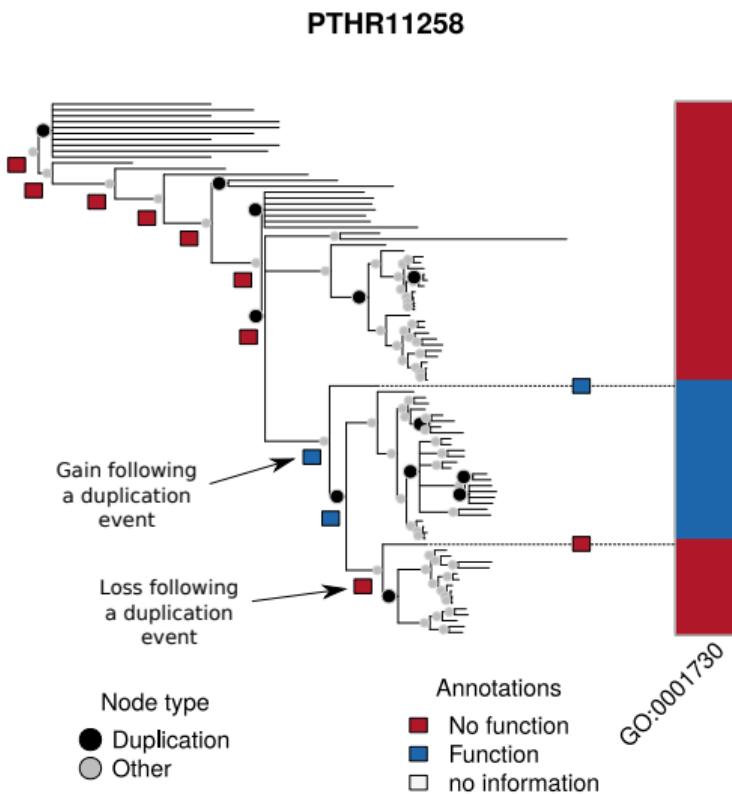
- ▶ Starting with the root node (no function in this case).
- ▶ Passes the baton to its offspring.
- ▶ Possibly without change.
- ▶ Or, with some probability, gaining... or loosing the function.

An evolutionary model of gene functions



- ▶ Starting with the root node (no function in this case).
- ▶ Passes the baton to its offspring.
- ▶ Possibly without change.
- ▶ Or, with some probability, gaining... or loosing the function.
- ▶ Until the baton reaches the end of the tree (modern genes).

An evolutionary model of gene functions



- ▶ Starting with the root node (no function in this case).
- ▶ Passes the baton to its offspring.
- ▶ Possibly without change.
- ▶ Or, with some probability, gaining... or loosing the function.
- ▶ Until the baton reaches the end of the tree (modern genes).

[► more on duplication](#)

[► alt view](#)

Example of Data + Predictions

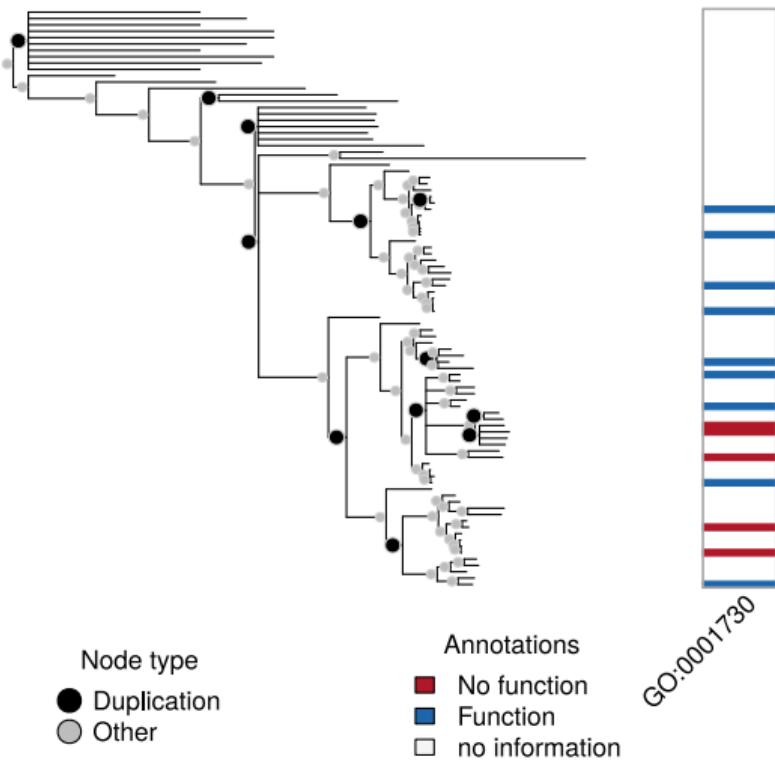
Family: PTHR11258

Type: Molecular Function

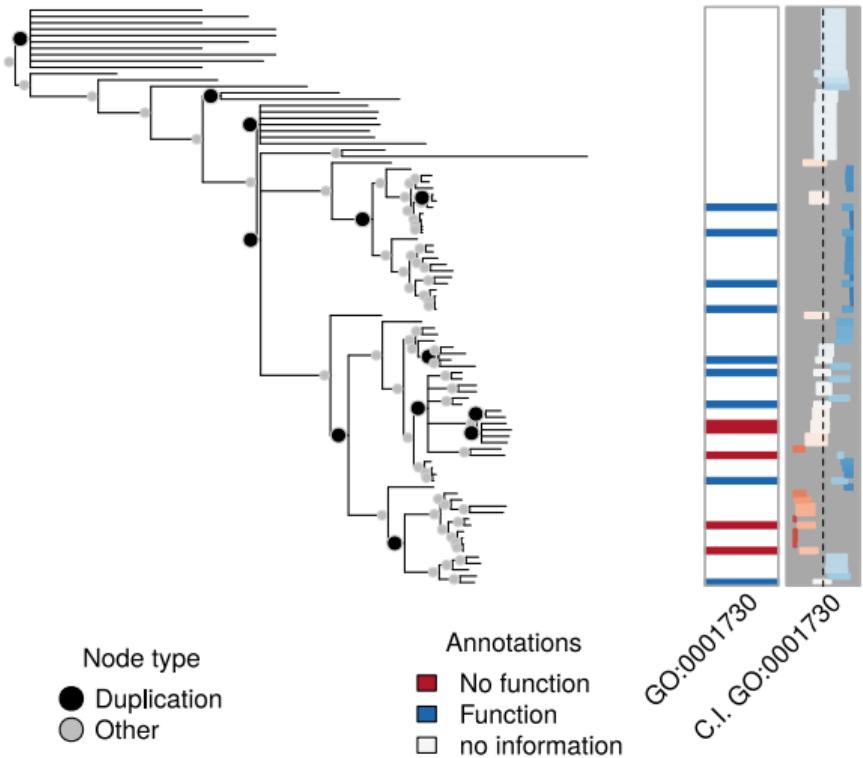
Name: 2'-5'-oligoadenylate synthetase activity

Desc: GO:0001730 involved in the process of cellular antiviral activity (wiki on [interferon](#)).

see a bad one



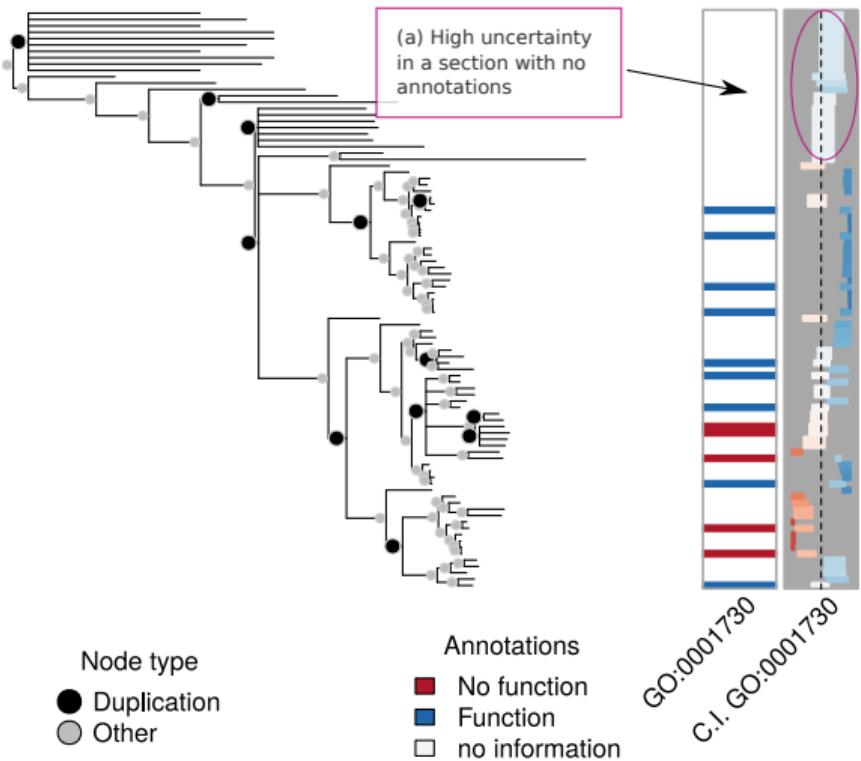
Example of Data + Predictions

Family: PTHR11258**Type:** Molecular Function**Name:** 2'-5'-oligoadenylate synthetase activity**Desc:** GO:0001730 involved in the process of cellular antiviral activity (wiki on [interferon](#)).**MAE:** 0.34**AUC:** 0.91[see a bad one](#)

Example of Data + Predictions

Family: PTHR11258**Type:** Molecular Function**Name:** 2'-5'-oligoadenylate synthetase activity**Desc:** GO:0001730 involved in the process of cellular antiviral activity (wiki on [interferon](#)).**MAE:** 0.34**AUC:** 0.91

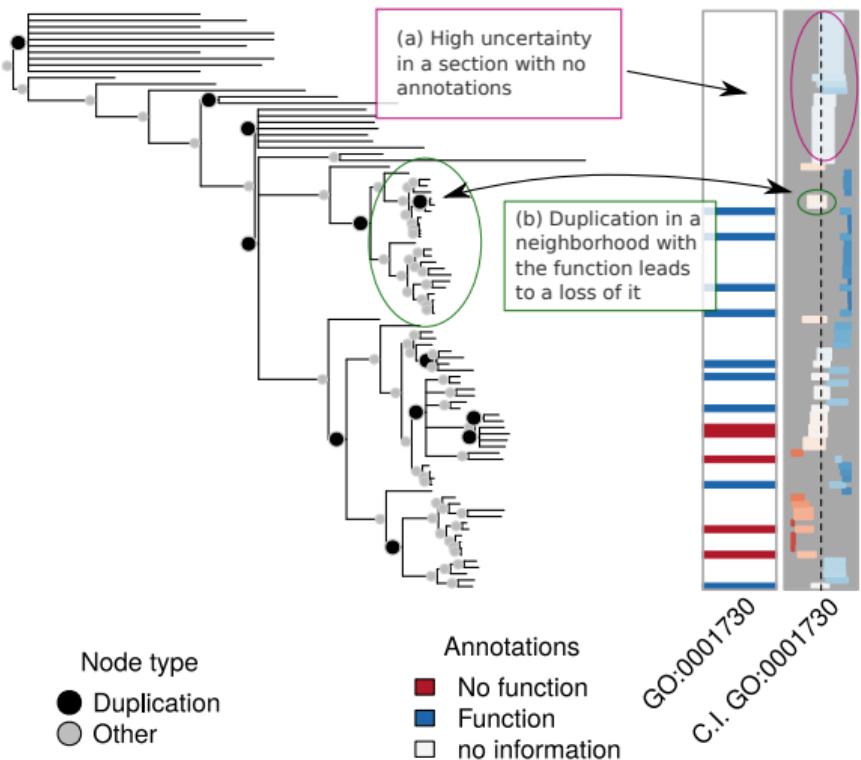
see a bad one



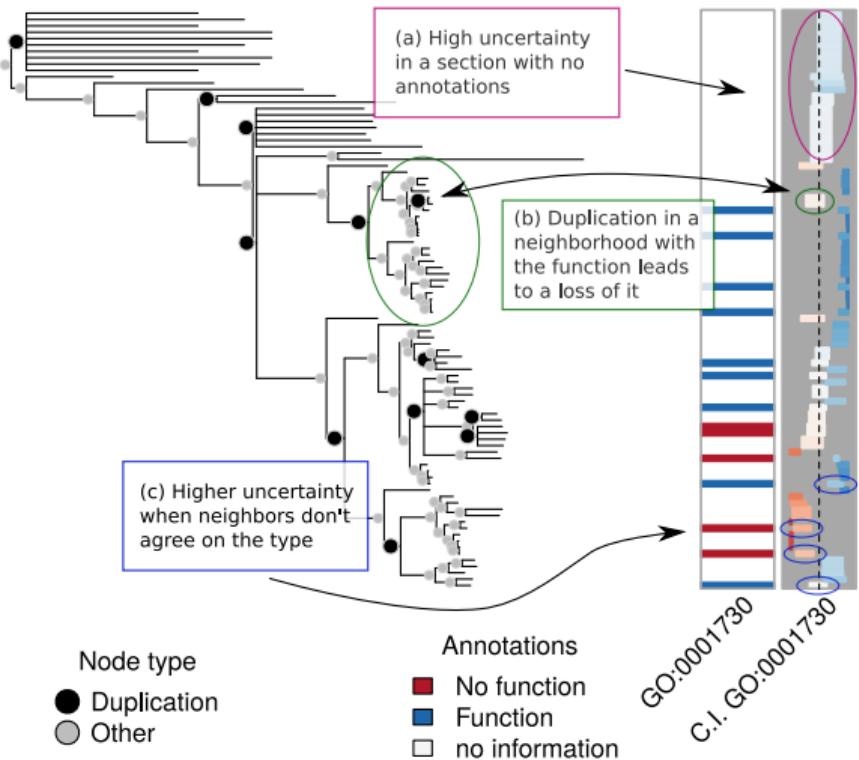
Example of Data + Predictions

Family: PTHR11258**Type:** Molecular Function**Name:** 2'-5'-oligoadenylate synthetase activity**Desc:** GO:0001730 involved in the process of cellular antiviral activity (wiki on [interferon](#)).**MAE:** 0.34**AUC:** 0.91

see a bad one



Example of Data + Predictions

Family: PTHR11258**Type:** Molecular Function**Name:** 2'-5'-oligoadenylate synthetase activity**Desc:** GO:0001730 involved in the process of cellular antiviral activity (wiki on [interferon](#)).**MAE:** 0.34**AUC:** 0.91[see a bad one](#)

Results from the first version

Scalable

Pooled-data model
including hundreds of
trees (thousands of
genes) fitted within
minutes.

Scalable

Pooled-data model including hundreds of trees (thousands of genes) fitted within minutes.

Robust

Accuracy and estimates are consistent regardless of the used prior.

Scalable

Pooled-data model including hundreds of trees (thousands of genes) fitted within minutes.

Robust

Accuracy and estimates are consistent regardless of the used prior.

Intuitive

Gains and losses are more likely to happen at **duplication** events.

Scalable

Pooled-data model including hundreds of trees (thousands of genes) fitted within minutes.

Robust

Accuracy and estimates are consistent regardless of the used prior.

Intuitive

Gains and losses are more likely to happen at **duplication** events.

Competitive

Matches state-of-the-art phylo-based prediction models with ~ 0.75 AUC.

Scalable

Pooled-data model including hundreds of trees (thousands of genes) fitted within minutes.

Robust

Accuracy and estimates are consistent regardless of the used prior.

Intuitive

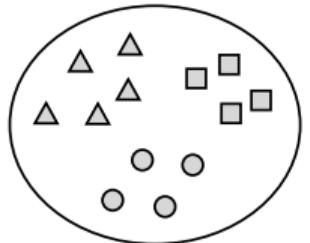
Gains and losses are more likely to happen at **duplication** events.

Competitive

Matches state-of-the-art phylo-based prediction models with ~ 0.75 AUC.

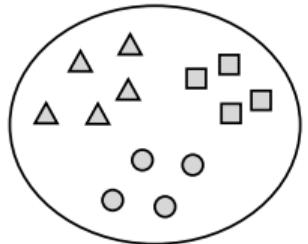
...all this assuming that all functions had the same gain/loss rate.

Phylogenetics Modeling: Pooling data



(a) Fixed rate
across functions

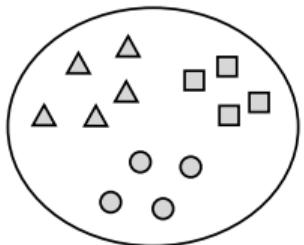
Phylogenetics Modeling: Pooling data



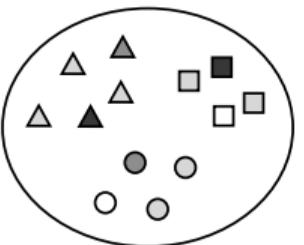
(a) Fixed rate
across functions

(a) Featured in the first version of the model.

Phylogenetics Modeling: Pooling data



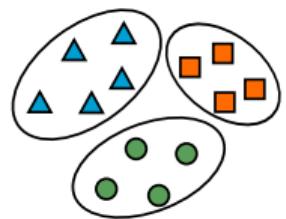
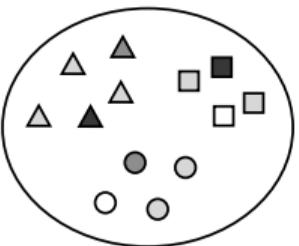
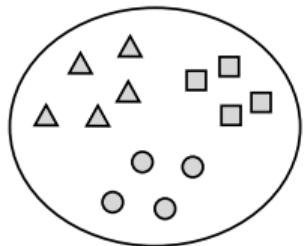
(a) Fixed rate
across functions



(b) Random rate
across functions

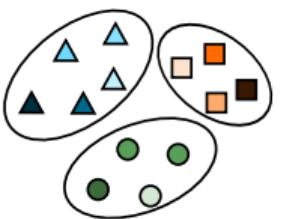
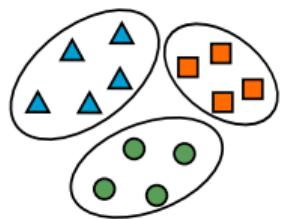
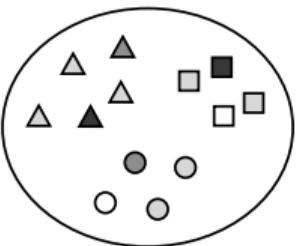
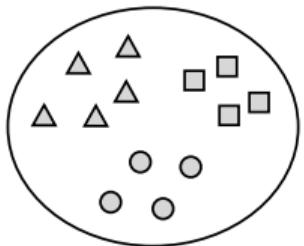
- (a) Featured in the first version of the model.
- (b) “Full glory” Hierarchical Bayes (1,001 parameters for the 141 functions).

Phylogenetics Modeling: Pooling data



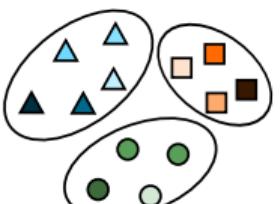
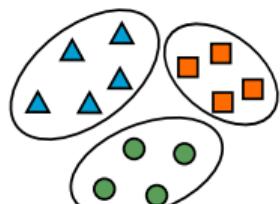
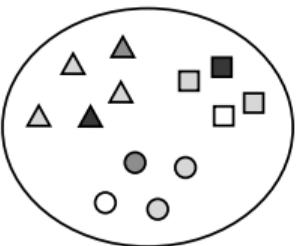
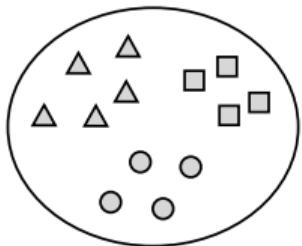
- (a) Featured in the first version of the model.
- (b) “Full glory” Hierarchical Bayes (1,001 parameters for the 141 functions).
- (c) Distilled version (a), improves accuracy.

Phylogenetics Modeling: Pooling data



- (a) Featured in the first version of the model.
- (b) “Full glory” Hierarchical Bayes (1,001 parameters for the 141 functions).
- (c) Distilled version (a), improves accuracy.
- (d) Model estimated for Molecular Function (using Empirical Bayes) without significant improvements.

