

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)

You can download the slides from <https://github.com/gvegayon/defense>

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)





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- ▶ About $\sim 550,000$ are on human genes.
- ▶ Yet, less than 10% of those annotations are based on experimental evidence.

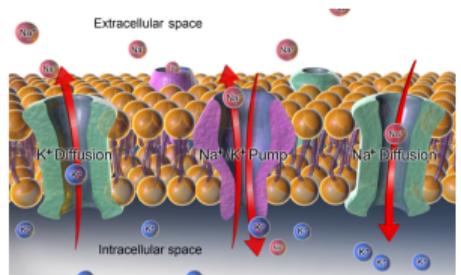
source: Statistics from <http://pantherdb.org> and <http://geneontology.org>

Gene functions can be classified in three types:

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Molecular function

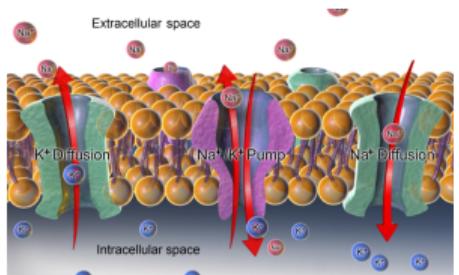
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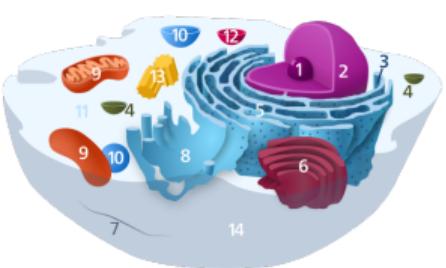
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Cellular component

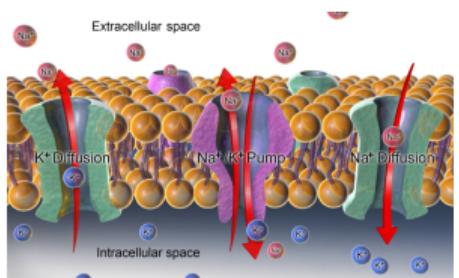
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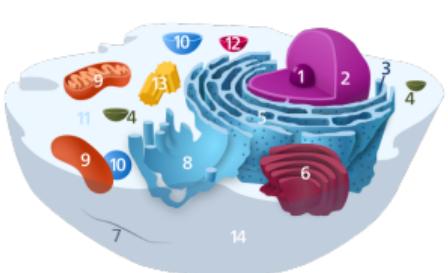
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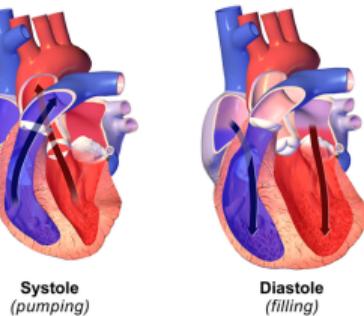
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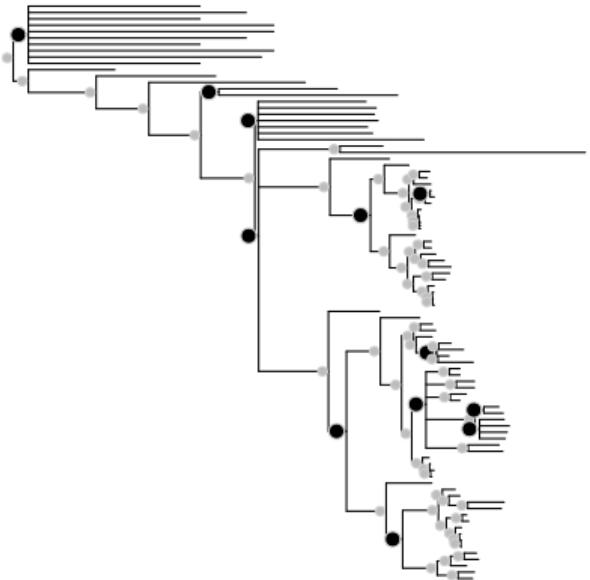
Biological process

Heart contraction GO:0060047



GO Annotations and Phylogenetic Trees

Family: PTHR11258



Node type

- Duplication
- Other

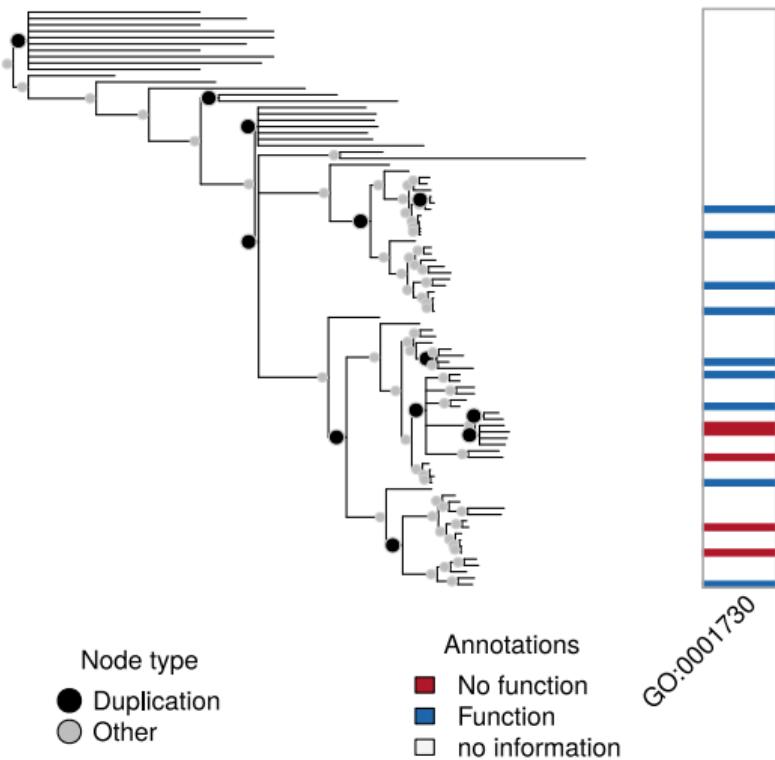
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An evolutionary model of gene functions

Imagine a relay race...