Phylogenetics Modeling: Pooling data



- (a) Featured in the first version of the model.
- (b) “Full glory” Hierarchical Bayes (1,001 parameters for the 141 functions).
- (c) Distilled version (a), improves accuracy.
- (d) Model estimated for Molecular Function (using Empirical Bayes) without significant improvements.

All methods are now available in the `aphylo` package: `aphylo_mle`, `aphylo_mcmc`, and `aphylo_hier`.

Overview of Prediction Results

	Pooled	Type of Annotation		
		Molecular Function	Biological Process	Cellular Component
Mislabeling				
ψ_{01}	0.23	0.18	0.09	
ψ_{10}	0.01	0.01	0.01	
Duplication Events				
μ_{d01}	0.97	0.97	0.10	
μ_{d10}	0.52	0.51	0.03	
Speciation Events				
μ_{s01}	0.05	0.05	0.05	
μ_{s10}	0.01	0.01	0.02	
Root node				
π	0.79	0.71	0.88	
Trees	141	74	45	22
Accuracy under the by-aspect model				
AUC	-	0.77	0.83	
MAE	-	0.34	0.26	
Accuracy under the pooled-data model				
AUC	-	0.77	0.75	
MAE	-	0.35	0.34	

Previously, joint estimates out-performed one-at-a-time

Overview of Prediction Results

	Pooled	Type of Annotation		
		Molecular Function	Biological Process	Cellular Component
Mislabeling				
ψ_{01}	0.23	0.18	0.09	
ψ_{10}	0.01	0.01	0.01	
Duplication Events				
μ_{d01}	0.97	0.97	0.10	
μ_{d10}	0.52	0.51	0.03	
Speciation Events				
μ_{s01}	0.05	0.05	0.05	
μ_{s10}	0.01	0.01	0.02	
Root node				
π	0.79	0.71	0.88	
Trees	141	74	45	22
Accuracy under the by-aspect model				
AUC	-	0.77	0.83	
MAE	-	0.34	0.26	
Accuracy under the pooled-data model				
AUC	-	0.77	0.75	
MAE	-	0.35	0.34	

Previously, joint estimates out-performed one-at-a-time

► **Molecular Function** No change.

Overview of Prediction Results

	Pooled	Type of Annotation		
		Molecular Function	Biological Process	Cellular Component
Mislabeling				
ψ_{01}	0.23	0.18	0.09	
ψ_{10}	0.01	0.01	0.01	
Duplication Events				
μ_{d01}	0.97	0.97	0.10	
μ_{d10}	0.52	0.51	0.03	
Speciation Events				
μ_{s01}	0.05	0.05	0.05	
μ_{s10}	0.01	0.01	0.02	
Root node				
π	0.79	0.71	0.88	
Trees	141	74	45	22
Accuracy under the by-aspect model				
AUC	-	0.77	0.83	
MAE	-	0.34	0.26	
Accuracy under the pooled-data model				
AUC	-	0.77	0.75	
MAE	-	0.35	0.34	

Previously, joint estimates out-performed one-at-a-time

► **Molecular Function** No change.

► **Biological Process** Significantly better.

Overview of Prediction Results

	Pooled	Type of Annotation		
		Molecular Function	Biological Process	Cellular Comp.
Mislabeling				
ψ_{01}	0.23	0.18	0.09	
ψ_{10}	0.01	0.01	0.01	
Duplication Events				
μ_{d01}	0.97	0.97	0.10	
μ_{d10}	0.52	0.51	0.03	
Speciation Events				
μ_{s01}	0.05	0.05	0.05	?
μ_{s10}	0.01	0.01	0.02	
Root node				
π	0.79	0.71	0.88	
Trees	141	74	45	22
Accuracy under the by-aspect model				
AUC	-	0.77	0.83	
MAE	-	0.34	0.26	
Accuracy under the pooled-data model				
AUC	-	0.77	0.75	
MAE	-	0.35	0.34	

Previously, joint estimates out-performed one-at-a-time

- ▶ **Molecular Function** No change.
- ▶ **Biological Process** Significantly better.
- ▶ **Cellular Component** Does not converge.

Overview of Prediction Results

	Pooled	Type of Annotation		
		Molecular Function	Biological Process	Cellular Component
Mislabeling				
ψ_{01}	0.23	0.18	0.09	
ψ_{10}	0.01	0.01	0.01	
Duplication Events				
μ_{d01}	0.97	0.97	0.10	
μ_{d10}	0.52	0.51	0.03	
Speciation Events				
μ_{s01}	0.05	0.05	0.05	?
μ_{s10}	0.01	0.01	0.02	
Root node				
π	0.79	0.71	0.88	
Trees	141	74	45	22
Accuracy under the by-aspect model				
AUC	-	0.77	0.83	
MAE	-	0.34	0.26	
Accuracy under the pooled-data model				
AUC	-	0.77	0.75	
MAE	-	0.35	0.34	

Previously, joint estimates out-performed one-at-a-time

- ▶ **Molecular Function** No change.
- ▶ **Biological Process** Significantly better.
- ▶ **Cellular Component** Does not converge.

Molecular Function \neq Biological Process ? Cellular Component

▶ data

Exponential Random Graph Models for Small Networks

Joint with: Andrew Slaughter and Kayla de la Haye
(Chapter 2)



Data: Friendship network of a UK university faculty

from `igraphdata`. Viz: R package `netplot` (yours truly,

github.com/usccana/netplot)

- ▶ If COVID-19 has taught us something it is that networks matter.



Data: Friendship network of a UK university faculty
from `igraphdata`. Viz: R package `netplot` (yours truly,
github.com/usccana/netplot)

- ▶ If COVID-19 has taught us something it is that networks matter.
- ▶ And especially small networks: Families, teams, friends, etc.



Data: Friendship network of a UK university faculty
from `igraphdata`. Viz: R package `netplot` (yours truly,
github.com/usccana/netplot)

- ▶ If COVID-19 has taught us something it is that networks matter.
- ▶ And especially small networks: Families, teams, friends, etc. The cornerstone of larger social systems.



Data: Friendship network of a UK university faculty
from `igraphdata`. Viz: R package `netplot` (yours truly,
github.com/usccana/netplot)

- ▶ If COVID-19 has taught us something it is that networks matter.
- ▶ And especially small networks: Families, teams, friends, etc. The cornerstone of larger social systems.
- ▶ We can study networks using ERGMs.

Data: Friendship network of a UK university faculty
from `igraphdata`. Viz: R package `netplot` (yours truly,
github.com/usccana/netplot)



What are Exponential Random Graph Models

Exponential Family Random Graph Models, aka ERGMs are:

What are Exponential Random Graph Models

Exponential Family Random Graph Models, aka **ERGMs** are:

- ▶ Statistical models of (social) networks.

What are Exponential Random Graph Models

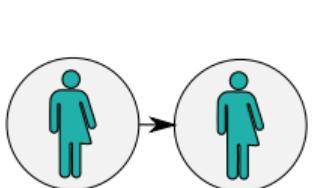
Exponential Family Random Graph Models, aka **ERGMs** are:

- ▶ Statistical models of (social) networks.
- ▶ Not about individual ties, but about local structures.

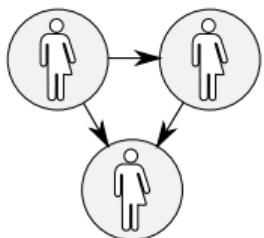
What are Exponential Random Graph Models

Exponential Family Random Graph Models, aka **ERGMs** are:

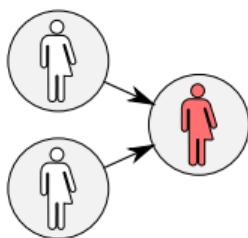
- ▶ Statistical models of (social) networks.
- ▶ Not about individual ties, but about local structures.



Homophily



Transitive Triad



Popularity

Discrete Exponential-Family Models

$$\mathbb{P}(\mathbf{G} = \mathbf{g} \mid X = x) = \frac{\exp\{\boldsymbol{\theta}^t s(\mathbf{g}, x)\}}{\sum_{\mathbf{g}' \in \mathcal{G}} \exp\{\boldsymbol{\theta}^t s(\mathbf{g}', x)\}}, \quad \forall \mathbf{g} \in \mathcal{G}$$

A vector of model parameters A vector of sufficient statistics

Observed data The normalizing constant All possible networks

Discrete Exponential-Family Models

$$\mathbb{P}(\mathbf{G} = \mathbf{g} \mid X = x) = \frac{\exp\{\theta^t s(\mathbf{g}, x)\}}{\sum_{\mathbf{g}' \in \mathcal{G}} \exp\{\theta^t s(\mathbf{g}', x)\}}, \quad \forall \mathbf{g} \in \mathcal{G}$$

A vector of model parameters A vector of sufficient statistics

Observed data The normalizing constant All possible networks

- ▶ For any 0/1 matrix of size $(n \times m)$, there are $2^{(n \times m)}$ possible realizations.

Discrete Exponential-Family Models

$$\mathbb{P}(\mathbf{G} = \mathbf{g} \mid X = x) = \frac{\exp\{\theta^t s(\mathbf{g}, x)\}}{\sum_{\mathbf{g}' \in \mathcal{G}} \exp\{\theta^t s(\mathbf{g}', x)\}}, \quad \forall \mathbf{g} \in \mathcal{G}$$

A vector of model parameters A vector of sufficient statistics

Observed data The normalizing constant All possible networks

- ▶ For any 0/1 matrix of size $(n \times m)$, there are $2^{(n \times m)}$ possible realizations.
- ▶ A directed graph of size 5 has 1,048,576 possible configurations!

Discrete Exponential-Family Models

$$\mathbb{P}(\mathbf{G} = \mathbf{g} \mid X = x) = \frac{\exp\{\boldsymbol{\theta}^t s(\mathbf{g}, x)\}}{\sum_{\mathbf{g}' \in \mathcal{G}} \exp\{\boldsymbol{\theta}^t s(\mathbf{g}', x)\}}, \quad \forall \mathbf{g} \in \mathcal{G}$$

A vector of model parameters A vector of sufficient statistics

Observed data The normalizing constant All possible networks

- ▶ For any 0/1 matrix of size $(n \times m)$, there are $2^{(n \times m)}$ possible realizations.
- ▶ A directed graph of size 5 has 1,048,576 possible configurations!
- ▶ Most (all) applications use **approximations**...

Discrete Exponential-Family Models

$$\mathbb{P}(\mathbf{G} = \mathbf{g} \mid X = x) = \frac{\exp \{ \theta^t s(\mathbf{g}, x) \}}{\sum_{\mathbf{g}' \in \mathcal{G}} \exp \{ \theta^t s(\mathbf{g}', x) \}}, \quad \forall \mathbf{g} \in \mathcal{G}$$

A vector of model parameters A vector of sufficient statistics

Observed data The normalizing constant All possible networks

- ▶ For any 0/1 matrix of size $(n \times m)$, there are $2^{(n \times m)}$ possible realizations.
- ▶ A directed graph of size 5 has 1,048,576 possible configurations!
- ▶ Most (all) applications use **approximations**... yet, for sufficiently small graphs we “can be exact”.

▶ more theory ▶ more terms

ergmito: Estimation of Small ERGM using Exact Statistics

Using exact statistics means:

- Higher convergence rate.
- Lower type-I error rate.
- Smaller bias.
- More power.
- Faster.
- More flexible.

CRAN - Package ergmito

ergmito: Exponential Random Graph Models for Small Networks

Simulation and estimation of Exponential Random Graph Models (ERGMs) for small networks using exact statistics. As a difference from the 'ergm' package, 'ergmito' circumvents using Markov-Chain Maximum Likelihood Estimator (MC-MLE) and instead uses Maximum Likelihood Estimator (MLE) to fit ERGMs for small networks. As exhaustive enumeration is computationally feasible for small networks, this R package takes advantage of this and provides tools for calculating likelihood functions, and other relevant functions, directly, meaning that in many cases both estimation and simulation of ERGMs for small networks can be faster and more accurate than simulation-based algorithms.

Version: 0.2-1
Depends: R (≥ 3.3.0)
Imports: ergm, network, MASS, Rcpp, texreg, stats, parallel, utils, methods, graphics
LinkingTo: Rcpp, RcppArmadillo
Suggests: covr, sna, lmtest, fmcmc, coda, knitr, rmarkdown, tinytest
Published: 2020-02-12
Author: George Vega Yon [cre, aut], Kayla de la Haye [ths], Army Research Laboratory and the U.S. Army Research Office [fnd] (Grant Number W911NF-15-1-0577)

Exponential Random Graph

ergmito 0.2-1-9999

ergmito: Exponential Random Graph Models for Small Networks

This R package, which has been developed on top of the amazing work that the Statnet team has done, implements estimation and simulation methods for Exponential Random Graph Models of small networks, in particular, less than 7 nodes. In the case of small networks, the calculation of the likelihood of ERGMs becomes computationally feasible, which allows us avoiding approximations and do exact calculation, ultimately obtaining MLEs directly.

Support

This material is based upon work support by, or in part by, the U.S. Army Research Laboratory and the U.S. Army Research Office under grant number W911NF-15-1-0577

Computation for the work described in this paper was supported by the University of Southern California's Center for High-Performance Computing (www.usc.edu/cmp).

more

ergmito: Estimation of Small ERGM using Exact Statistics

Using exact statistics means:

- Higher convergence rate.
- Lower type-I error rate.
- Smaller bias.
- More power.
- Faster.
- More flexible.

CRAN - Package ergmito

ergmito: Exponential Random Graph Models for Small Networks

Simulation and estimation of Exponential Random Graph Models (ERGMs) for small networks using exact statistics. As a difference from the 'ergm' package, 'ergmito' circumvents using Markov-Chain Maximum Likelihood Estimator (MC-MLE) and instead uses Maximum Likelihood Estimator (MLE) to fit ERGMs for small networks. As exhaustive enumeration is computationally feasible for small networks, this R package takes advantage of this and provides tools for calculating likelihood functions, and other relevant functions, directly, meaning that in many cases both estimation and simulation of ERGMs for small networks can be faster and more accurate than simulation-based algorithms.

Version: 0.2-1
Depends: R (≥ 3.3.0)
Imports: ergm, network, MASS, Rcpp, texreg, stats, parallel, utils, methods, graphics
LinkingTo: Rcpp, RcppArmadillo
Suggests: covr, sna, lmtest, fmcmc, coda, knitr, rmarkdown, tinytest
Published: 2020-02-12
Author: George Vega Yon [cre, aut], Kayla de la Haye [ths], Army Research Laboratory and the U.S. Army Research Office [fnd] (Grant Number W911NF-15-1-0577)

Exponential Random Graph

ergmito 0.2-1-9999

ergmito: Exponential Random Graph Models for Small Networks

This R package, which has been developed on top of the amazing work that the Statnet team has done, implements estimation and simulation methods for Exponential Random Graph Models of small networks, in particular, less than 7 nodes. In the case of small networks, the calculation of the likelihood of ERGMs becomes computationally feasible, which allows us avoiding approximations and do exact calculation, ultimately obtaining MLEs directly.

Support

This material is based upon work support by, or in part by, the U.S. Army Research Laboratory and the U.S. Army Research Office under grant number W911NF-15-1-0577

Computation for the work described in this paper was supported by the University of Southern California's Center for High-Performance Computing (www.usc.edu/cmp).

more

ergmito: Estimation of Small ERGM using Exact Statistics

Using exact statistics means:

- Higher convergence rate.
- Lower type-I error rate.
- Smaller bias.
- More power.
- Faster.
- More flexible.

CRAN - Package ergmito

ergmito: Exponential Random Graph Models for Small Networks

Simulation and estimation of Exponential Random Graph Models (ERGMs) for small networks using exact statistics. As a difference from the 'ergm' package, 'ergmito' circumvents using Markov-Chain Maximum Likelihood Estimator (MC-MLE) and instead uses Maximum Likelihood Estimator (MLE) to fit ERGMs for small networks. As exhaustive enumeration is computationally feasible for small networks, this R package takes advantage of this and provides tools for calculating likelihood functions, and other relevant functions, directly, meaning that in many cases both estimation and simulation of ERGMs for small networks can be faster and more accurate than simulation-based algorithms.

Version: 0.2-1
 Depends: R (≥ 3.3.0)
 Imports: ergm, network, MASS, Rcpp, texreg, stats, parallel, utils, methods, graphics
 LinkingTo: Rcpp, RcppArmadillo
 Suggests: covr, sna, lmtest, fmcmc, coda, knitr, rmarkdown, tinytest
 Published: 2020-02-12
 Author: George Vega Yon [cre, aut], Kayla de la Haye [ths], Army Research Laboratory and the U.S. Army Research Office [fnd] (Grant Number W911NF-15-1-0577)

Exponential Random Graph

ergmito 0.2-1-9999

ergmito: Exponential Random Graph Models for Small Networks



This R package, which has been developed on top of the amazing work that the Statnet team has done, implements estimation and simulation methods for Exponential Random Graph Models of small networks, in particular, less than 7 nodes. In the case of small networks, the calculation of the likelihood of ERGMs becomes computationally feasible, which allows us avoiding approximations and do exact calculation, ultimately obtaining MLEs directly.

Support

This material is based upon work support by, or in part by, the U.S. Army Research Laboratory and the U.S. Army Research Office under grant number W911NF-15-1-0577

Computation for the work described in this paper was supported by the University of Southern California's Center for High-Performance Computing (www.usc.edu/cmp).

more

ergmito: Estimation of Small ERGM using Exact Statistics

Using exact statistics means:

- Higher convergence rate.
- Lower type-I error rate.
- Smaller bias.
- More power.
- Faster.
- More flexible.

CRAN - Package ergmito

ergmito: Exponential Random Graph Models for Small Networks

Simulation and estimation of Exponential Random Graph Models (ERGMs) for small networks using exact statistics. As a difference from the 'ergm' package, 'ergmito' circumvents using Markov-Chain Maximum Likelihood Estimator (MC-MLE) and instead uses Maximum Likelihood Estimator (MLE) to fit ERGMs for small networks. As exhaustive enumeration is computationally feasible for small networks, this R package takes advantage of this and provides tools for calculating likelihood functions, and other relevant functions, directly, meaning that in many cases both estimation and simulation of ERGMs for small networks can be faster and more accurate than simulation-based algorithms.

Version: 0.2-1
Depends: R (≥ 3.3.0)
Imports: ergm, network, MASS, Rcpp, texreg, stats, parallel, utils, methods, graphics
LinkingTo: Rcpp, RcppArmadillo
Suggests: covr, sna, lmtest, fmcmc, coda, knitr, rmarkdown, tinytest
Published: 2020-02-12
Author: George Vega Yon [cre, aut], Kayla de la Haye [ths], Army Research Laboratory and the U.S. Army Research Office [fnd] (Grant Number W911NF-15-1-0577)

Exponential Random Graph

ergmito 0.2-1-9999

ergmito: Exponential Random Graph Models for Small Networks



This R package, which has been developed on top of the amazing work that the Statnet team has done, implements estimation and simulation methods for Exponential Random Graph Models of small networks, in particular, less than 7 nodes. In the case of small networks, the calculation of the likelihood of ERGMs becomes computationally feasible, which allows us avoiding approximations and do exact calculation, ultimately obtaining MLEs directly.

Support

This material is based upon work support by, or in part by, the U.S. Army Research Laboratory and the U.S. Army Research Office under grant number W911NF-15-1-0577

Computation for the work described in this paper was supported by the University of Southern California's Center for High-Performance Computing (www.usc.edu/cmp).

more

ergmito: Estimation of Small ERGM using Exact Statistics

Using exact statistics means:

- Higher convergence rate.
- Lower type-I error rate.
- Smaller bias.
- More power.
- Faster.
- More flexible.

CRAN - Package ergmito

ergmito: Exponential Random Graph Models for Small Networks

Simulation and estimation of Exponential Random Graph Models (ERGMs) for small networks using exact statistics. As a difference from the 'ergm' package, 'ergmito' circumvents using Markov-Chain Maximum Likelihood Estimator (MC-MLE) and instead uses Maximum Likelihood Estimator (MLE) to fit ERGMs for small networks. As exhaustive enumeration is computationally feasible for small networks, this R package takes advantage of this and provides tools for calculating likelihood functions, and other relevant functions, directly, meaning that in many cases both estimation and simulation of ERGMs for small networks can be faster and more accurate than simulation-based algorithms.

Version: 0.2-1
Depends: R (≥ 3.3.0)
Imports: ergm, network, MASS, Rcpp, texreg, stats, parallel, utils, methods, graphics
LinkingTo: Rcpp, RcppArmadillo
Suggests: covr, sna, lmtest, fmcmc, coda, knitr, rmarkdown, tinytest
Published: 2020-02-12
Author: George Vega Yon [cre, aut], Kayla de la Haye [ths], Army Research Laboratory and the U.S. Army Research Office [fnd] (Grant Number W911NF-15-1-0577)

Exponential Random Graph

ergmito 0.2-1-9999

ergmito: Exponential Random Graph Models for Small Networks



This R package, which has been developed on top of the amazing work that the Statnet team has done, implements estimation and simulation methods for Exponential Random Graph Models of small networks, in particular, less than 7 nodes. In the case of small networks, the calculation of the likelihood of ERGMs becomes computationally feasible, which allows us avoiding approximations and do exact calculation, ultimately obtaining MLEs directly.

Support

This material is based upon work support by, or in part by, the U.S. Army Research Laboratory and the U.S. Army Research Office under grant number W911NF-15-1-0577

Computation for the work described in this paper was supported by the University of Southern California's Center for High-Performance Computing (www.usc.edu/cmp).

more

ergmito: Estimation of Small ERGM using Exact Statistics

Using exact statistics means:

- Higher convergence rate.
- Lower type-I error rate.
- Smaller bias.
- More power.
- Faster.
- More flexible.

CRAN - Package ergmito

ergmito: Exponential Random Graph Models for Small Networks

Simulation and estimation of Exponential Random Graph Models (ERGMs) for small networks using exact statistics. As a difference from the 'ergm' package, 'ergmito' circumvents using Markov-Chain Maximum Likelihood Estimator (MC-MLE) and instead uses Maximum Likelihood Estimator (MLE) to fit ERGMs for small networks. As exhaustive enumeration is computationally feasible for small networks, this R package takes advantage of this and provides tools for calculating likelihood functions, and other relevant functions, directly, meaning that in many cases both estimation and simulation of ERGMs for small networks can be faster and more accurate than simulation-based algorithms.

Version: 0.2-1
 Depends: R (≥ 3.3.0)
 Imports: ergm, network, MASS, Rcpp, texreg, stats, parallel, utils, methods, graphics
 LinkingTo: Rcpp, RcppArmadillo
 Suggests: covr, sna, lmtest, fmcmc, coda, knitr, rmarkdown, tinytest
 Published: 2020-02-12
 Author: George Vega Yon [cre, aut], Kayla de la Haye [ths], Army Research Laboratory and the U.S. Army Research Office [fnd] (Grant Number W911NF-15-1-0577)

Exponential Random Graph

ergmito 0.2-1-9999

ergmito: Exponential Random Graph Models for Small Networks



This R package, which has been developed on top of the amazing work that the Statnet team has done, implements estimation and simulation methods for Exponential Random Graph Models of small networks, in particular, less than 7 nodes. In the case of small networks, the calculation of the likelihood of ERGMs becomes computationally feasible, which allows us avoiding approximations and do exact calculation, ultimately obtaining MLEs directly.

Support

This material is based upon work support by, or in part by, the U.S. Army Research Laboratory and the U.S. Army Research Office under grant number W911NF-15-1-0577

Computation for the work described in this paper was supported by the University of Southern California's Center for High-Performance Computing (www.usc.edu/cmp).

more

ergmito: Estimation of Small ERGM using Exact Statistics

Using exact statistics means:

- Higher convergence rate.
- Lower type-I error rate.
- Smaller bias.
- More power.
- Faster.
- More flexible.

CRAN - Package ergmito

ergmito: Exponential Random Graph Models for Small Networks

Simulation and estimation of Exponential Random Graph Models (ERGMs) for small networks using exact statistics. As a difference from the 'ergm' package, 'ergmito' circumvents using Markov-Chain Maximum Likelihood Estimator (MC-MLE) and instead uses Maximum Likelihood Estimator (MLE) to fit ERGMs for small networks. As exhaustive enumeration is computationally feasible for small networks, this R package takes advantage of this and provides tools for calculating likelihood functions, and other relevant functions, directly, meaning that in many cases both estimation and simulation of ERGMs for small networks can be faster and more accurate than simulation-based algorithms.

Version: 0.2-1
Depends: R (≥ 3.3.0)
Imports: ergm, network, MASS, Rcpp, texreg, stats, parallel, utils, methods, graphics
LinkingTo: Rcpp, RcppArmadillo
Suggests: covr, sna, lmtest, fmcmc, coda, knitr, rmarkdown, tinytest
Published: 2020-02-12
Author: George Vega Yon [cre, aut], Kayla de la Haye [ths], Army Research Laboratory and the U.S. Army Research Office [fnd] (Grant Number W911NF-15-1-0577)

Exponential Random Graph

ergmito 0.2-1-9999

ergmito: Exponential Random Graph Models for Small Networks



This R package, which has been developed on top of the amazing work that the Statnet team has done, implements estimation and simulation methods for Exponential Random Graph Models of small networks, in particular, less than 7 nodes. In the case of small networks, the calculation of the likelihood of ERGMs becomes computationally feasible, which allows us avoiding approximations and do exact calculation, ultimately obtaining MLEs directly.

Support

This material is based upon work support by, or in part by, the U.S. Army Research Laboratory and the U.S. Army Research Office under grant number W911NF-15-1-0577

Computation for the work described in this paper was supported by the University of Southern California's Center for High-Performance Computing (www.usc.edu/cmp).

more

ergmito: Estimation of Small ERGM using Exact Statistics

Using exact statistics means:

- Higher convergence rate.
- Lower type-I error rate.
- Smaller bias.
- More power.
- Faster.
- More flexible.

downloads 2593

CRAN - Package ergmito

ergmito: Exponential Random Graph Models for Small Networks

Simulation and estimation of Exponential Random Graph Models (ERGMs) for small networks using exact statistics. As a difference from the 'ergm' package, 'ergmito' circumvents using Markov-Chain Maximum Likelihood Estimator (MC-MLE) and instead uses Maximum Likelihood Estimator (MLE) to fit ERGMs for small networks. As exhaustive enumeration is computationally feasible for small networks, this R package takes advantage of this and provides tools for calculating likelihood functions, and other relevant functions, directly, meaning that in many cases both estimation and simulation of ERGMs for small networks can be faster and more accurate than simulation-based algorithms.

Version: 0.2-1
Depends: R (≥ 3.3.0)
Imports: ergm, network, MASS, Rcpp, texreg, stats, parallel, utils, methods, graphics
LinkingTo: Rcpp, RcppArmadillo
Suggests: covr, sna, lmtest, fmcmc, coda, knitr, rmarkdown, tinytest
Published: 2020-02-12
Author: George Vega Yon [cre, aut], Kayla de la Haye [ths], Army Research Laboratory and the U.S. Army Research Office [fnd] (Grant Number W911NF-15-1-0577)

Exponential Random Graph

ergmito 0.2-1-9999

ergmito: Exponential Random Graph Models for Small Networks

This R package, which has been developed on top of the amazing work that the Statnet team has done, implements estimation and simulation methods for Exponential Random Graph Models of small networks, in particular, less than 7 nodes. In the case of small networks, the calculation of the likelihood of ERGMs becomes computationally feasible, which allows us avoiding approximations and do exact calculation, ultimately obtaining MLEs directly.

Support

This material is based upon work support by, or in part by, the U.S. Army Research Laboratory and the U.S. Army Research Office under grant number W911NF-15-1-0577

Computation for the work described in this paper was supported by the University of Southern California's Center for High-Performance Computing (www.usc.edu/cmp).

▶ more

Featured Application: Small Teams

Sample

Featured Application: Small Teams

Sample

- ▶ 31 mixed-gender teams (4-5 members).

Featured Application: Small Teams

Sample

- ▶ 31 mixed-gender teams (4-5 members).
- ▶ University students.

Featured Application: Small Teams

Sample

- ▶ 31 mixed-gender teams (4-5 members).
- ▶ University students.
- ▶ Don't know each other.

Featured Application: Small Teams

Sample

- ▶ 31 mixed-gender teams (4-5 members).
- ▶ University students.
- ▶ Don't know each other.
- ▶ At least one female/male per team.

Featured Application: Small Teams

Sample

- ▶ 31 mixed-gender teams (4-5 members).
- ▶ University students.
- ▶ Don't know each other.
- ▶ At least one female/male per team.

Experiment

Featured Application: Small Teams

Sample

- ▶ 31 mixed-gender teams (4-5 members).
- ▶ University students.
- ▶ Don't know each other.
- ▶ At least one female/male per team.

Experiment

- ▶ Complete 1 hour of group tasks.

Featured Application: Small Teams

Sample

- ▶ 31 mixed-gender teams (4-5 members).
- ▶ University students.
- ▶ Don't know each other.
- ▶ At least one female/male per team.

Experiment

- ▶ Complete 1 hour of group tasks.
- ▶ Captured network data using name generator survey: *Who did you go to for advice, information or help to complete the group task?*

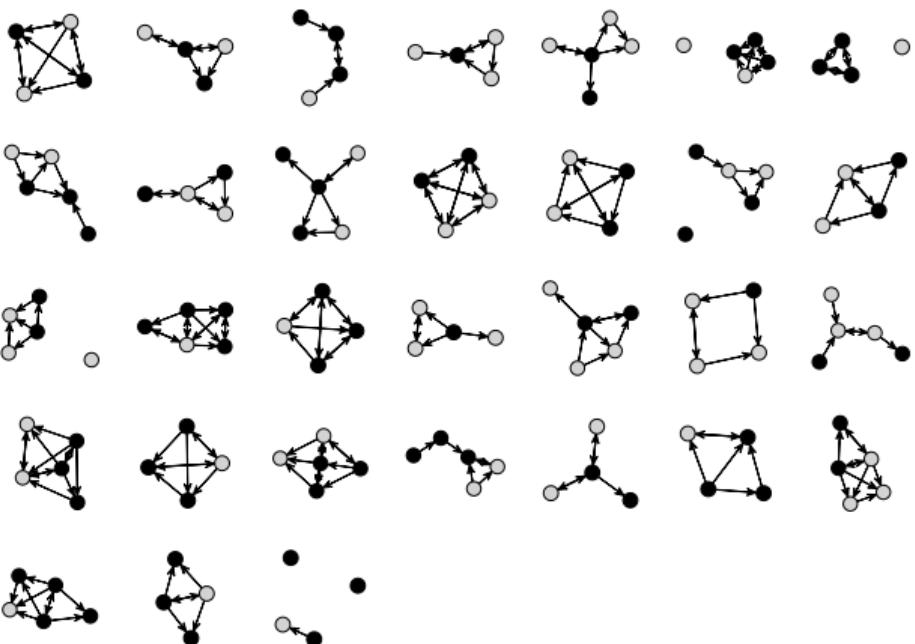
Featured Application: Small Teams

Sample

- ▶ 31 mixed-gender teams (4-5 members).
- ▶ University students.
- ▶ Don't know each other.
- ▶ At least one female/male per team.

Experiment

- ▶ Complete 1 hour of group tasks.
- ▶ Captured network data using name generator survey: *Who did you go to for advice, information or help to complete the group task?*



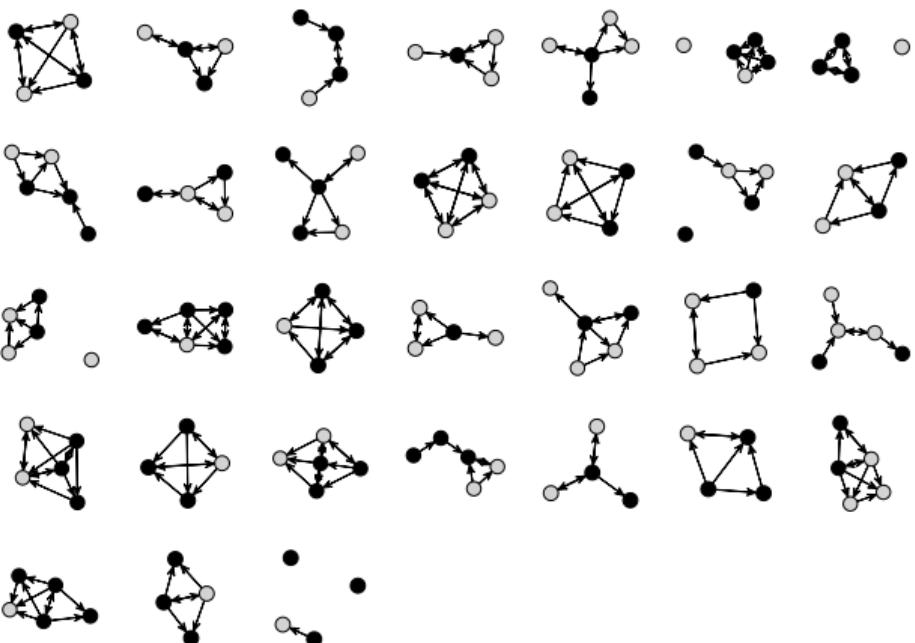
Featured Application: Small Teams

Sample

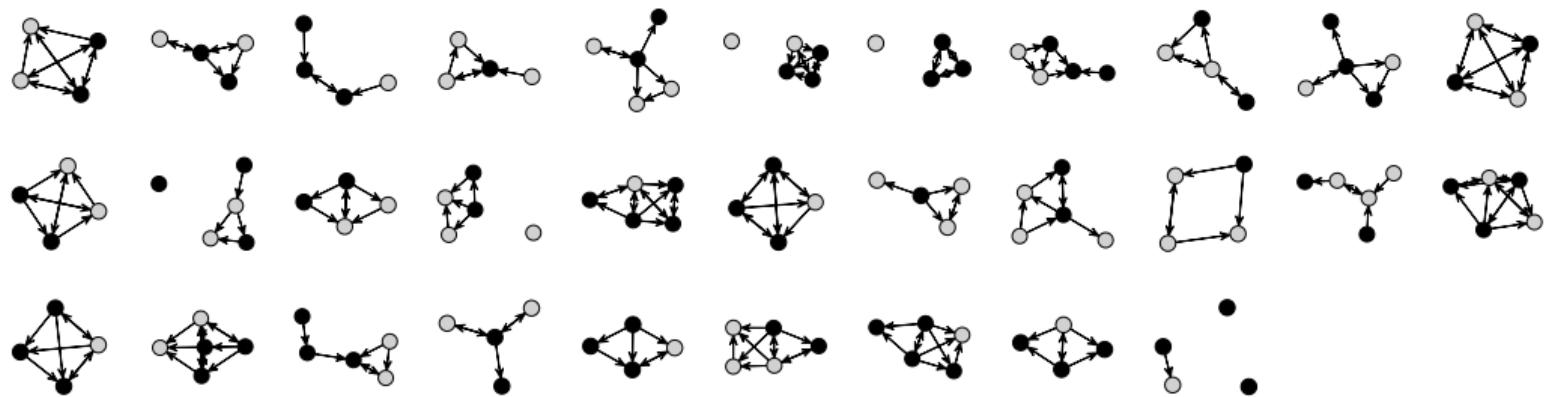
- ▶ 31 mixed-gender teams (4-5 members).
- ▶ University students.
- ▶ Don't know each other.
- ▶ At least one female/male per team.

Experiment

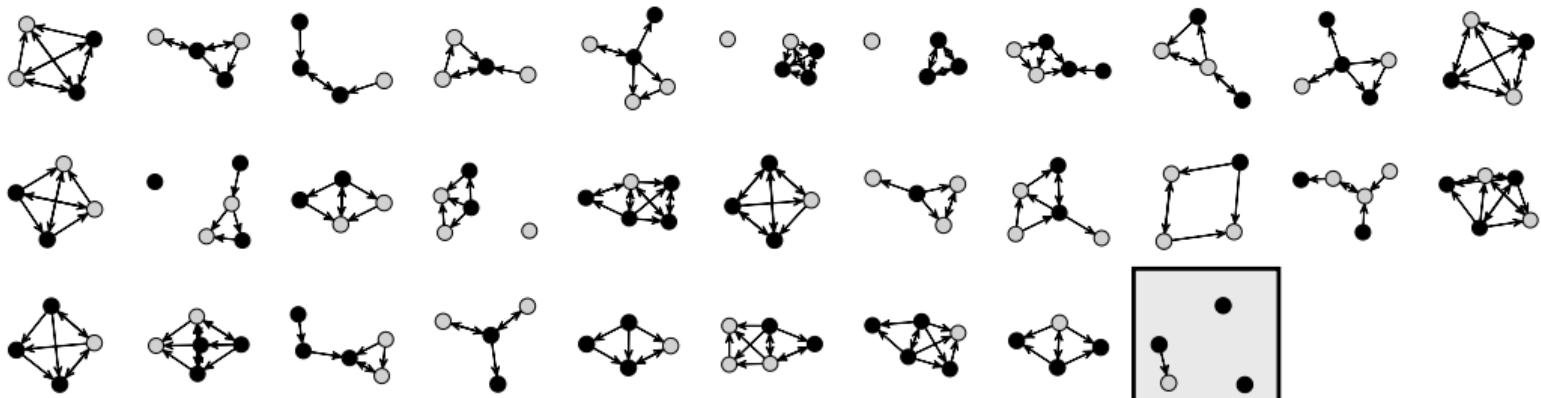
- ▶ Complete 1 hour of group tasks.
- ▶ Captured network data using name generator survey: *Who did you go to for advice, information or help to complete the group task?*



Is Gender Homophily a feature of these graphs?

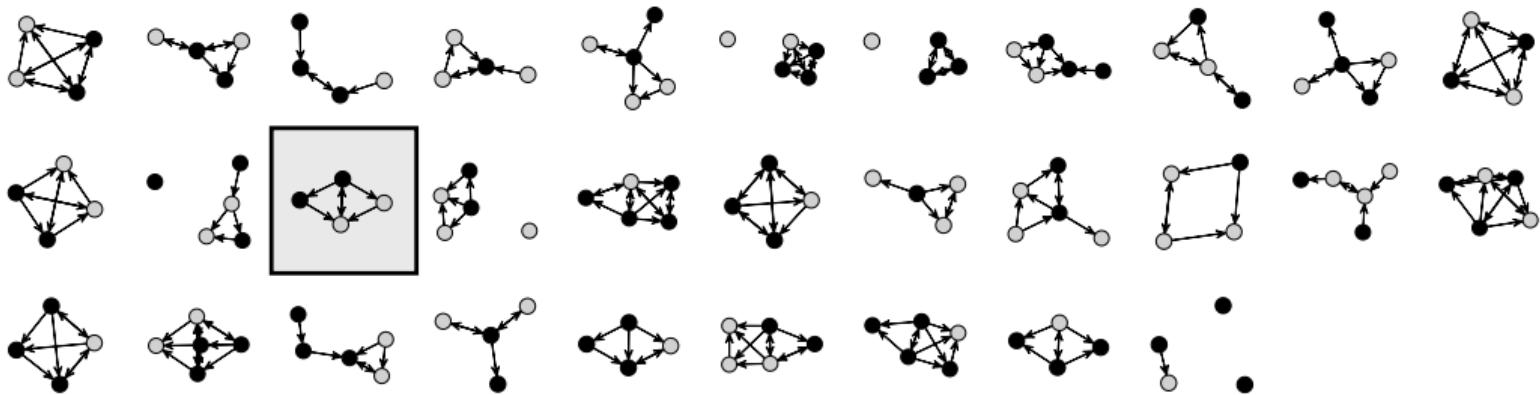


Key findings



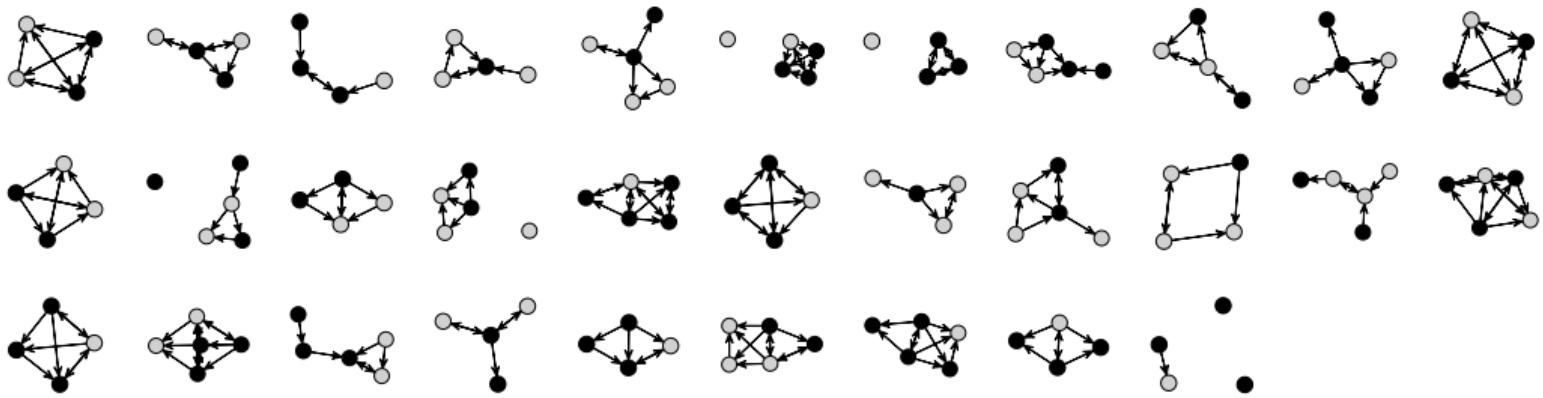
Key findings

- ▶ Low density.