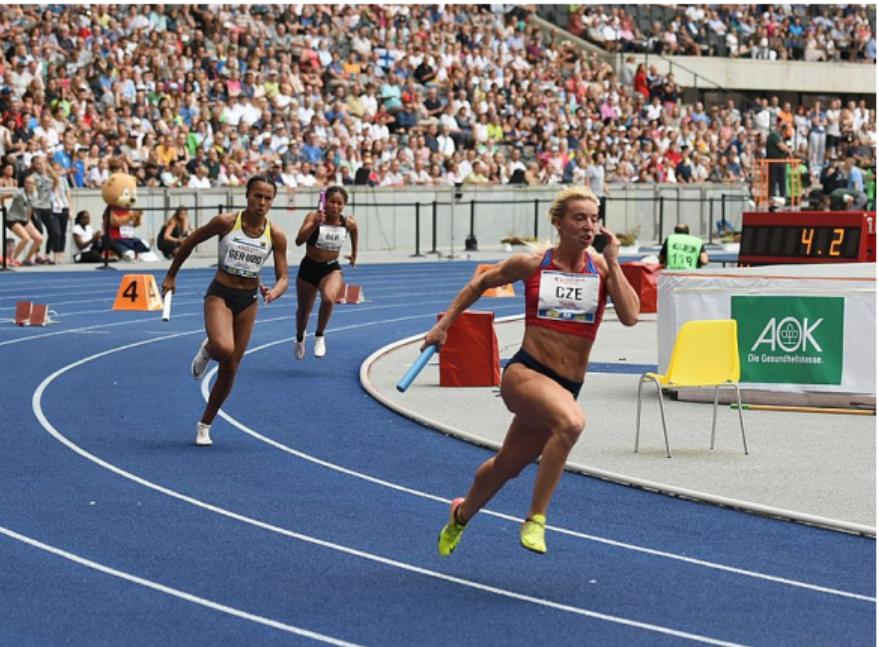
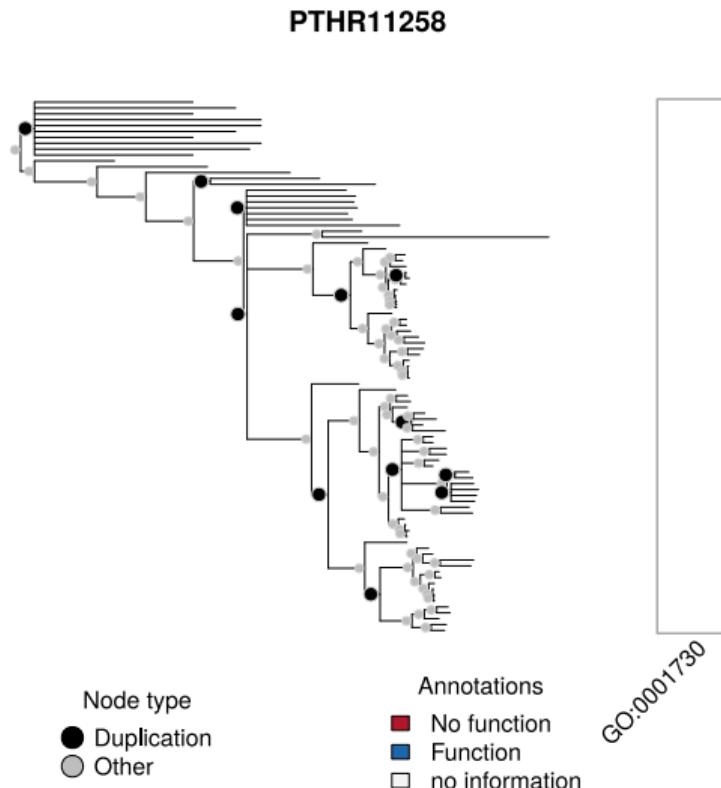
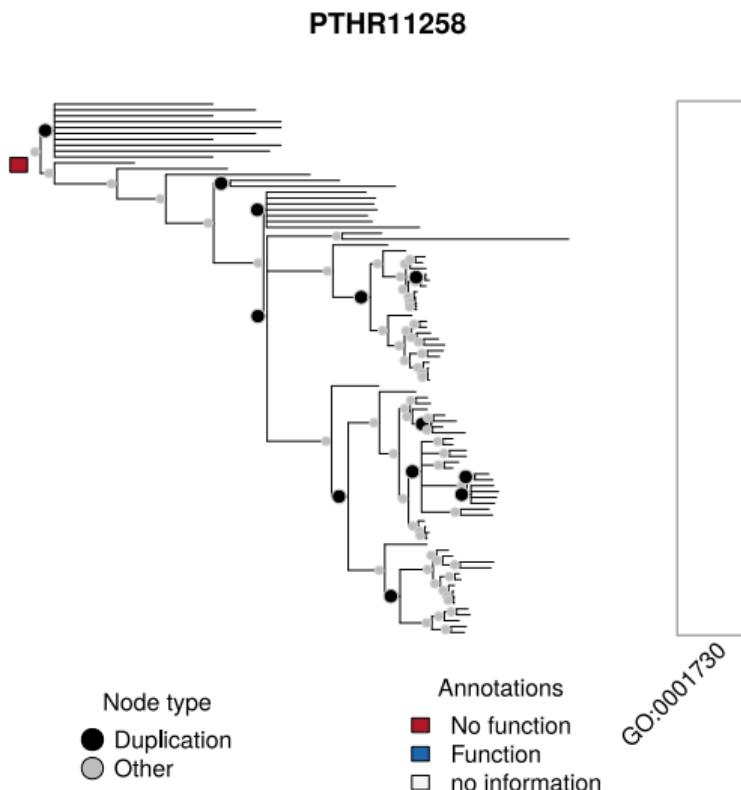


Figure 1 ISTAF 2019 4 × 100 m relay race (Martin Rulsch, wikimedia)

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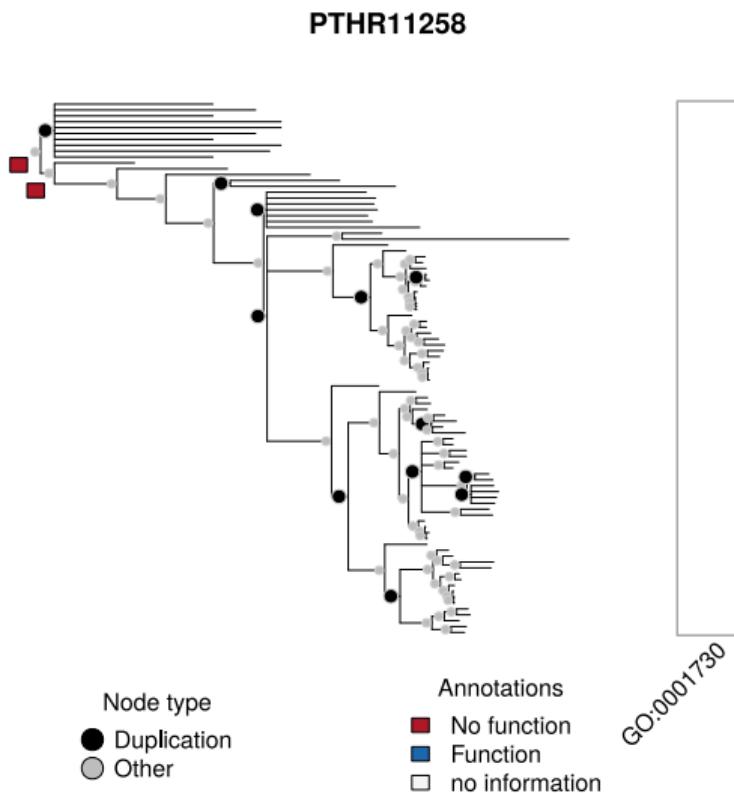