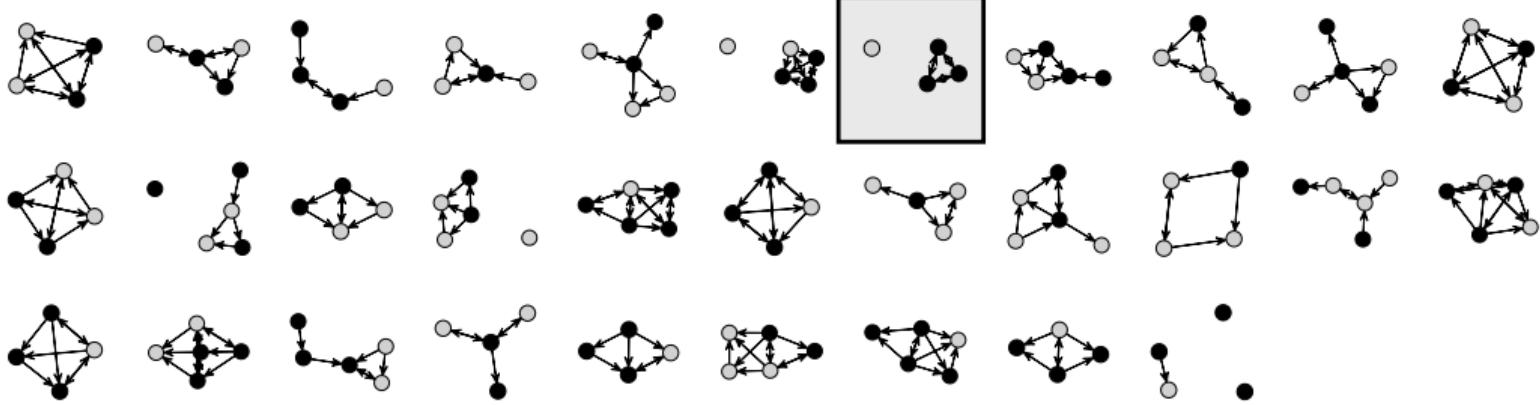
Key findings

- ▶ Low density.
- ▶ High balance (transitive triads).



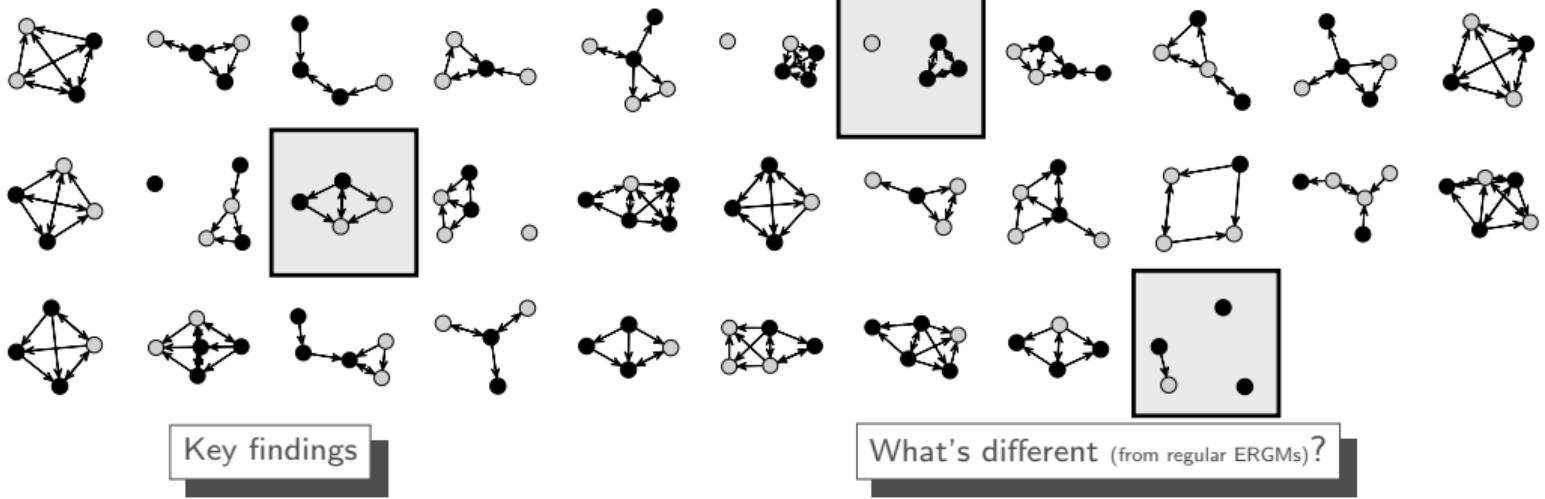
Key findings

- ▶ Low density.
- ▶ High balance (transitive triads).
- ▶ No evidence of gender homophily.

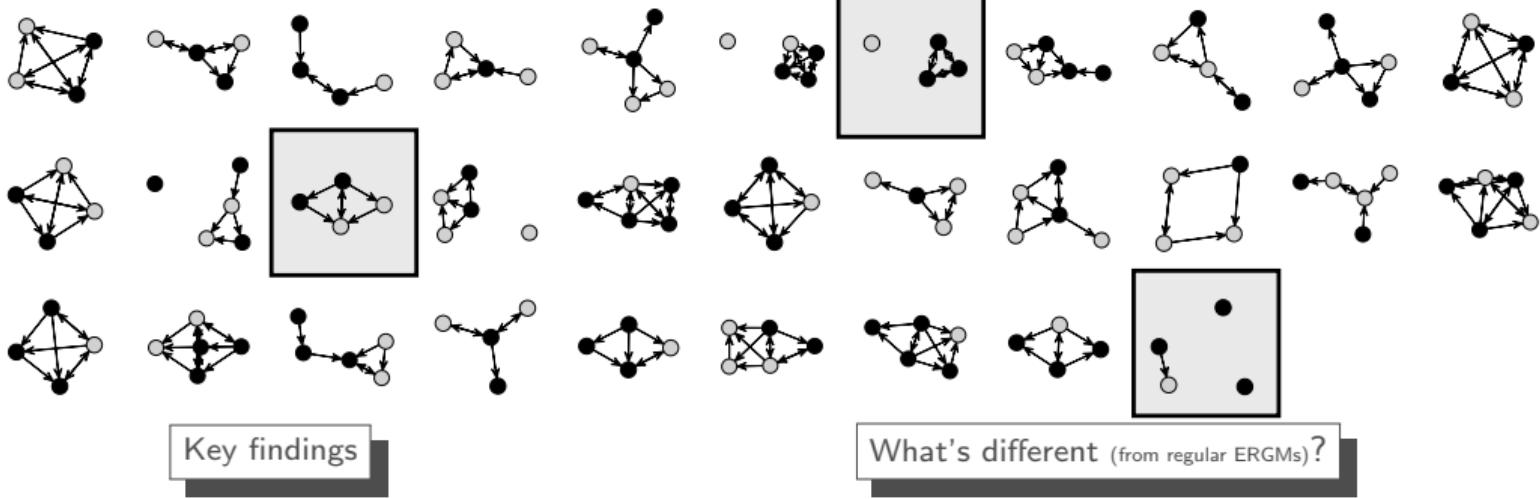


Key findings

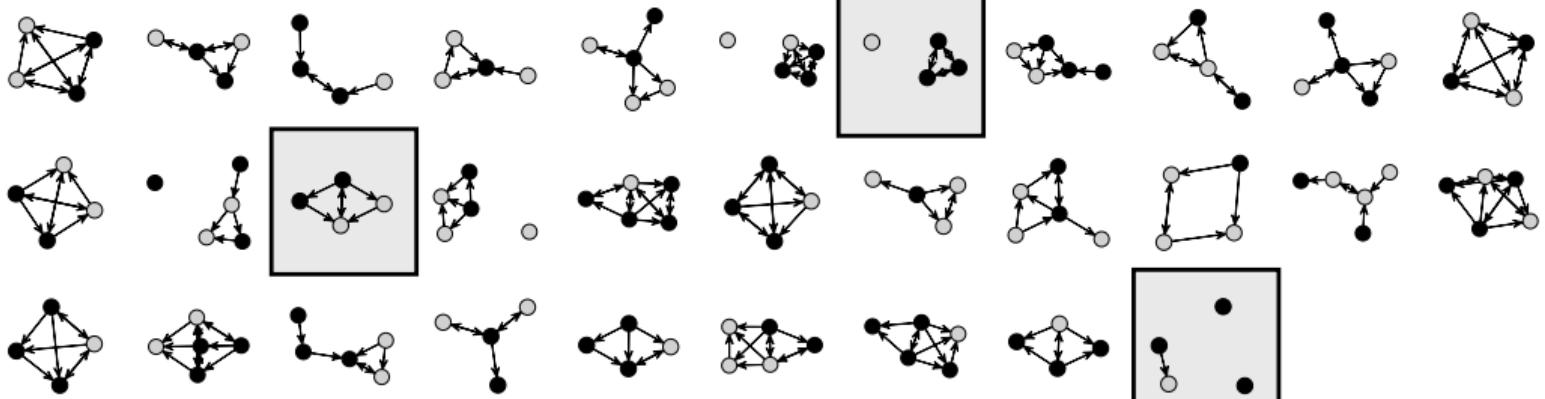
- ▶ Low density.
- ▶ High balance (transitive triads).
- ▶ No evidence of gender homophily.
- ▶ Females are more likely to ask for advice.



- ▶ Low density.
- ▶ High balance (transitive triads).
- ▶ No evidence of gender homophily.
- ▶ Females are more likely to ask for advice.



- ▶ Low density.
- ▶ High balance (transitive triads).
- ▶ No evidence of gender homophily.
- ▶ Females are more likely to ask for advice.
- ▶ Interaction effects: edges $\times \mathbf{1}$ ($n = 5$).

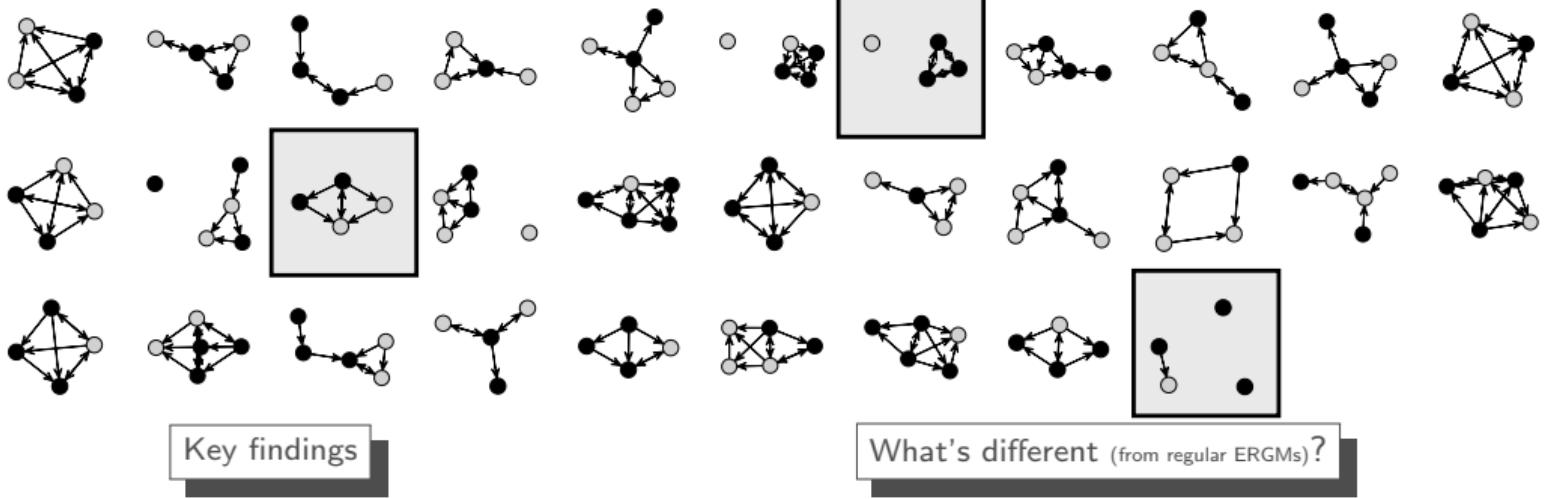


Key findings

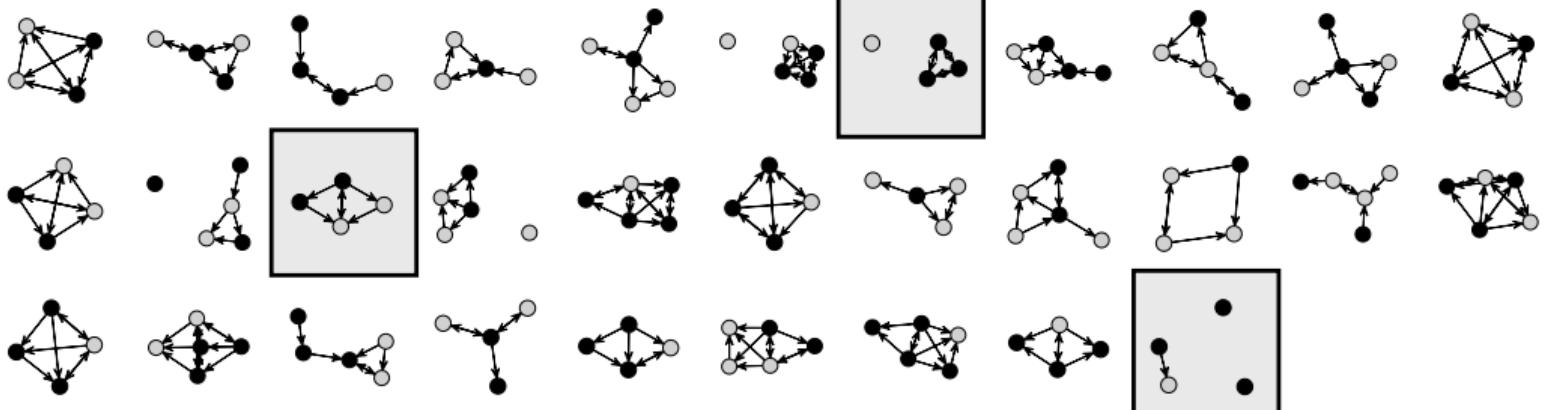
- ▶ Low density.
- ▶ High balance (transitive triads).
- ▶ No evidence of gender homophily.
- ▶ Females are more likely to ask for advice.

What's different (from regular ERGMs)?

- ▶ Interaction effects: edges \times 1 ($n = 5$).
- ▶ Constrained support: edge > 4 .



- ▶ Low density.
- ▶ High balance (transitive triads).
- ▶ No evidence of gender homophily.
- ▶ Females are more likely to ask for advice.
- ▶ Interaction effects: edges $\times \mathbf{1}$ ($n = 5$).
- ▶ Constrained support: edge > 4 .
- ▶ Transformed variables: $(\text{Homophily})^{1/2}$.

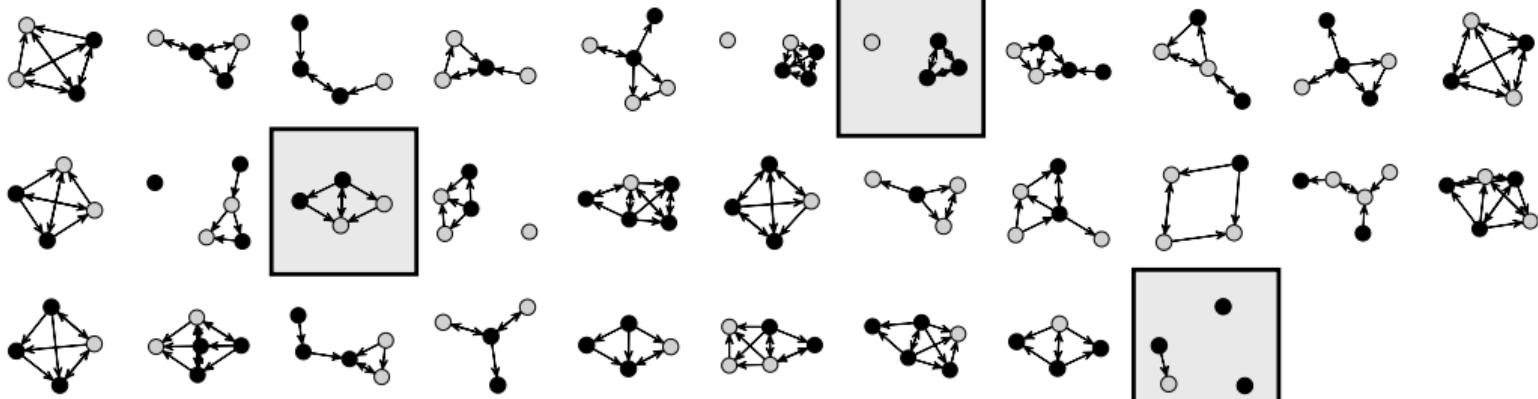


Key findings

- ▶ Low density.
- ▶ High balance (transitive triads).
- ▶ No evidence of gender homophily.
- ▶ Females are more likely to ask for advice.

What's different (from regular ERGMs)?

- ▶ Interaction effects: edges $\times 1$ ($n = 5$).
- ▶ Constrained support: edge > 4 .
- ▶ Transformed variables: $(\text{Homophily})^{1/2}$.
- ▶ Bootstrapping: 1,000 replicates in less than 1.5 minutes...



Key findings

- ▶ Low density.
- ▶ High balance (transitive triads).
- ▶ No evidence of gender homophily.
- ▶ Females are more likely to ask for advice.

What's different (from regular ERGMs)?

- ▶ Interaction effects: edges $\times 1$ ($n = 5$).
- ▶ Constrained support: edge > 4 .
- ▶ Transformed variables: $(\text{Homophily})^{1/2}$.
- ▶ Bootstrapping: 1,000 replicates in less than 1.5 minutes...
... if you are lucky, using “regular” ERGMs would take you about 5 hours.

Goodness-of-fit for Small Networks

(Chapters 3 and 6)

Goodness-of-fit: Conditional Distributions

“Does the model edges+transitivity capture the observed path-length distribution?”

“Does the model edges+transitivity capture the observed path-length distribution?”

- ▶ The current Goodness-of-fit (GOF) for ERGMs does not fit ERGMitos.

“Does the model edges+transitivity capture the observed path-length distribution?”