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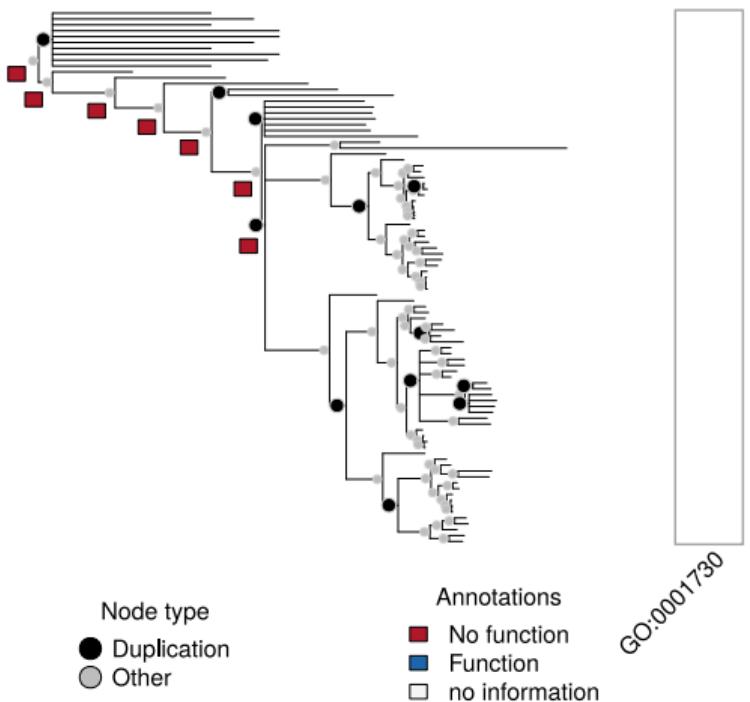
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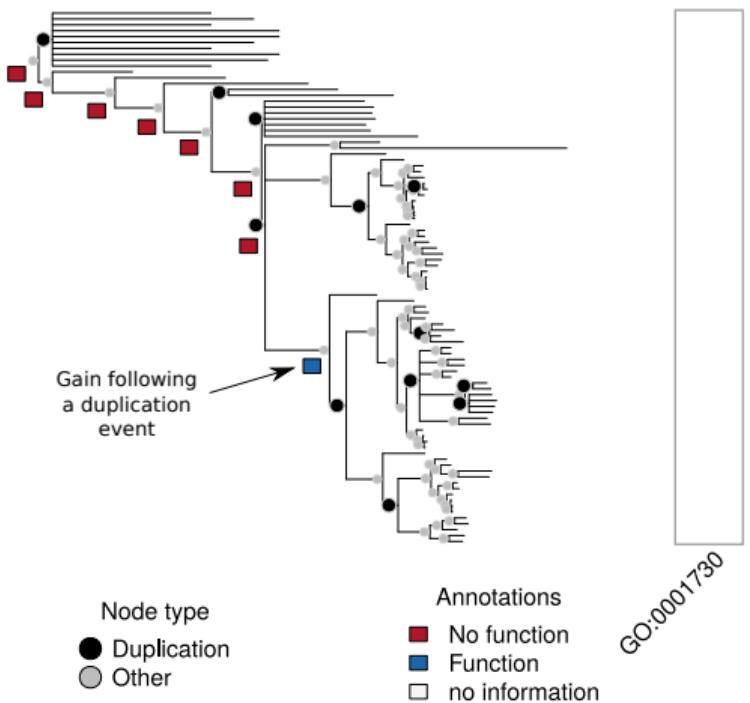
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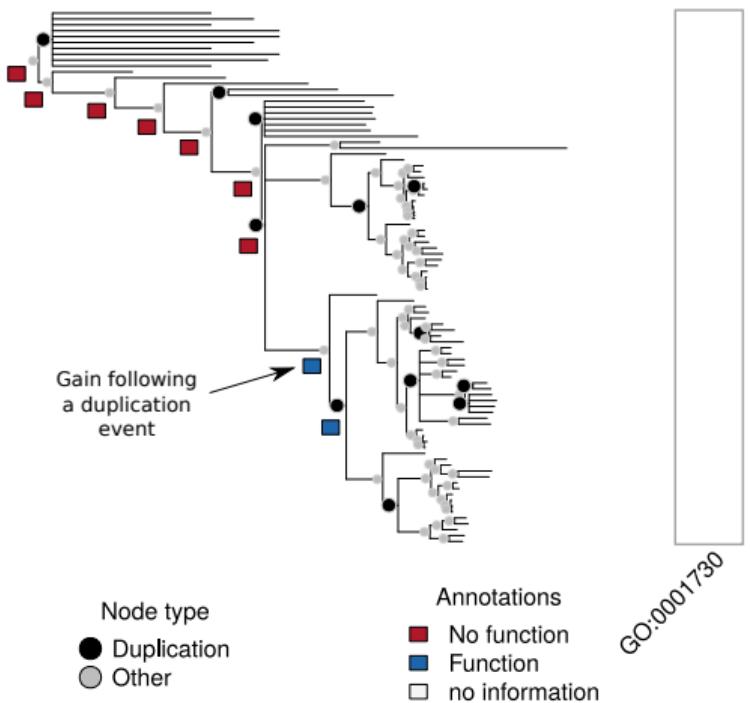
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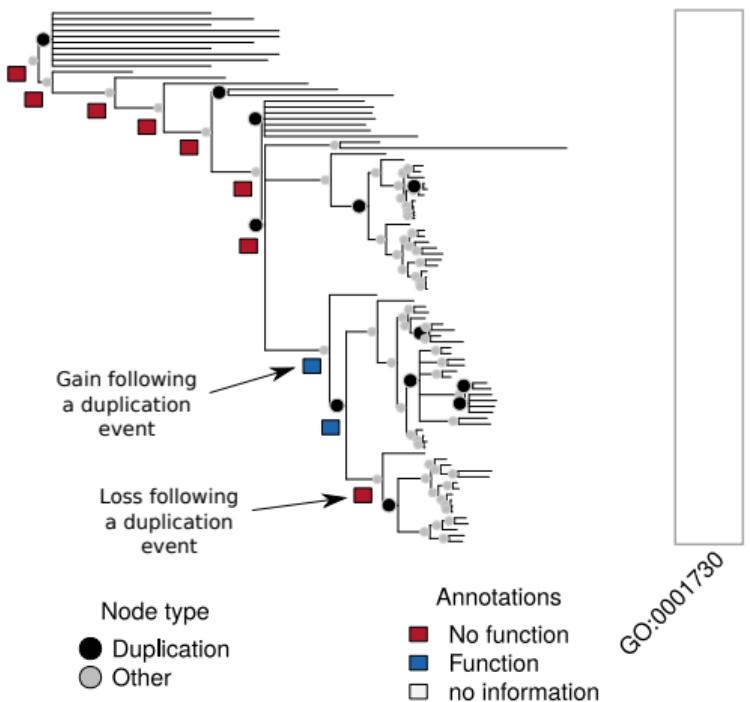
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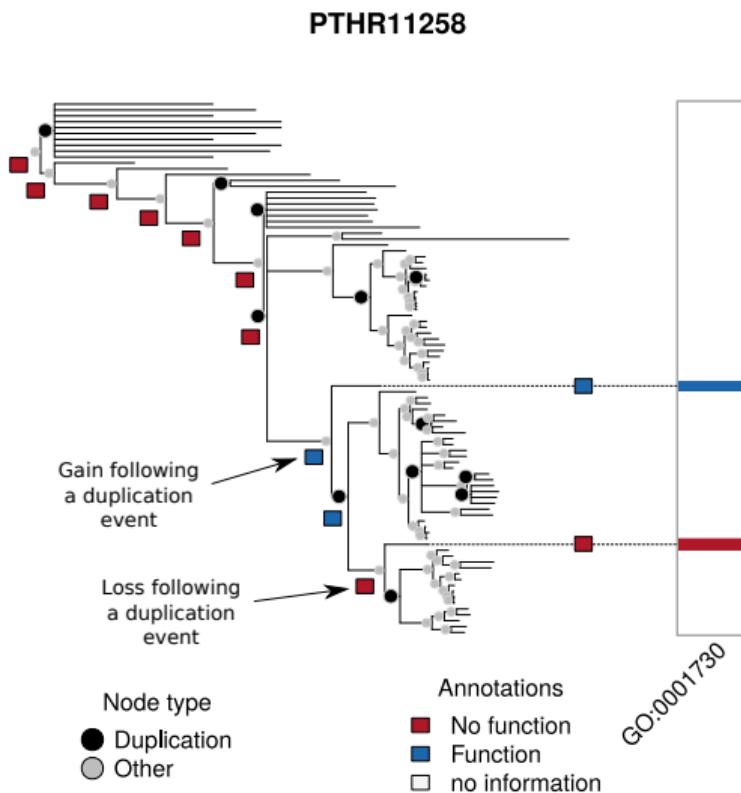
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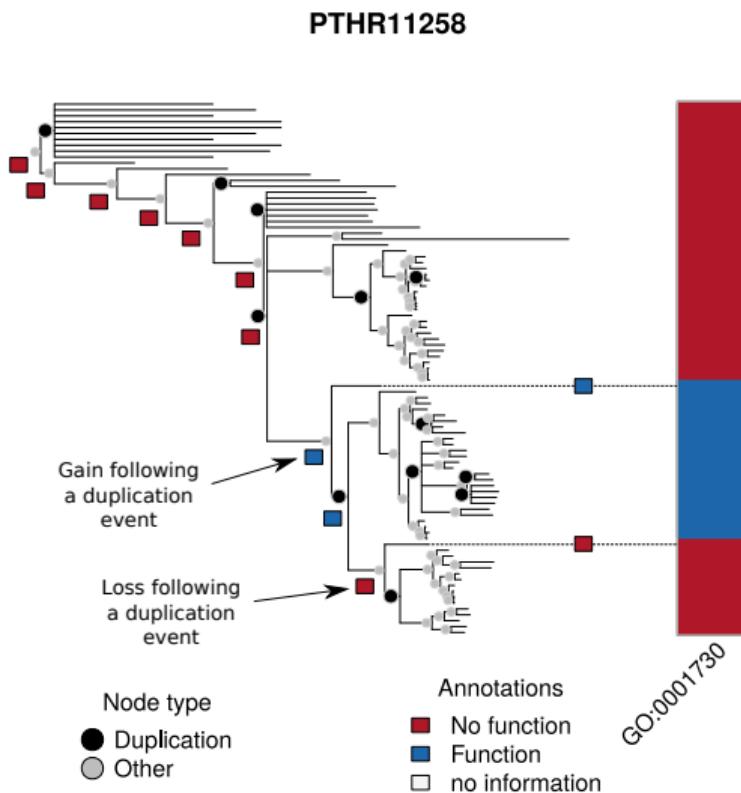
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▶ more on duplication

▶ alt view

Example of Data + Predictions

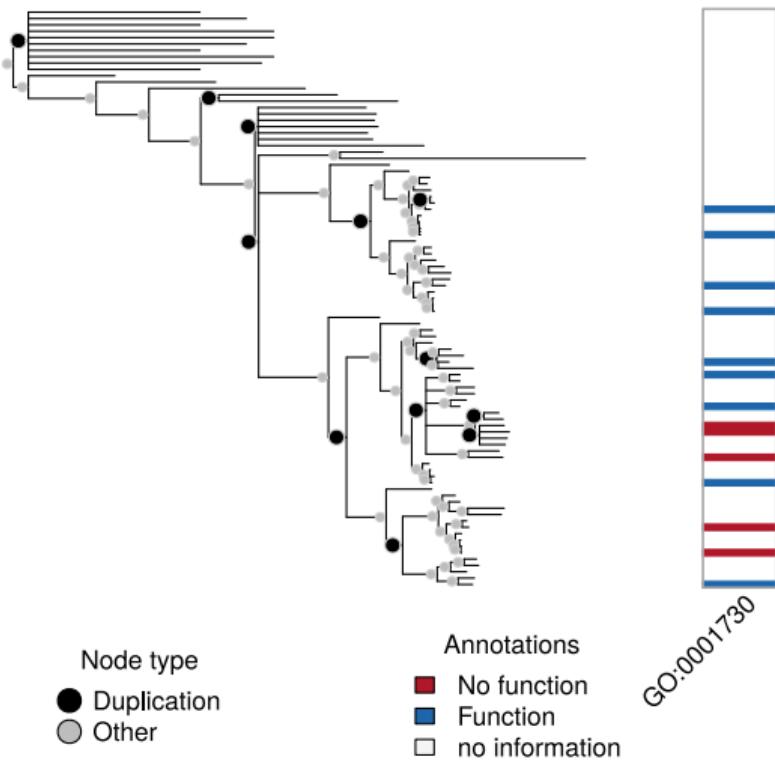
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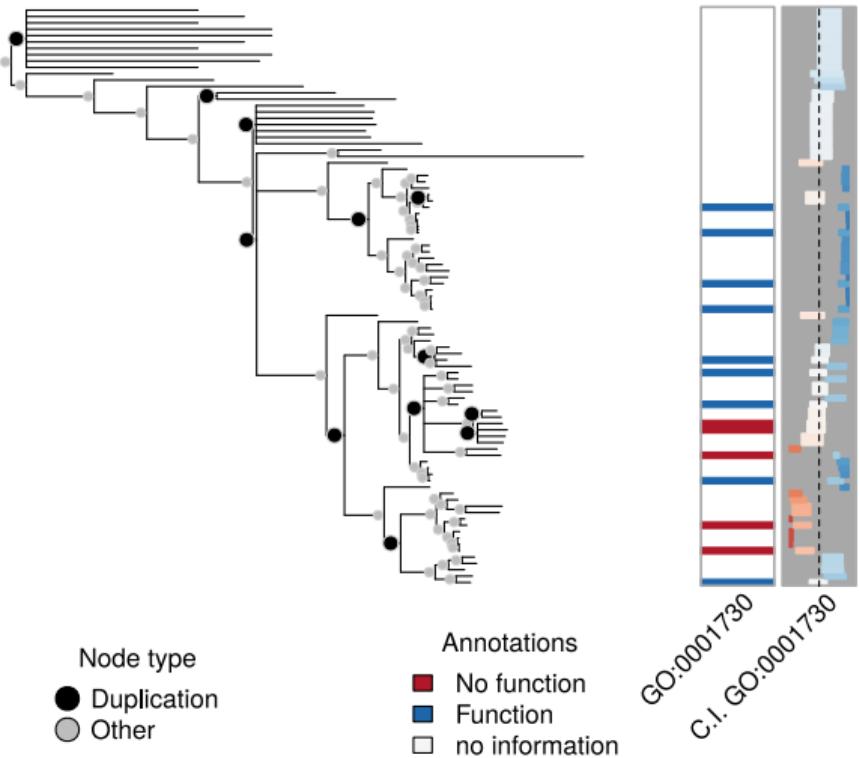
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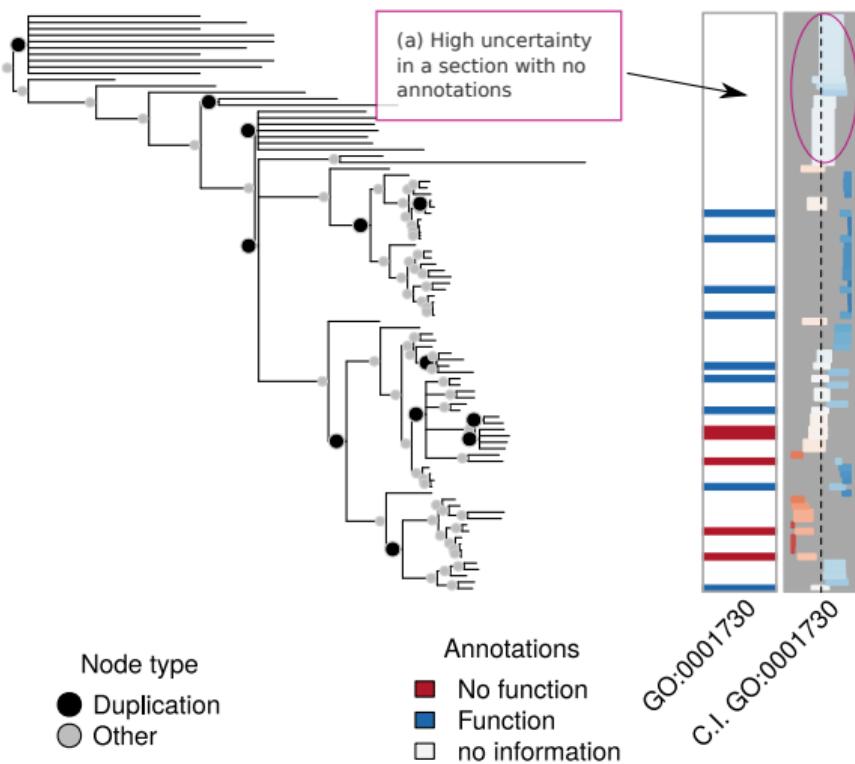
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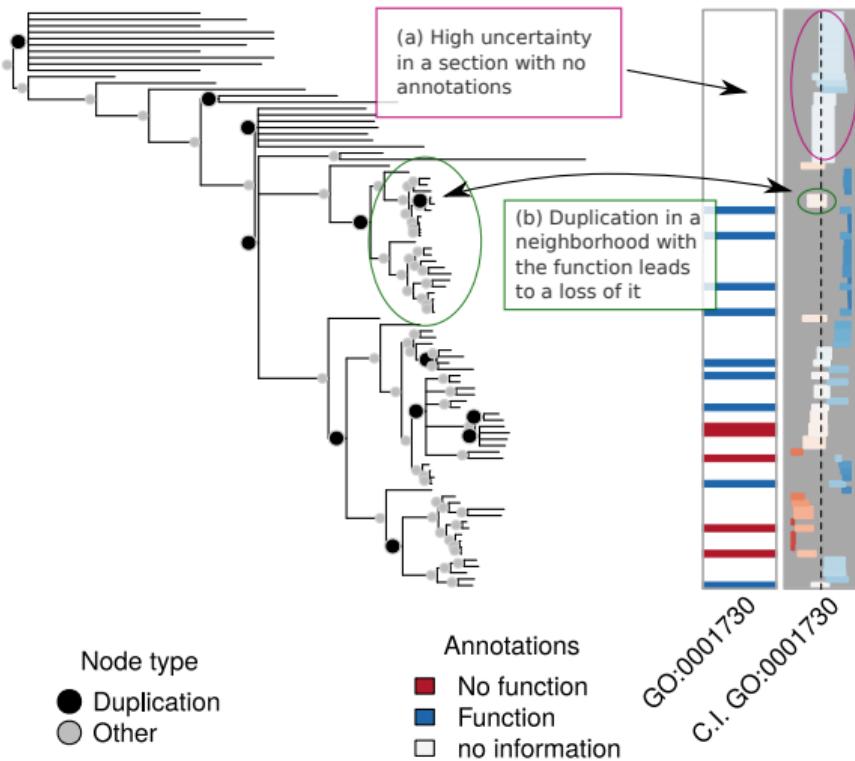
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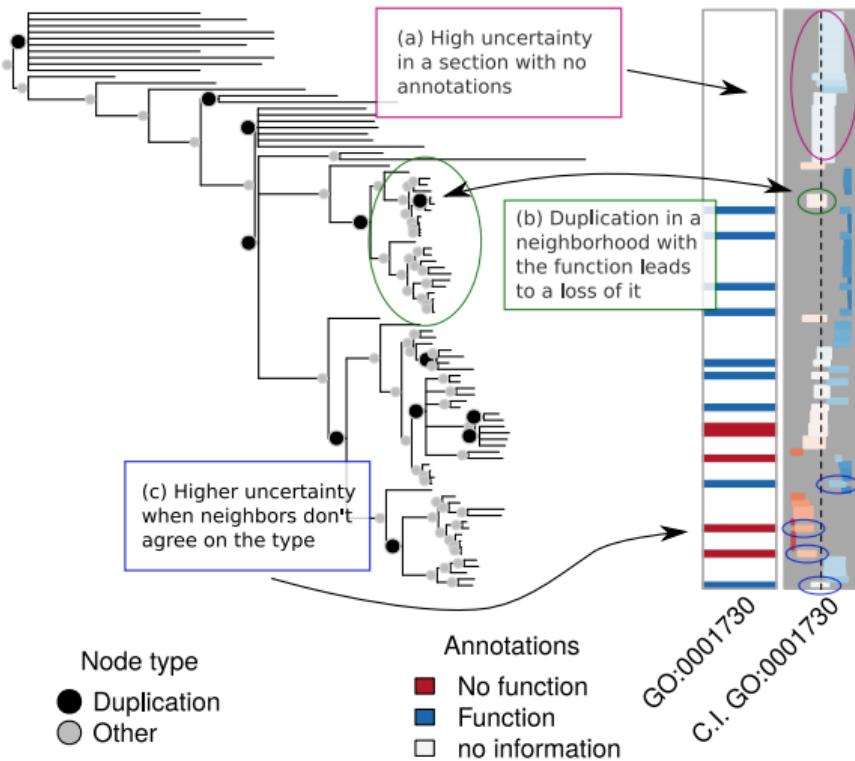
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Results from the first version