- ▶ The current Goodness-of-fit (GOF) for ERGMs does not fit ERGMitos.
- ▶ A closely related idea: Conditional Distributions.

How much does *Term B* can tell us about *Term A*?

Goodness-of-fit: Conditional Distributions

“Does the model edges+transitivity capture the observed path-length distribution?”

- ▶ The current Goodness-of-fit (GOF) for ERGMs does not fit ERGMitos.
- ▶ A closely related idea: Conditional Distributions.

How much does *Term B* can tell us about *Term A*?

- ▶ Brief study: Analyze the prediction capability that **Mutuals**, **Transitive Triads**, **Homophily**, and **Receiver Effect** terms have on each other.

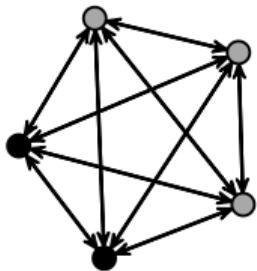
Goodness-of-fit: Conditional Distributions

“Does the model edges+transitivity capture the observed path-length distribution?”

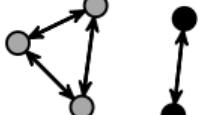
- ▶ The current Goodness-of-fit (GOF) for ERGMs does not fit ERGMitos.
- ▶ A closely related idea: Conditional Distributions.

How much does *Term B* can tell us about *Term A*?

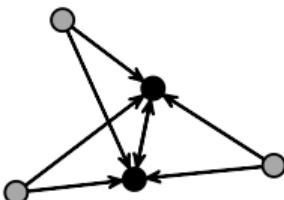
- ▶ Brief study: Analyze the prediction capability that **Mutuals**, **Transitive Triads**, **Homophily**, and **Receiver Effect** terms have on each other.



(a) Mutual Ties and
Transitive Triads



(b) Homophilic
Ties



(c) Attribute
Receiver Effect

How much does *Term B* can tell us about
Term A?

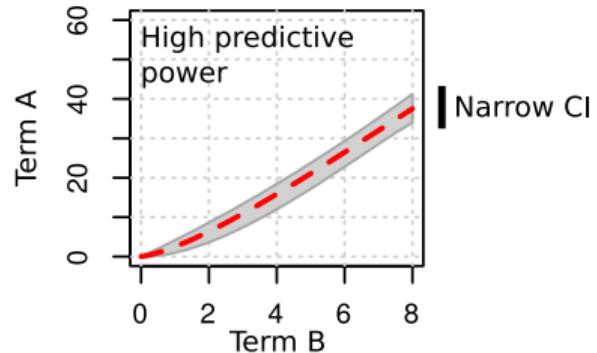
How much does *Term B* can tell us about
Term A?

- ▶ High predictive power ($\text{Term A} \mid \text{Term B}$):

(All this is based on Chapters 3 and 6)

How much does *Term B* can tell us about *Term A*?

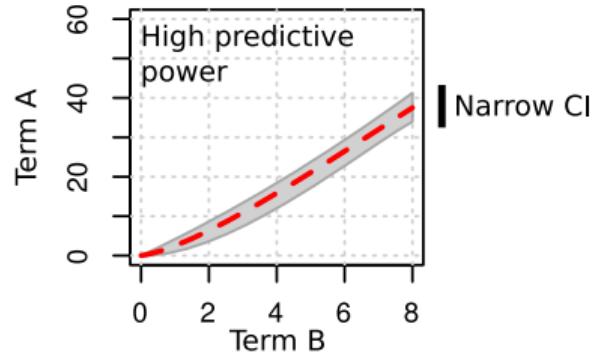
- ▶ High predictive power ($\text{Term A} \mid \text{Term B}$):
 - ▶ Stepped slope.
 - ▶ Narrow Confidence Interval (CI).



(All this is based on Chapters 3 and 6)

How much does *Term B* can tell us about *Term A*?

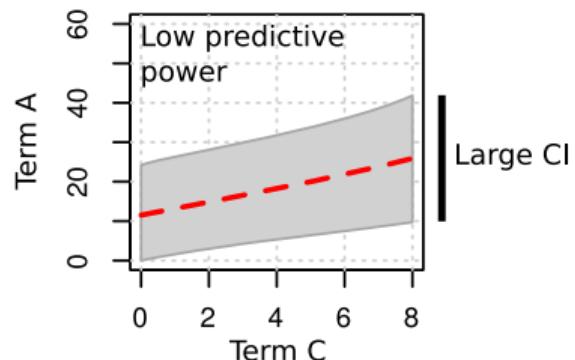
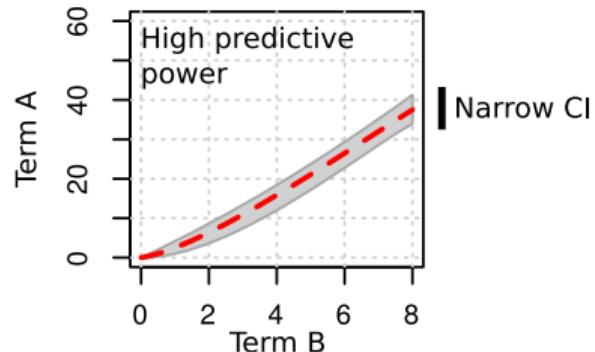
- ▶ High predictive power (*Term A* | *Term B*):
 - ▶ Stepped slope.
 - ▶ Narrow Confidence Interval (CI).
- ▶ Low predictive power (*Term A* | *Term C*):



(All this is based on Chapters 3 and 6)

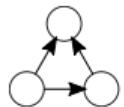
How much does *Term B* can tell us about *Term A*?

- ▶ High predictive power (*Term A* | *Term B*):
 - ▶ Stepped slope.
 - ▶ Narrow Confidence Interval (CI).
- ▶ Low predictive power (*Term A* | *Term C*):
 - ▶ Positive slope (both increase b/c density increases).
 - ▶ Large CI.



(All this is based on Chapters 3 and 6)

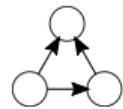
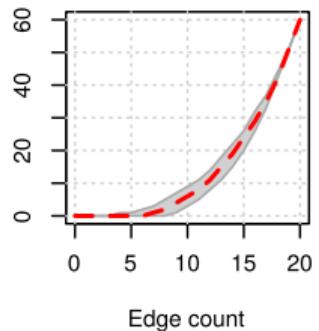
Conditional Distribution: Transitive Triads



▶ more examples

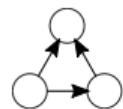
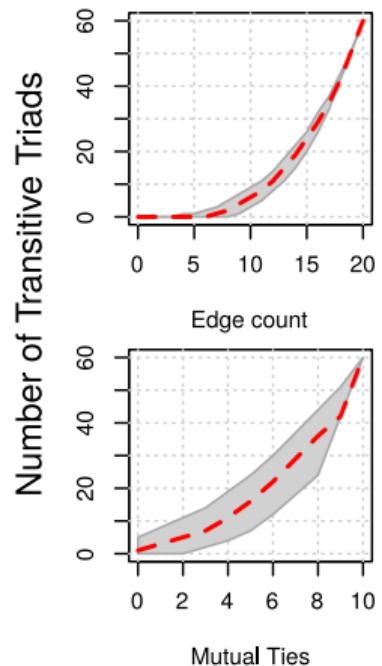
Conditional Distribution: Transitive Triads

Number of Transitive Triads



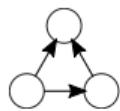
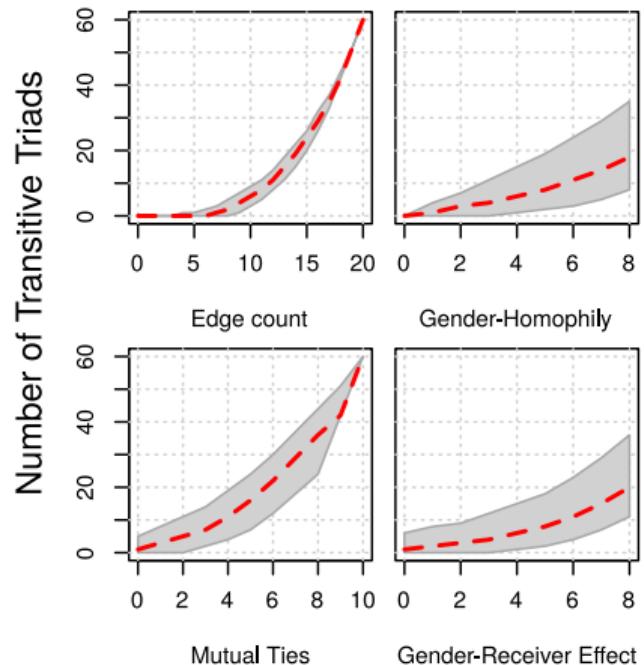
► more examples

Conditional Distribution: Transitive Triads



▶ more examples

Conditional Distribution: Transitive Triads

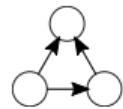
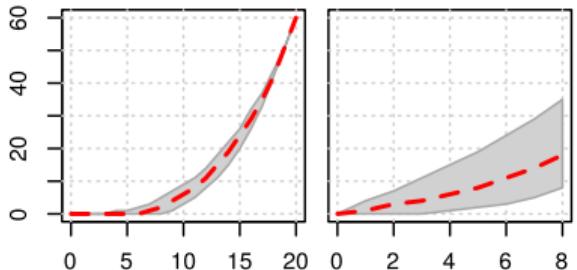


▶ more examples

Conditional Distribution: Transitive Triads

$$\theta_{\text{triads}} = 0$$

Number of Transitive Triads



Edge count

Gender-Homophily

Mutual Ties

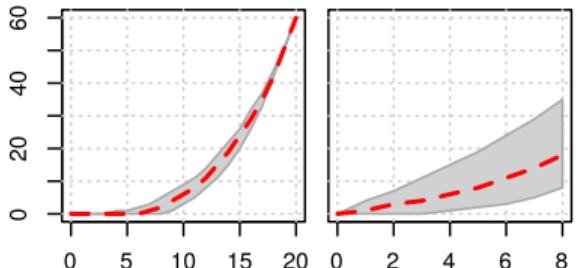
Gender-Receiver Effect

▶ more examples

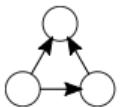
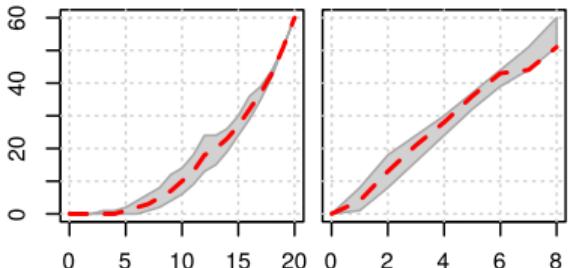
Conditional Distribution: Transitive Triads

$$\theta_{\text{triads}} = 0$$

Number of Transitive Triads

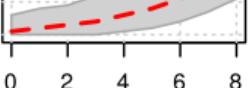
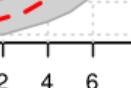


$$\theta_{\text{triads}} = 1$$



Edge count

Gender-Homophily

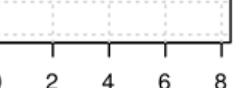
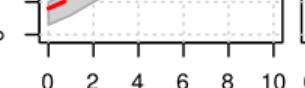


Mutual Ties

Gender-Receiver Effect

Edge count

Gender-Homophily



Mutual Ties

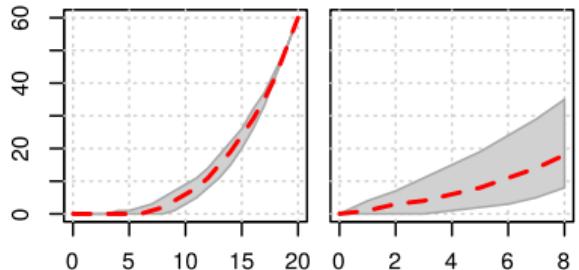
Gender-Receiver Effect

► more examples

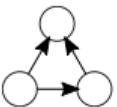
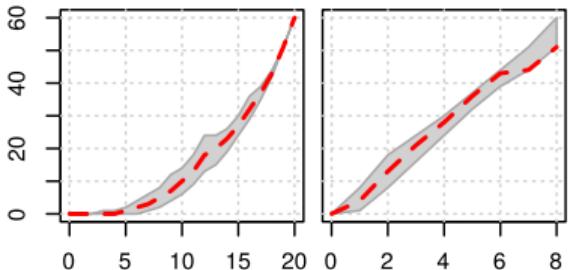
Conditional Distribution: Transitive Triads

$$\theta_{\text{triads}} = 0$$

Number of Transitive Triads



$$\theta_{\text{triads}} = 1$$

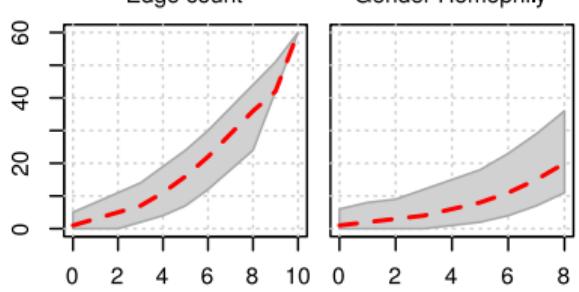


- ▶ Edge count and mutuality are good predictors of transitivity.

Edge count

Gender-Homophily

Mutual Ties



Edge count

Gender-Homophily

Mutual Ties

Gender-Receiver Effect

Mutual Ties

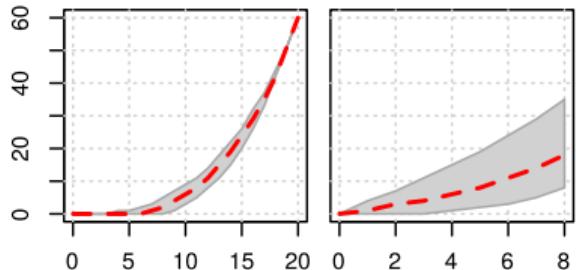
Gender-Receiver Effect

▶ more examples

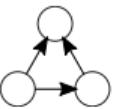
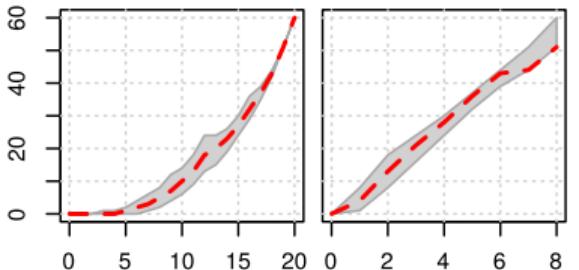
Conditional Distribution: Transitive Triads

$$\theta_{\text{triads}} = 0$$

Number of Transitive Triads



$$\theta_{\text{triads}} = 1$$



- ▶ Edge count and mutuality are good predictors of transitivity.
- ▶ Prevalence (θ_{triads}) narrows the confidence intervals.

Edge count

Gender-Homophily

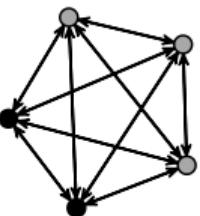
Mutual Ties

Gender-Receiver Effect

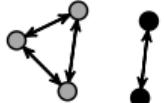
GOF for Small Networks

1. Markov structures (involve two or more ties) are better predictors of each other.

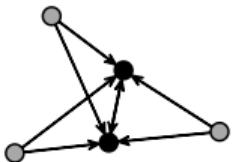
1. Markov structures (involve two or more ties) are better predictors of each other.
2. *Miopic* terms: fast saturation implies poor information, e.g. homophily and receiver effect
saturate at 8/20 ties:



(a) Mutual Ties and
Transitive Triads

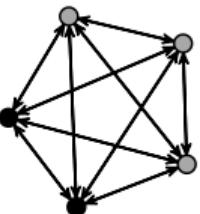


(b) Homophilic
Ties

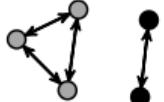


(c) Attribute
Receiver Effect

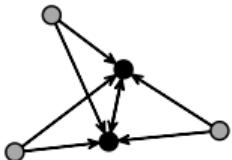
1. Markov structures (involve two or more ties) are better predictors of each other.
2. *Miopic* terms: fast saturation implies poor information, e.g. homophily and receiver effect
saturate at 8/20 ties:



(a) Mutual Ties and
Transitive Triads



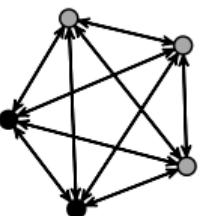
(b) Homophilic
Ties



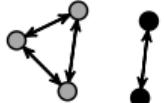
(c) Attribute
Receiver Effect

3. Not only GOF:

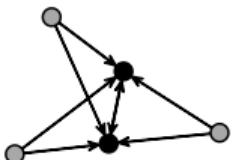
1. Markov structures (involve two or more ties) are better predictors of each other.
2. *Miopic* terms: fast saturation implies poor information, e.g. homophily and receiver effect
saturate at 8/20 ties:



(a) Mutual Ties and
Transitive Triads



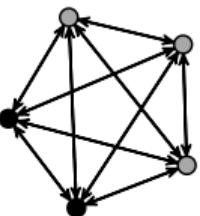
(b) Homophilic
Ties



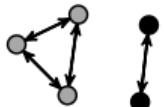
(c) Attribute
Receiver Effect

3. Not only GOF:
 - **Co-linearity** How correlated are A and B?

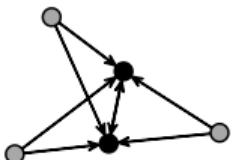
1. Markov structures (involve two or more ties) are better predictors of each other.
2. *Miopic* terms: fast saturation implies poor information, e.g. homophily and receiver effect saturate at 8/20 ties:



(a) Mutual Ties and
Transitive Triads



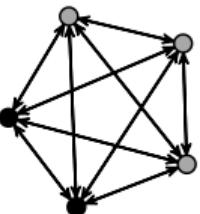
(b) Homophilic
Ties



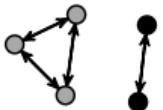
(c) Attribute
Receiver Effect

3. Not only GOF:
 - **Co-linearity** How correlated are A and B?
 - **Parsimony** Improve prediction while keeping the number of terms small.

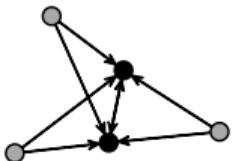
1. Markov structures (involve two or more ties) are better predictors of each other.
2. *Miopic* terms: fast saturation implies poor information, e.g. homophily and receiver effect
saturate at 8/20 ties:



(a) Mutual Ties and
Transitive Triads



(b) Homophilic
Ties



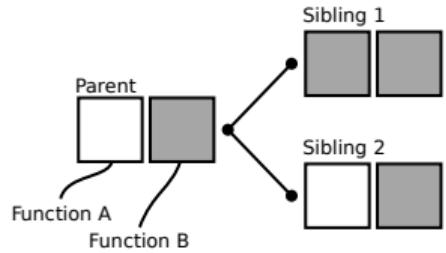
(c) Attribute
Receiver Effect

3. Not only GOF:
 - **Co-linearity** How correlated are A and B?
 - **Parsimony** Improve prediction while keeping the number of terms small.
 - **The right permutation** Evaluate how stringent a permutation test would be.