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Pooled-data model
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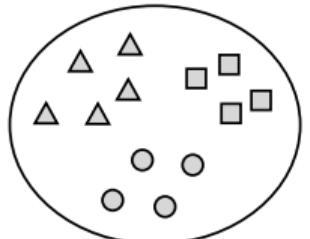
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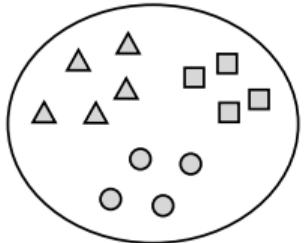
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...all this assuming that all functions had the same gain/loss rate.

Phylogenetics Modeling: Pooling data



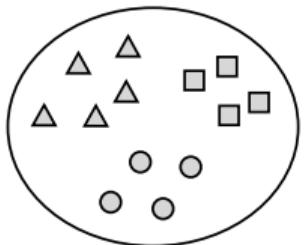
(a) Fixed rate
across functions



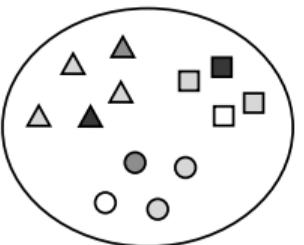
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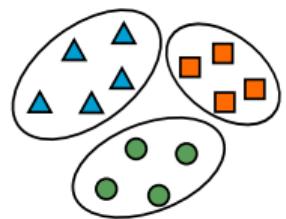
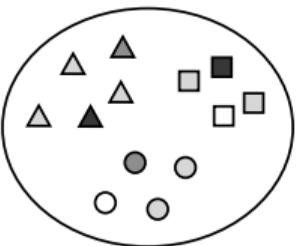
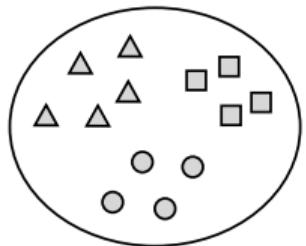
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(b) Random rate
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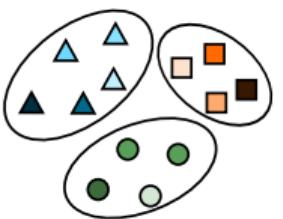
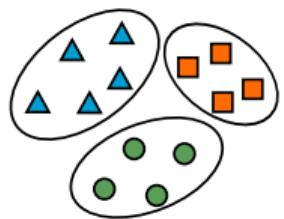
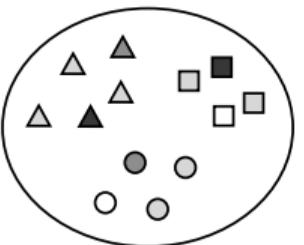
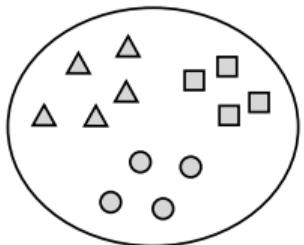
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- (b) “Full glory” Hierarchical Bayes (1,001 parameters for the 141 functions).