Connecting the Dots: Phylogenetic Modeling with ERGMs

(Chapter 4)

Phylogenetics Modeling Strategies

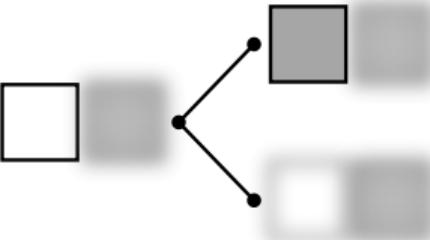
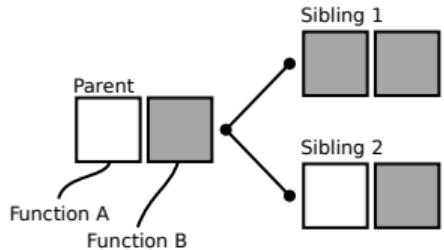


Has the function

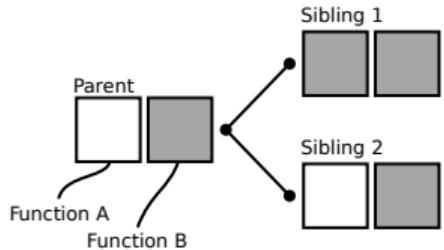


Doesn't have the function

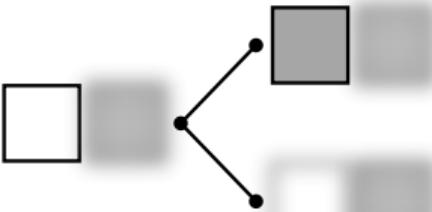
Phylogenetics Modeling Strategies



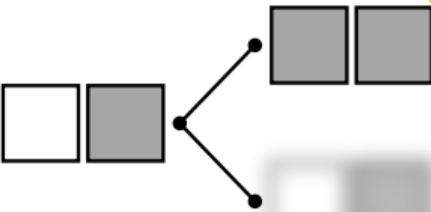
(a) Sibling and Function
Conditional Independence



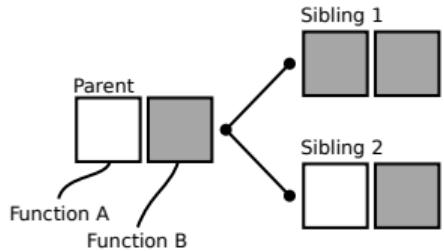
- [White Square] Has the function
- [Gray Square] Doesn't have the function



(a) Sibling and Function Conditional Independence



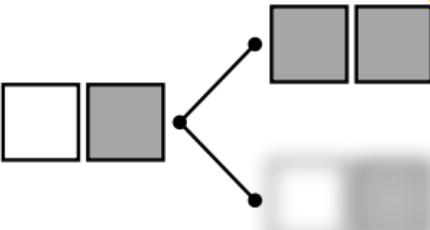
(b) Sibling Conditional Independence



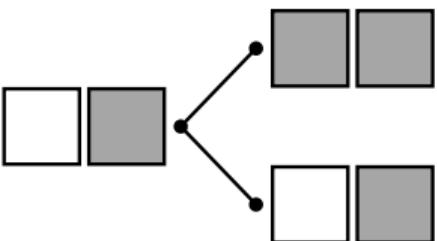
Has the function
 Doesn't have the function



(a) Sibling and Function Conditional Independence



(b) Sibling Conditional Independence



(c) No conditional independence

What Drives Evolution

Imagine that we have 3 functions (rows) and that each node has 2 siblings (columns)

		Transitions to	
		Case 1	Case 2
Parent	A	$\begin{bmatrix} 0 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
	B	$\begin{bmatrix} 1 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}$
	C	$\begin{bmatrix} 1 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

What Drives Evolution

Imagine that we have 3 functions (rows) and that each node has 2 siblings (columns)

		Transitions to	
		Case 1	Case 2
Parent	A	$\begin{bmatrix} 0 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
	B	$\begin{bmatrix} 1 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}$
	C	$\begin{bmatrix} 1 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

Sufficient statistics

What Drives Evolution

Imagine that we have 3 functions (rows) and that each node has 2 siblings (columns)

		Transitions to	
		Case 1	Case 2
Parent	A	$\begin{bmatrix} 0 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
	B	$\begin{bmatrix} 1 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}$
	C	$\begin{bmatrix} 1 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

Sufficient statistics

Gains 1 1

What Drives Evolution

Imagine that we have 3 functions (rows) and that each node has 2 siblings (columns)

		Transitions to	
		Case 1	Case 2
Parent	A	$\begin{bmatrix} 0 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
	B	$\begin{bmatrix} 1 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}$
	C	$\begin{bmatrix} 1 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix}$

Sufficient statistics

# Gains	1	1
Only one offspring changes (yes/no)	1	0

What Drives Evolution

Imagine that we have 3 functions (rows) and that each node has 2 siblings (columns)

		Transitions to	
		Case 1	Case 2
Parent	A	$\begin{bmatrix} 0 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
	B	$\begin{bmatrix} 1 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
	C	$\begin{bmatrix} 1 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

Sufficient statistics

# Gains	1	1
Only one offspring changes (yes/no)	1	0
# Changes (gain+loss)	2	3

Imagine that we have 3 functions (rows) and that each node has 2 siblings (columns)

		Transitions to	
		Case 1	Case 2
Parent	A	$\begin{bmatrix} 0 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
	B	$\begin{bmatrix} 1 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
	C	$\begin{bmatrix} 1 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

Sufficient statistics

# Gains	1	1
Only one offspring changes (yes/no)	1	0
# Changes (gain+loss)	2	3
Subfunctionalization (yes/no)	0	1

What Drives Evolution: a game changer

In the model with 3 functions and 2 offspring per node:

What Drives Evolution: a game changer

In the model with 3 functions and 2 offspring per node:

- ▶ Full Markov transition matrix: $2^3 \times 2^6 = 512$

What Drives Evolution: a game changer

In the model with 3 functions and 2 offspring per node:

- ▶ Full Markov transition matrix: $2^3 \times 2^6 = 512$
- ▶ Using sufficient statistics:

What Drives Evolution: a game changer

In the model with 3 functions and 2 offspring per node:

- ▶ Full Markov transition matrix: $2^3 \times 2^6 = 512$
- ▶ Using sufficient statistics:

Pairwise co-evolution: 3 terms,

What Drives Evolution: a game changer

In the model with 3 functions and 2 offspring per node:

- ▶ Full Markov transition matrix: $2^3 \times 2^6 = 512$

- ▶ Using sufficient statistics:

 - Pairwise co-evolution: 3 terms,

 - Pairwise Neofunctionalization: 3 terms,

What Drives Evolution: a game changer

In the model with 3 functions and 2 offspring per node:

- ▶ Full Markov transition matrix: $2^3 \times 2^6 = 512$

- ▶ Using sufficient statistics:

 - Pairwise co-evolution: 3 terms,

 - Pairwise Neofunctionalization: 3 terms,

 - Pairwise Subfunctionalization: 3 terms,

What Drives Evolution: a game changer

In the model with 3 functions and 2 offspring per node:

- ▶ Full Markov transition matrix: $2^3 \times 2^6 = 512$

- ▶ Using sufficient statistics:

 - Pairwise co-evolution: 3 terms,

 - Pairwise Neofunctionalization: 3 terms,

 - Pairwise Subfunctionalization: 3 terms,

 - Function specific gain: 3 terms,

What Drives Evolution: a game changer

In the model with 3 functions and 2 offspring per node:

- ▶ Full Markov transition matrix: $2^3 \times 2^6 = 512$

- ▶ Using sufficient statistics:

 - Pairwise co-evolution: 3 terms,

 - Pairwise Neofunctionalization: 3 terms,

 - Pairwise Subfunctionalization: 3 terms,

 - Function specific gain: 3 terms,

 - Function specific loss: 3 terms,

What Drives Evolution: a game changer

In the model with 3 functions and 2 offspring per node:

- ▶ Full Markov transition matrix: $2^3 \times 2^6 = 512$

- ▶ Using sufficient statistics:

 - Pairwise co-evolution: 3 terms,

 - Pairwise Neofunctionalization: 3 terms,

 - Pairwise Subfunctionalization: 3 terms,

 - Function specific gain: 3 terms,

 - Function specific loss: 3 terms,

Total: 15 parameters.

What Drives Evolution: a game changer

In the model with 3 functions and 2 offspring per node:

- ▶ Full Markov transition matrix: $2^3 \times 2^6 = 512$
- ▶ Using sufficient statistics:

Pairwise co-evolution: 3 terms,

Pairwise Neofunctionalization: 3 terms,

Pairwise Subfunctionalization: 3 terms,

Function specific gain: 3 terms,

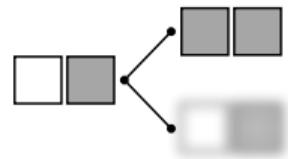
Function specific loss: 3 terms,

Total: 15 parameters.

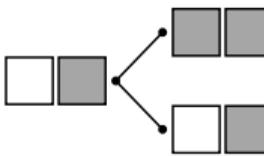
- ▶ Easier to fit and interpret.



(a) Sibling and Function
Conditional Independence



(b) Sibling Conditional
Independence



(c) No conditional
independence

Next Steps (Chapter 7)

barray:

C++ header-only library for counting structures in binary arrays

Barry:

C++ header-only library for counting structures in binary arrays

“The Sniffing Accountant” (Seinfeld, Season 5, Episode 4)

- ▶ Sparse matrix represented using double hashmaps (fast row/column access).

[https://USCbiostats.github.io/
binaryarrays](https://USCbiostats.github.io/binaryarrays)

- ▶ Sparse matrix represented using double hashmaps (fast row/column access).
- ▶ Template implementation for flexible weights and metadata.

[https://USCbiostats.github.io/
binaryarrays](https://USCbiostats.github.io/binaryarrays)

- ▶ Sparse matrix represented using double hashmaps (fast row/column access).
- ▶ Template implementation for flexible weights and metadata.
- ▶ Fast counting using change statistics (Ch. 4).

[https://USCbiostats.github.io/
binaryarrays](https://USCbiostats.github.io/binaryarrays)

- ▶ Sparse matrix represented using double hashmaps (fast row/column access).
- ▶ Template implementation for flexible weights and metadata.
- ▶ Fast counting using change statistics (Ch. 4).
- ▶ Calculation of support for sufficient stats.

[https://USCbiostats.github.io/
binaryarrays](https://USCbiostats.github.io/binaryarrays)

Barry: your go-to *motif* accountant

- ▶ Sparse matrix represented using double hashmaps (fast row/column access).
- ▶ Template implementation for flexible weights and metadata.
- ▶ Fast counting using change statistics (Ch. 4).
- ▶ Calculation of support for sufficient stats.

[https://USCbiostats.github.io/
binaryarrays](https://USCbiostats.github.io/binaryarrays)



Figure 2 Screenshots from the project's website on GitHub.

Barry: your go-to *motif* accountant

- ▶ Sparse matrix represented using double hashmaps (fast row/column access).
- ▶ Template implementation for flexible weights and metadata.
- ▶ Fast counting using change statistics (Ch. 4).
- ▶ Calculation of support for sufficient stats.

[https://USCbiostats.github.io/
binaryarrays](https://USCbiostats.github.io/binaryarrays)

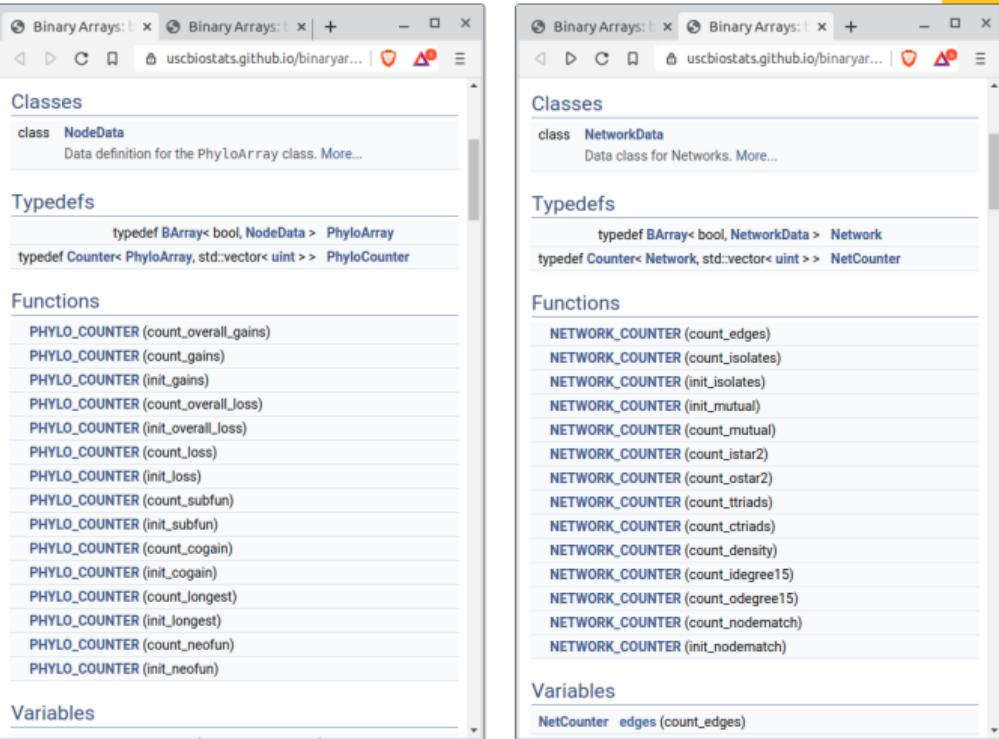


Figure 2 Screenshots from the project's website on GitHub.

Concluding Remarks

Concluding Remarks

Before my dissertation

Predicting gene functions

- ▶ “Small scale”.
- ▶ Detached from theory.

Concluding Remarks

Before my dissertation

Predicting gene functions

- ▶ “Small scale”.
- ▶ Detached from theory.

ERGMs

- ▶ Only approximations.
- ▶ Small networks overlooked.
- ▶ Limited alternatives for small nets.

Concluding Remarks

Before my dissertation

After my dissertation

Predicting gene functions

- ▶ “Small scale”.
- ▶ Detached from theory.

ERGMs

- ▶ Only approximations.
- ▶ Small networks overlooked.
- ▶ Limited alternatives for small nets.

Predicting gene functions

- ▶ Scale-up the problem.
- ▶ More biology (via ERGMs).
- ▶ New ways to look at phylo data.

Concluding Remarks

Before my dissertation

After my dissertation

Predicting gene functions

- ▶ “Small scale”.
- ▶ Detached from theory.

ERGMs

- ▶ Only approximations.
- ▶ Small networks overlooked.
- ▶ Limited alternatives for small nets.

Predicting gene functions

- ▶ Scale-up the problem.
- ▶ More biology (via ERGMs).
- ▶ New ways to look at phylo data.

ERGMs

- ▶ Revisited exact methods.
- ▶ New light on small networks.
- ▶ Many opportunities for methodological innovations.

Concluding Remarks

Before my dissertation

Predicting gene functions

- ▶ “Small scale”.
- ▶ Detached from theory.

ERGMs

- ▶ Only approximations.
- ▶ Small networks overlooked.
- ▶ Limited alternatives for small nets.

After my dissertation

Predicting gene functions

- ▶ Scale-up the problem.
- ▶ More biology (via ERGMs).
- ▶ New ways to look at phylo data.

ERGMs

- ▶ Revisited exact methods.
- ▶ New light on small networks.
- ▶ Many opportunities for methodological innovations.

Products

Publications

6 journal publications (Journal of Open Source Software, Stata Journal, Journal of health and social behavior, Translational behavioral medicine, Social Science & Medicine)

Concluding Remarks

Before my dissertation

Predicting gene functions

- ▶ “Small scale”.
- ▶ Detached from theory.

ERGMs

- ▶ Only approximations.
- ▶ Small networks overlooked.
- ▶ Limited alternatives for small nets.

After my dissertation

Predicting gene functions

- ▶ Scale-up the problem.
- ▶ More biology (via ERGMs).
- ▶ New ways to look at phylo data.

ERGMs

- ▶ Revisited exact methods.
- ▶ New light on small networks.
- ▶ Many opportunities for methodological innovations.

Products

Publications

6 journal publications (*Journal of Open Source Software, Stata Journal, Journal of health and social behavior, Translational behavioral medicine, Social Science & Medicine*) +2 submitted
(*PLOS Comp. Bio, Social Networks*)

Concluding Remarks

Before my dissertation

Predicting gene functions

- ▶ “Small scale”.
- ▶ Detached from theory.

ERGMs

- ▶ Only approximations.
- ▶ Small networks overlooked.
- ▶ Limited alternatives for small nets.

After my dissertation

Predicting gene functions

- ▶ Scale-up the problem.
- ▶ More biology (via ERGMs).
- ▶ New ways to look at phylo data.

ERGMs

- ▶ Revisited exact methods.
- ▶ New light on small networks.
- ▶ Many opportunities for methodological innovations.

Products

Publications

6 journal publications (*Journal of Open Source Software*, *Stata Journal*, *Journal of health and social behavior*, *Translational behavioral medicine*, *Social Science & Medicine*) +2 submitted
(*PLOS Comp. Bio*, *Social Networks*)

Published software

- ▶ `ergmito` downloads 2593
- ▶ `slurmR` downloads 2667
- ▶ `fmcmc` downloads 4305
- ▶ `netdiffuseR` downloads 17K

Concluding Remarks

Before my dissertation

Predicting gene functions

- ▶ “Small scale”.
- ▶ Detached from theory.

ERGMs

- ▶ Only approximations.
- ▶ Small networks overlooked.
- ▶ Limited alternatives for small nets.

After my dissertation

Predicting gene functions

- ▶ Scale-up the problem.
- ▶ More biology (via ERGMs).
- ▶ New ways to look at phylo data.

ERGMs

- ▶ Revisited exact methods.
- ▶ New light on small networks.
- ▶ Many opportunities for methodological innovations.

Products

Publications

6 journal publications (*Journal of Open Source Software, Stata Journal, Journal of health and social behavior, Translational behavioral medicine, Social Science & Medicine*) +2 submitted
(*PLOS Comp. Bio, Social Networks*)

Published software

- ▶ ergmito downloads 2593
- ▶ slurmR downloads 2667
- ▶ fmcmc downloads 4305
- ▶ netdiffuseR downloads 17K

Other tools

similR, gnet, aphylo, polygons, pruner, netplot, rphyloxml, jsPhyloSVG,

Concluding Remarks

Before my dissertation

Predicting gene functions

- ▶ “Small scale”.
- ▶ Detached from theory.

ERGMs

- ▶ Only approximations.
- ▶ Small networks overlooked.
- ▶ Limited alternatives for small nets.

After my dissertation

Predicting gene functions

- ▶ Scale-up the problem.
- ▶ More biology (via ERGMs).
- ▶ New ways to look at phylo data.

ERGMs

- ▶ Revisited exact methods.
- ▶ New light on small networks.
- ▶ Many opportunities for methodological innovations.

Products

Publications

6 journal publications (*Journal of Open Source Software*, *Stata Journal*, *Journal of health and social behavior*, *Translational behavioral medicine*, *Social Science & Medicine*) +2 submitted
(*PLOS Comp. Bio*, *Social Networks*)

Published software

- ▶ ergmito downloads 2593
- ▶ slurmR downloads 2667
- ▶ fmcmc downloads 4305
- ▶ netdiffuseR downloads 17K

Other tools

similR, gnet, aphylo, polygons, pruner, netplot, rphyloxml, jsPhyloSVG, and **Barry**

Acknowledgments

Acknowledgments

- ▶ Prof. Paul Marjoram
- ▶ Prof. Kayla de la Haye
- ▶ Prof. Paul D Thomas
- ▶ Prof. Duncan C Thomas
- ▶ Prof. Emilio Ferrara

Acknowledgments

- ▶ Prof. Paul Marjoram
- ▶ Prof. Kayla de la Haye
- ▶ Prof. Paul D Thomas
- ▶ Prof. Duncan C Thomas
- ▶ Prof. Emilio Ferrara
- ▶ Prof. Kim Siegmund
- ▶ Prof. Jim Gauderman
- ▶ Prof. Tom Valente

Acknowledgments

- ▶ Prof. Paul Marjoram
 - ▶ Prof. Kayla de la Haye
 - ▶ Prof. Paul D Thomas
 - ▶ Prof. Duncan C Thomas
 - ▶ Prof. Emilio Ferrara
 - ▶ Prof. Kim Siegmund
 - ▶ Prof. Jim Gauderman
 - ▶ Prof. Tom Valente
 - ▶ Colleagues at USC
- ▶ Coauthors

Acknowledgments

- ▶ Prof. Paul Marjoram
- ▶ Prof. Kayla de la Haye
- ▶ Prof. Paul D Thomas
- ▶ Prof. Duncan C Thomas
- ▶ Prof. Emilio Ferrara
- ▶ Prof. Kim Siegmund
- ▶ Prof. Jim Gauderman
- ▶ Prof. Tom Valente
- ▶ Colleagues at USC
- ▶ Coauthors
- ▶ Members of the P01 group
- ▶ Members of the CANA group

Acknowledgments

- ▶ Prof. Paul Marjoram
- ▶ Prof. Kayla de la Haye
- ▶ Prof. Paul D Thomas
- ▶ Prof. Duncan C Thomas
- ▶ Prof. Emilio Ferrara
- ▶ Prof. Kim Siegmund
- ▶ Prof. Jim Gauderman
- ▶ Prof. Tom Valente
- ▶ Colleagues at USC
- ▶ Coauthors
- ▶ Members of the P01 group
- ▶ Members of the CANA group
- ▶ Department of Preventive medicine

Acknowledgments

- ▶ Prof. Paul Marjoram
- ▶ Prof. Kayla de la Haye
- ▶ Prof. Paul D Thomas
- ▶ Prof. Duncan C Thomas
- ▶ Prof. Emilio Ferrara
- ▶ Prof. Kim Siegmund
- ▶ Prof. Jim Gauderman
- ▶ Prof. Tom Valente
- ▶ Colleagues at USC
- ▶ Coauthors
- ▶ Members of the P01 group
- ▶ Members of the CANA group
- ▶ Department of Preventive medicine
- ▶ Friends and family

Acknowledgments

- ▶ Prof. Paul Marjoram
- ▶ Prof. Kayla de la Haye
- ▶ Prof. Paul D Thomas
- ▶ Prof. Duncan C Thomas
- ▶ Prof. Emilio Ferrara
- ▶ Prof. Kim Siegmund
- ▶ Prof. Jim Gauderman
- ▶ Prof. Tom Valente
- ▶ Colleagues at USC
- ▶ Coauthors
- ▶ Members of the P01 group
- ▶ Members of the CANA group
- ▶ Department of Preventive medicine
- ▶ Friends and family
- ▶ Mateo (4yo)
- ▶ Tomas ($\lim_{\varepsilon \downarrow 0} \{3 - \exp\{\varepsilon\}\}$)yo)
- ▶ Valentina (my wife)

And many more...

Essays on Bioinformatics and Social Network Analysis
Statistical and Computational Methods for Complex Systems



Thank you!

References |

-  Dodd, Diane M. B. (1989). "Reproductive Isolation as a Consequence of Adaptive Divergence in *Drosophila pseudoobscura*". In: *Evolution* 43.6, pp. 1308–1311. ISSN: 00143820, 15585646. URL: <http://www.jstor.org/stable/2409365>.
-  Handcock, Mark S. (2003). "Assessing Degeneracy in Statistical Models of Social Networks". In: *Working Paper No. 39* 76.39, pp. 33–50. ISSN: 1936900X. DOI: 10.1.1.81.5086. URL: <http://citeseerx.ist.psu.edu/viewdoc/summary?doi=10.1.1.81.5086>.

The Gene Ontology Project

Example of GO term

Accession	GO:0060047
Name	heart contraction
Ontology	biological_process
Synonyms	heart beating, cardiac contraction, hemolymph circulation
Alternate IDs	None
Definition	The multicellular organismal process in which the heart decreases in volume in a characteristic way to propel blood through the body. Source: GOC:dph

Table 1 Heart Contraction Function. source: amigo.geneontology.org

You know what is interesting about this function?

◀ go back

These four species have a gene with that function... and two of these are part of the same evolutionary tree!



Felis catus pthr10037



Oryzias latipes pthr11521



Anolis carolinensis pthr11521



Equus caballus pthr24356

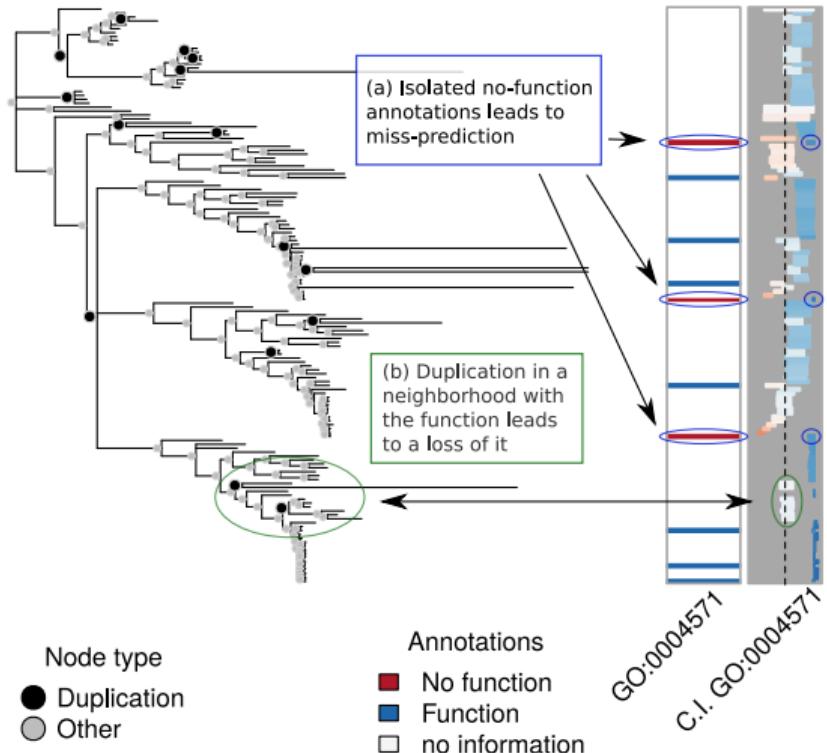
[◀ go back](#)

Example 2: Bad quality prediction

MAE: 0.52

AUC: 0.33

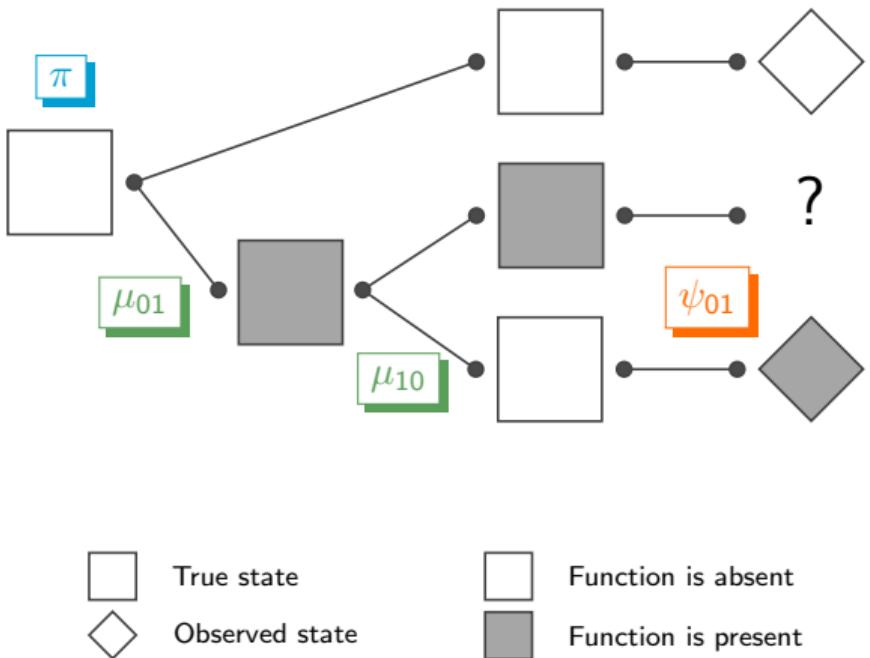
Type: Molecular Function

Name: mannosyl-oligosaccharide
1,2-alpha-mannosidase activityDesc: GO:0004571 involved in
synthesis of glycoproteins ([wiki](#)
and [examples](#)).[◀ go back](#)

		Pooled-data	One-at-a-time	
		Beta prior	Unif. prior	Beta Prior
Pooled-data				
Unif. prior	Beta prior	[-0.02,-0.01]	[-0.14,-0.10]	[-0.06,-0.03]
	Beta prior	-	[-0.12,-0.09]	[-0.04,-0.01]
One-at-a-time				
Unif. prior		-	-	[0.06, 0.09]

Table 2 Differences in Mean Absolute Error [MAE]. Each cell shows the 95% confidence interval for the difference in MAE resulting from two methods (row method minus column method). Cells are color coded blue when the method on that row has a significantly smaller MAE than the method on that column; Conversely, cells are colored red when the method in that column outperforms the method in that row. Overall, predictions calculated using the parameter estimates from *pooled-data* predictions outperform *one-at-a-time*.

An evolutionary model of gene functions



- ▶ Root has the function.
- ▶ Gain and loss (also depends on the type of event [► more](#)).
- ▶ Observed annotations may be incorrect.
- ▶ Only a fraction of the known genes have some form of annotation.

◀ go back

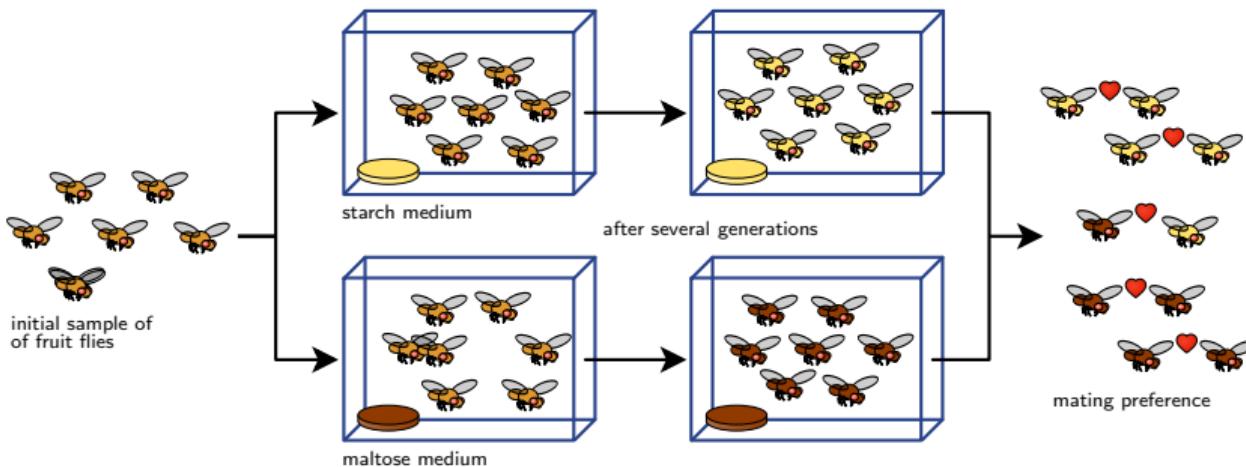


Figure 3 Dodd 1989: After one year of isolation, flies showed a significant level of assortativity in mating (wikimedia)

Duplication

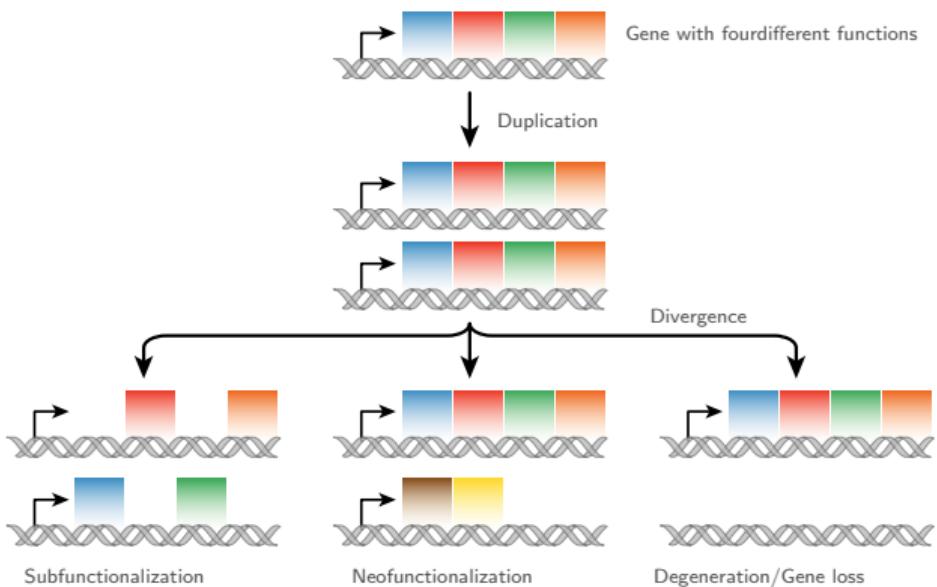


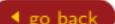
Figure 4 A key part of molecular innovation, gene duplication provides opportunity for new functions to emerge
(wikimedia)

◀ go back

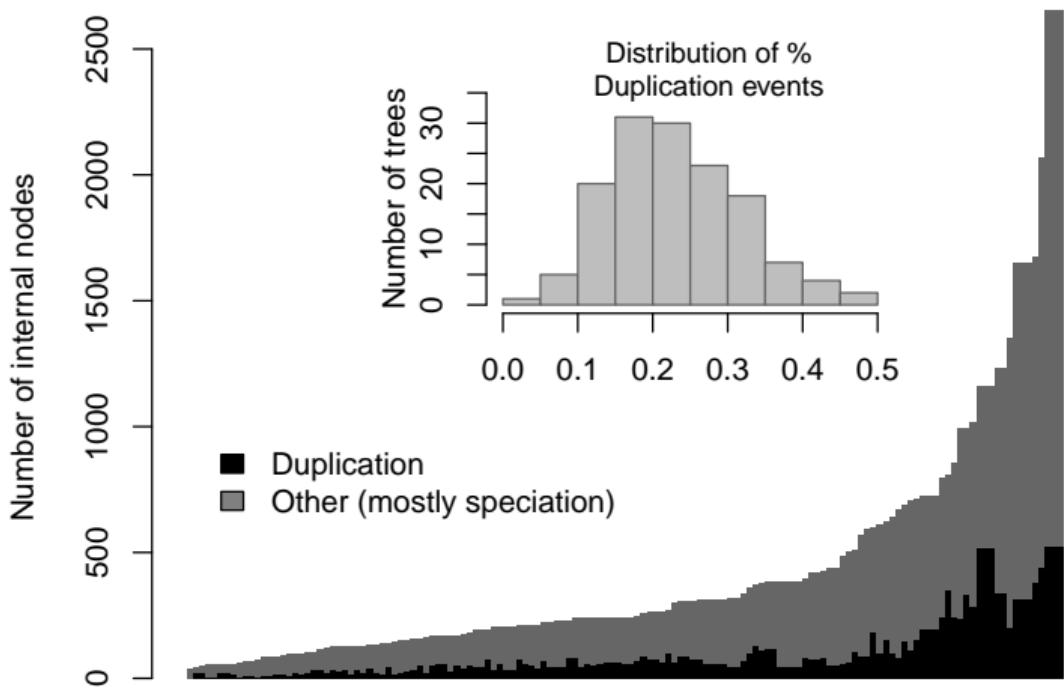
Data: Phylogenetic trees

Sample of annotations (first 10 in a single tree, Phosphoserine Phosphatase [PTHR10000])

Internal id	Branch Length	type	ancestor
AN0		S	LUCA
AN1	0.06	S	Archaea-Eukaryota
AN2	0.24	S	Eukaryota
AN3	0.44	S	Unikonts
AN4	0.42	S	Opisthokonts
AN6	0.68	D	
AN9	0.79	S	Amoebozoa
AN10	0.18	D	
AN15	0.57	S	Dictyostelium
AN18	0.52	S	Alveolata-Stramenopiles

◀ go back

Data: Node type (events)

[◀ go back](#)

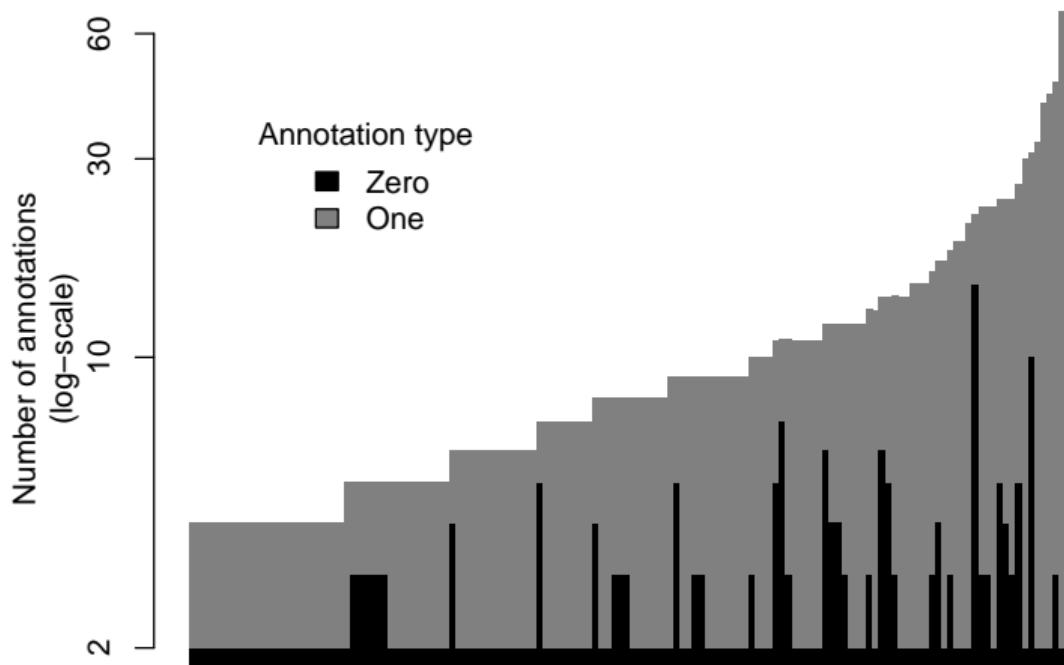
Data: Annotations (example)

This is the first 10 of ~ 400,000 experimental annotations used:

	Family	Id	GO term	Qualifier
1	PTHR12345	HUMAN HGNC=15756 UniProtKB=Q9H190	GO:0005546	
2	PTHR11361	HUMAN HGNC=7325 UniProtKB=P43246	GO:0016887	CONTRIBUTES_TO
3	PTHR10782	MOUSE MGI=MGI=3040693 UniProtKB=Q6P1E1	GO:0045582	
4	PTHR23086	ARATH TAIR=AT3G09920 UniProtKB=Q8L850	GO:0006520	
5	PTHR32061	RAT RGD=619819 UniProtKB=Q9EPI6	GO:0043197	
6	PTHR46870	ARATH TAIR=AT3G46870 UniProtKB=Q9STF9	GO:1990825	
7	PTHR15204	MOUSE MGI=MGI=1919439 UniProtKB=Q9Z1R2	GO:0045861	
8	PTHR22928	DROME FlyBase=FBgn0050085 UniProtKB=Q9XZ34	GO:0030174	
9	PTHR35972	HUMAN HGNC=34401 UniProtKB=A2RU48	GO:0005515	
10	PTHR10133	DROME FlyBase=FBgn0002905 UniProtKB=O18475	GO:0097681	

◀ go back

Data: Experimental Annotations



◀ go back

Asymptotic Behavior of ERGMs

- ▶ In the case that $s_l = s(\mathbf{g}, x)$ is on the boundary: $s_l \rightarrow \pm\infty$
- ▶ Since the support space of $s(\mathbf{g}, x) \in \mathcal{S}$ is bounded, e.g. # edges $\in [0, n \times (n - 1)]$, we have:

$$\lim_{\theta_l \rightarrow \infty} l(\theta), \quad \lim_{\theta_l \rightarrow \infty} \nabla l(\theta), \quad \lim_{\theta_l \rightarrow \infty} \mathbf{H}(\theta)$$

log-likelihood, its gradient, and hessian are finite.

- ▶ The direct implication is that, while $s(\mathbf{g}, x)$ is on the boundary, the MLE for the other statistics exists.¹
- ▶ All equations ultimately involve realizations of $s(\mathbf{g}', x)$ that equal s_l , relevant in: Simulations, Bootstrapping, etc.

◀ go back

¹Handcock 2003 briefly mentions this

- ▶ Long history in (soc.) network science.
- ▶ Common usage: Hypothesis test prevalence of a feature.

Is the observed count of XYZ within the expected in a Bernoulli graph?