Phylogenetics Modeling: Pooling data



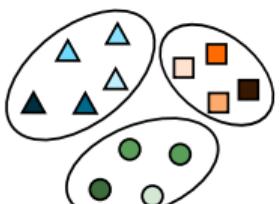
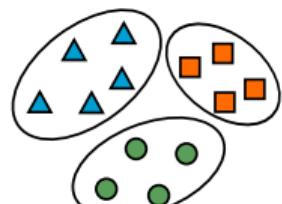
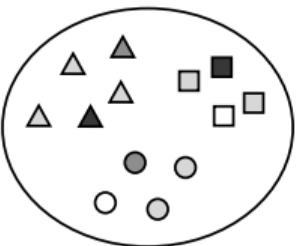
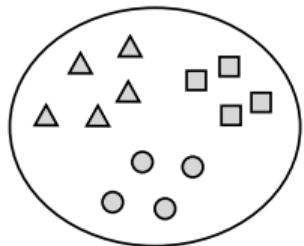
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All methods are now available in the `aphylo` package: `aphylo_mle`, `aphylo_mcmc`, and `aphylo_hier`.

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	
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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	
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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.



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- ▶ If COVID-19 has taught us something it is that networks matter.
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- ▶ We can study networks using ERGMs.

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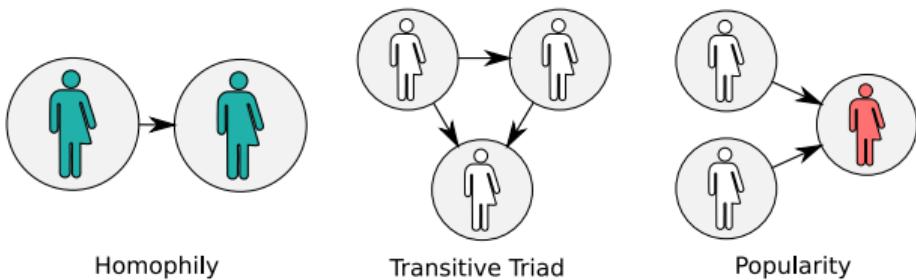
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Discrete Exponential-Family Models