Are statistics A, B, and C different from graphs with 5 triangles?

- ▶ Different names, same thing, e.g. CUG tests and rewiring algorithms.
- ▶ $\{\text{CUG, Rewiring}\} \subset \text{ERGM}$
- ▶ We can talk about *Conditional* ERGMs.

$$\mathbb{P}(s(\mathbf{G})_k = s_k \mid s(\mathbf{G})_l = s_l, \theta) = \frac{\exp\{\theta_{-l}^T s(\mathbf{g})_{-l}\}}{\sum_{\mathbf{g}' : s(\mathbf{g}')_l = s(\mathbf{g})_l} \exp\{\theta_{-l}^T s(\mathbf{g}')_{-l}\}} \quad (\text{Eq in 3.5 thesis})$$

In this equation, the marginal distribution of $s(\mathbf{g})_k$ is orthogonal (independent) from θ_l .

◀ go back

Sufficient statistics have various forms

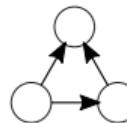
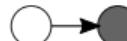
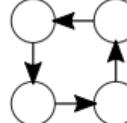
Representation	Description
	Mutual Ties (Reciprocity) $\sum_{i \neq j} y_{ij} y_{ji}$
	Transitive Triad (Balance) $\sum_{i \neq j \neq k} y_{ij} y_{jk} y_{ik}$
	Homophily $\sum_{i \neq j} y_{ij} \mathbf{1}(x_i = x_j)$
	Attribute-receiver effect $\sum_{i \neq j} y_{ij} x_j$
	Four Cycle $\sum_{i \neq j \neq k \neq l} y_{ij} y_{jk} y_{kl} y_{li}$

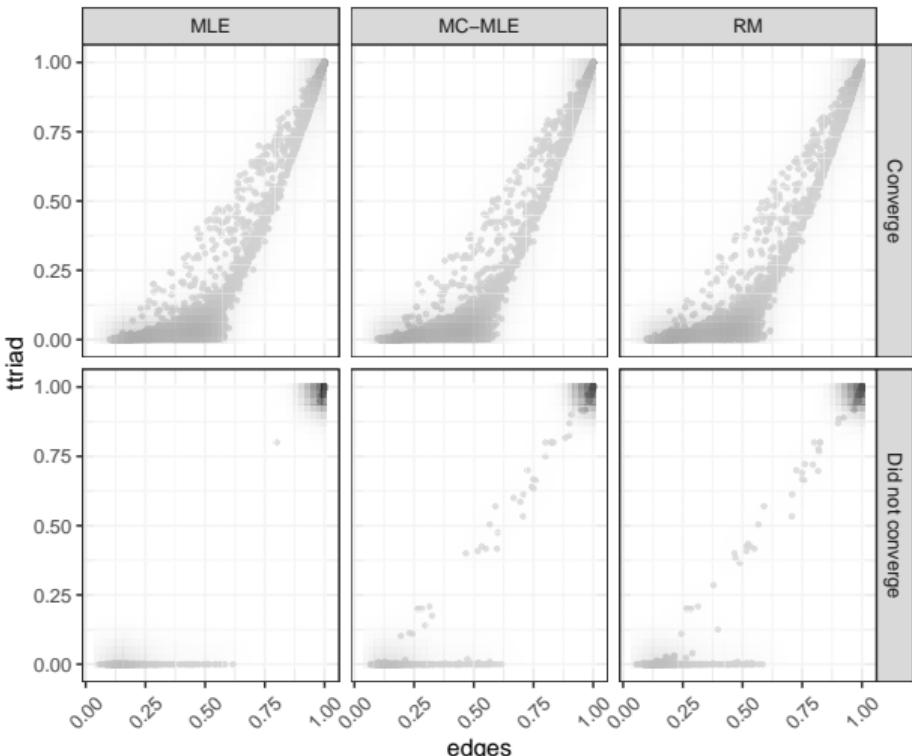
Figure 5 Besides the common edge count statistic (number of ties in a graph), ERGMs allow measuring other more complex structures that can be captured as sufficient statistics.

◀ go back

Simulation Study

1. Higher convergence rate

◀ return



Simulation Study

1. Higher convergence rate
2. **Smaller bias**

◀ return

	MLE	MC-MLE	RM
edges	[0.27, 0.36]	[1.23, 1.65]	[0.55, 1.54]
ttriads	[-0.05, -0.03]	[-0.22, -0.16]	[-0.15, 0.48]

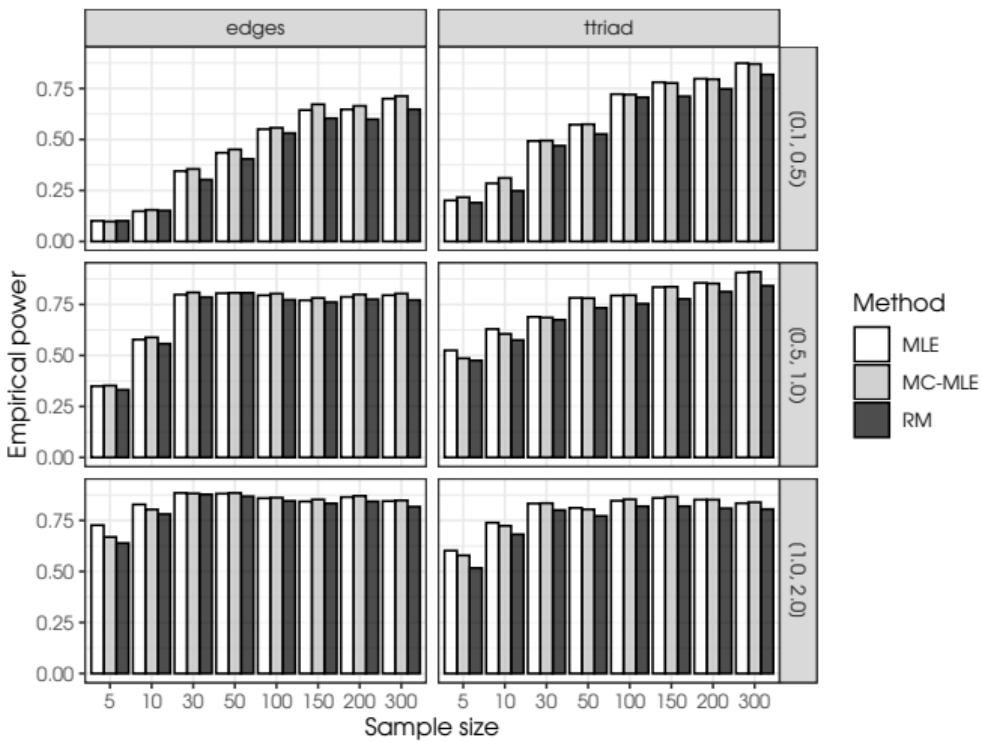
Table 3 Empirical bias. Each cell shows the 95% confidence interval of each methods' empirical bias.

▶ alt take

Simulation Study

1. Higher convergence rate
2. Smaller bias
3. **Higher power**

◀ return



Simulation Study

1. Higher convergence rate
2. Smaller bias
3. Higher power
4. **Smaller type I error**

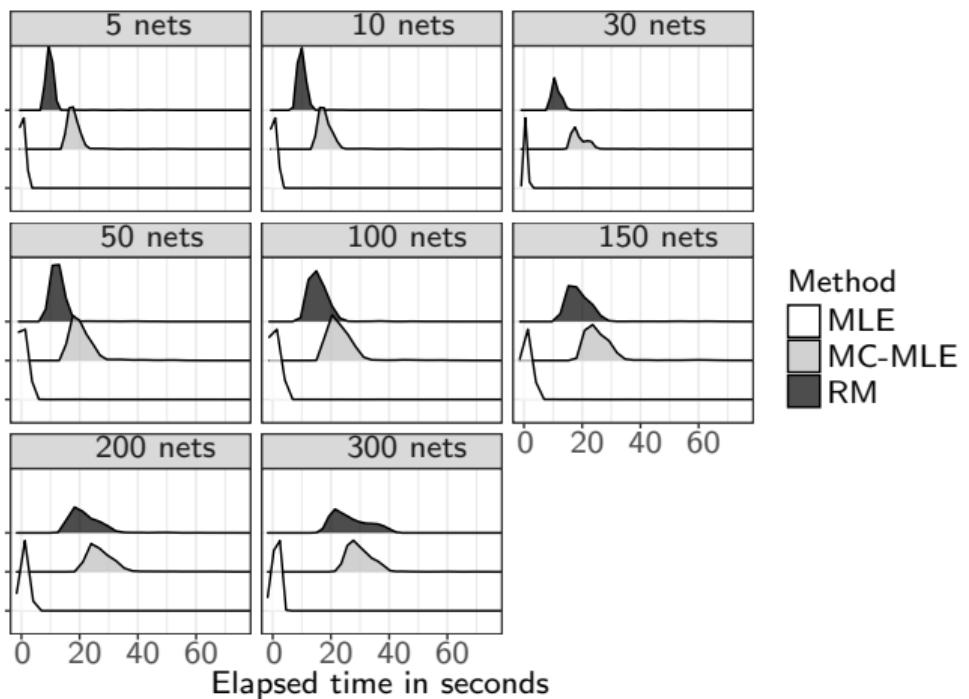
[◀ return](#)

	Sample size	N. Sims.	P(Type I error)		χ^2 (vs MLE)		RM
			MLE	MC-MLE	RM	MC-MLE	
	5	4,325	0.066	0.086	0.086	11.36 ***	11.36 ***
	10	4,677	0.063	0.078	0.073	8.44 ***	3.73 *
	15	4,818	0.060	0.072	0.063	5.50 **	0.41
	20	4,889	0.054	0.065	0.061	5.30 **	2.05
	30	4,946	0.053	0.059	0.055	1.60	0.07
	50	4,987	0.053	0.055	0.047	0.16	1.67
	100	4,999	0.054	0.054	0.050	0.00	0.81

Simulation Study

1. Higher convergence rate
2. Smaller bias
3. Higher power
4. Smaller type I error
5. **Elapsed time**

◀ return



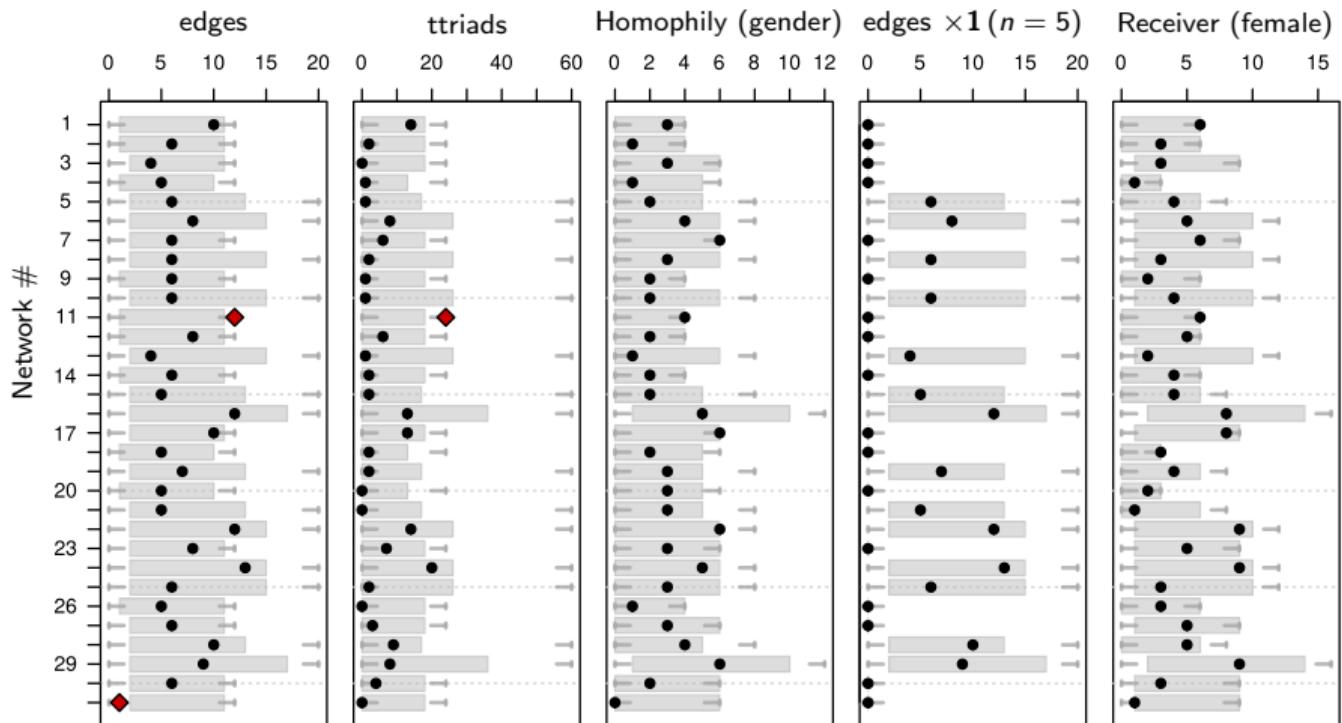
	(1)	(2)	(3)	(4)	(5)	(4b)
edges	-0.52** (0.17)	-0.91*** (0.23)	-0.54** (0.18)	-0.72*** (0.19)	-0.48* (0.19)	-0.72*** (0.17)
ttriads	0.36*** (0.06)	0.46*** (0.06)	0.37*** (0.06)	0.36*** (0.06)	0.36*** (0.06)	0.36*** (0.05)
Homophily (gender)	-0.03 (0.20)	-0.01 (0.21)	-0.20 (0.46)	-0.12 (0.20)	-0.01 (0.20)	-0.12 (0.20)
edges × 1 ($n = 5$)	-0.53*** (0.12)	-0.47** (0.16)	-0.52*** (0.13)	-0.53*** (0.13)	-0.53*** (0.12)	-0.53*** (0.13)
(Homophily) $^{1/2}$			0.54 (1.32)			
Sender (female)				0.46* (0.18)		0.46* (0.18)
Receiver (female)					-0.08 (0.18)	
<i>Constraint (offset)</i>						
edge > 4		Yes				
AIC	639.26	569.93	641.08	634.68	641.07	634.68
BIC	655.99	586.66	661.99	655.59	661.98	655.59
Num. networks	31	28	31	31	31	31
Time (seconds)	2.26	2.32	2.28	5.10	5.19	83.97
N replicates					1000	

*** $p < 0.001$, ** $p < 0.01$, * $p < 0.05$

1. Interaction effects: seemingly included.
2. Transformed variables: also easy to add.
3. Using offset terms, we can constrain the support.
4. Each 1,000 bootstrap replicates took roughly 0.08 secs.
5. No support for gender homophily, but evidence of females sending more ties.

What about goodness-of-fit?

What About Goodness-of-fit?

[◀ go back](#)

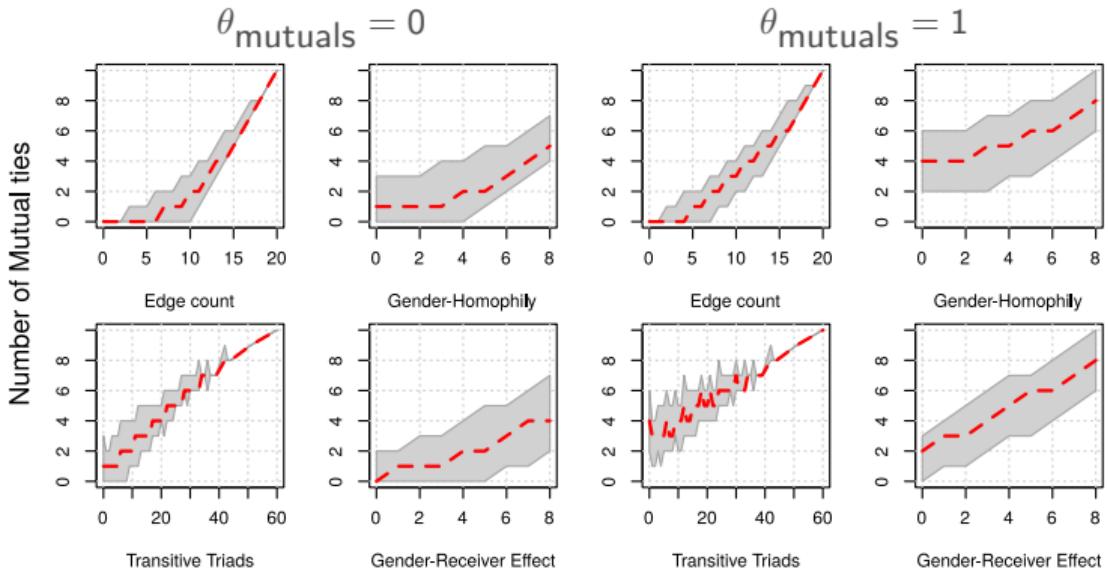
(1)	(2)	(3)	(4)	(5)	(6)
Size (n)	edges	ttriads	edges \times $\mathbf{1} (n = 5)$	ttriads \times $\mathbf{1} (n = 5)$	edges \times $\log \{1/n\}$
4	10	14	0	0	-13.86
4	6	2	0	0	-8.32
4	4	0	0	0	-5.55
5	6	1	6	1	-9.66
5	8	8	8	8	-12.88
5	6	2	6	2	-9.66
... 25 more rows...					

Table 4 Example of observed sufficient statistics for the team advice networks. Pooled-data ERGMs have multiple observed sufficient statistics (also known as target statistics). Furthermore, as shown here, we can manipulate common statistics as *edges* (2) and *ttriads* (3) to include, e.g. interaction effects (4) and (5), or more complex transformations, e.g. (6).

Conditional Distribution: Mutual Ties

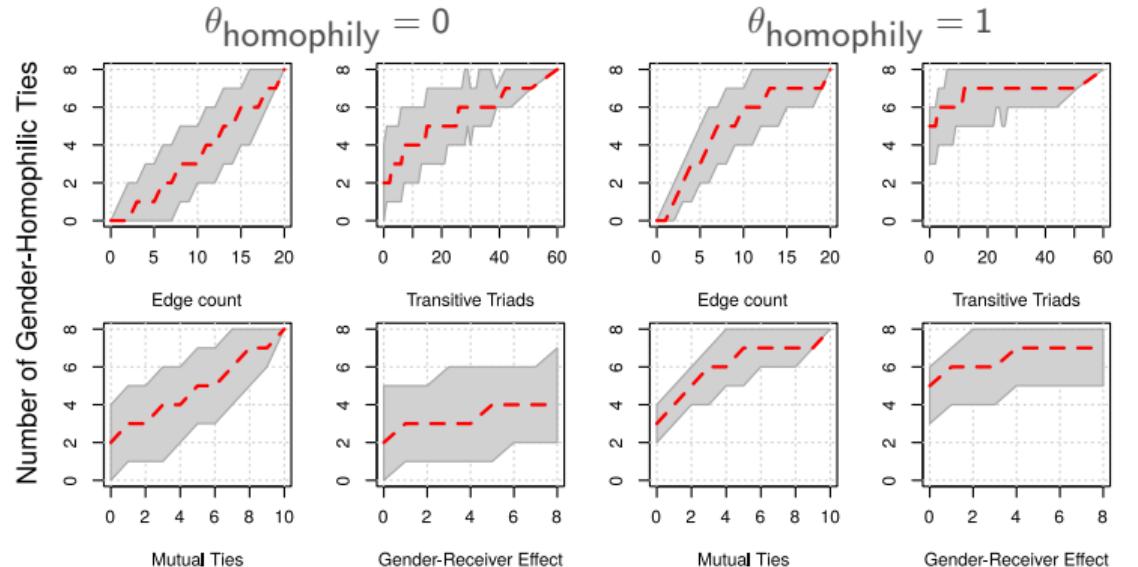


- ▶ Better predicted by other Markov structures.
- ▶ Non-Markov structures = poor prediction.
- ▶ No big impact of prevalence (θ_{mutual}).



◀ go back

Conditional Distribution: Homophily



- ▶ No structure has high predictive power.
- ▶ Almost zero association with Receiver Effect.
- ▶ Prevalence ($\theta_{\text{homophily}}$) has no effect.

◀ go back