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

A vector of model parameters A vector of sufficient statistics

Observed data The normalizing constant All possible networks

Discrete Exponential-Family Models

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

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▶ more theory ▶ more terms

ergmito: Estimation of Small ERGM using Exact Statistics

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- Lower type-I error rate.
- Smaller bias.
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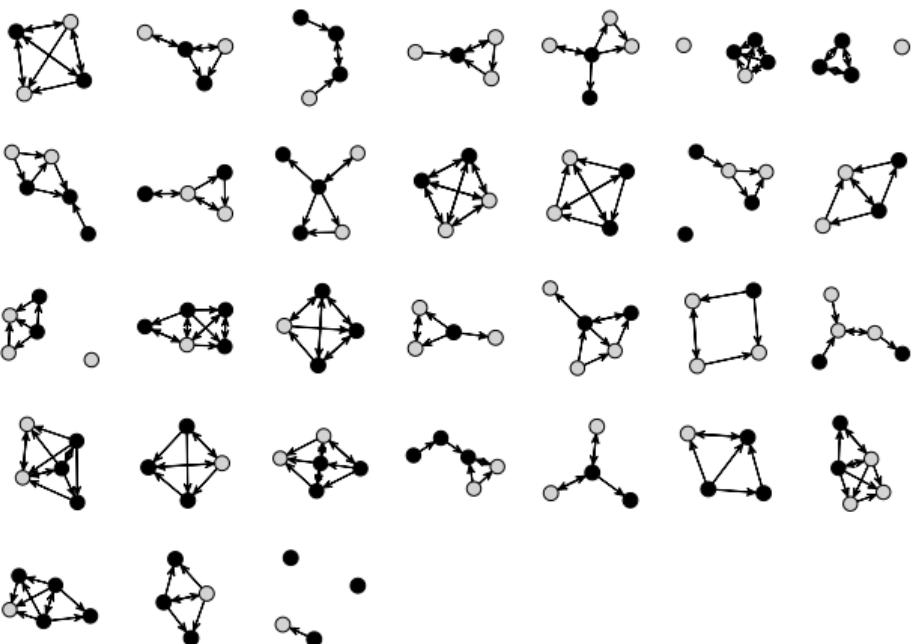
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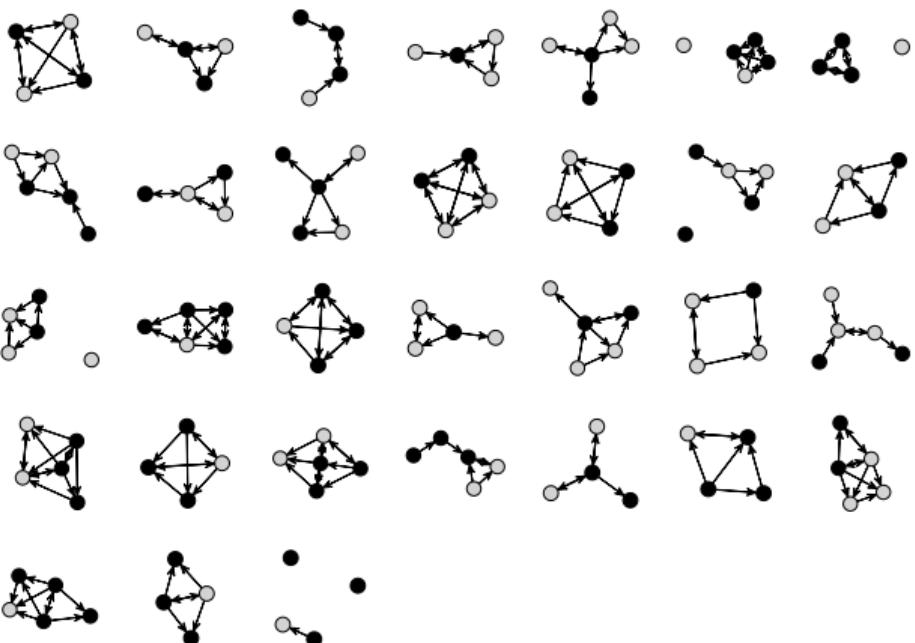
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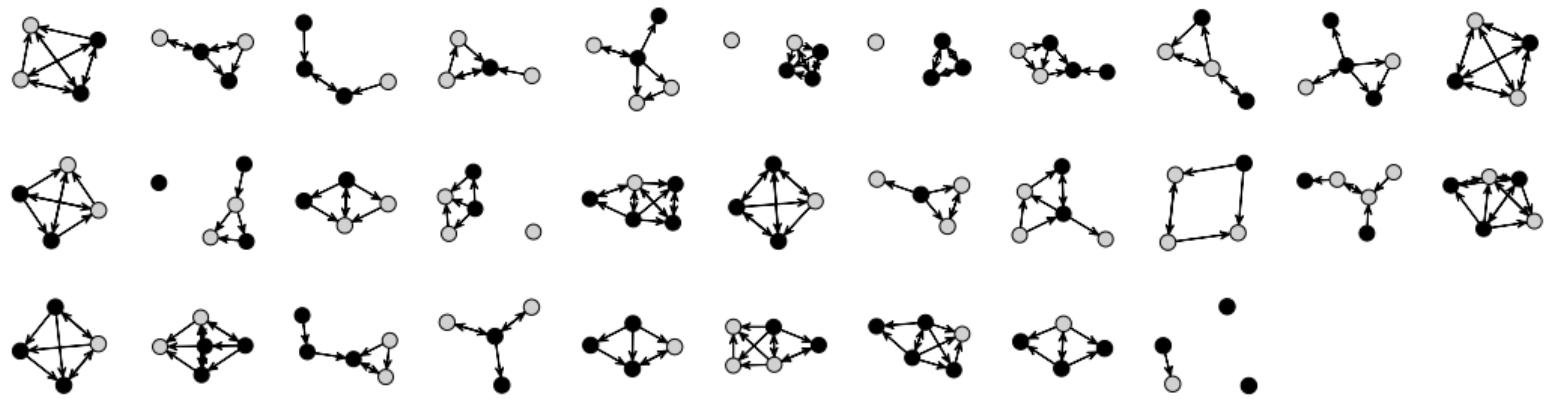
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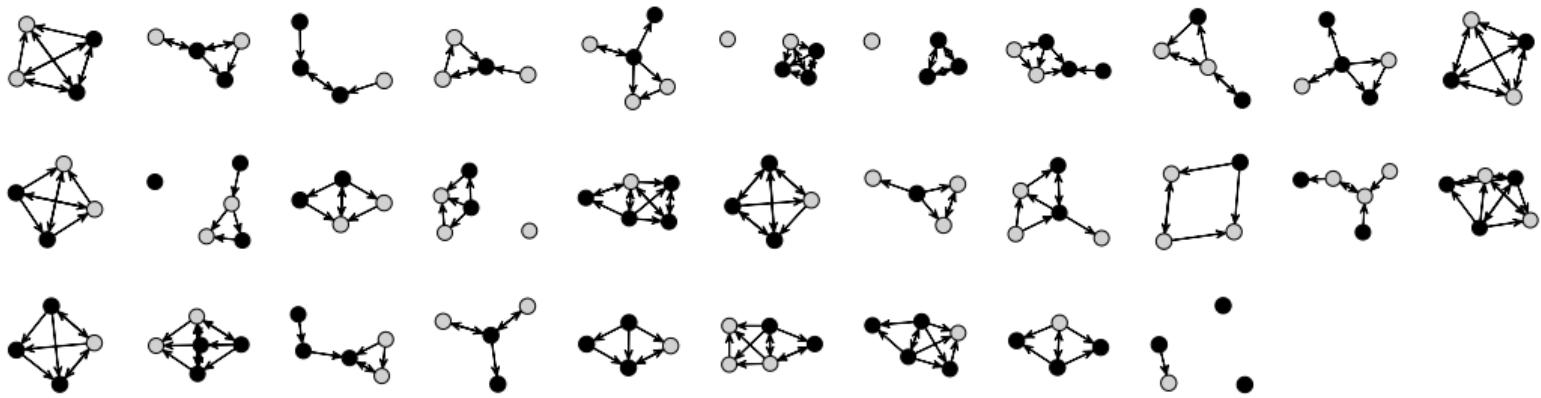
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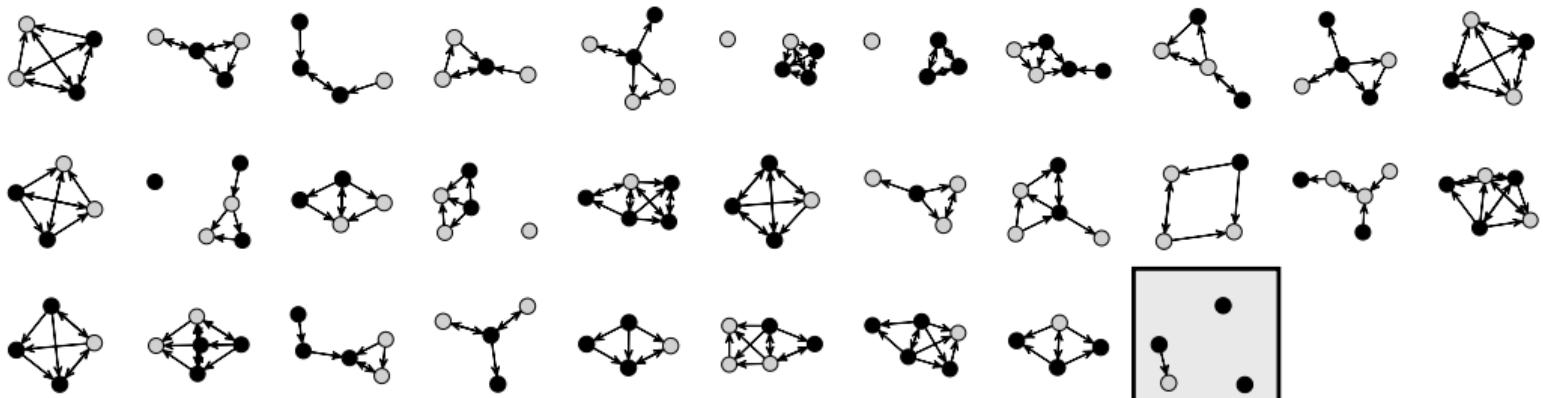


Is Gender Homophily a feature of these graphs?



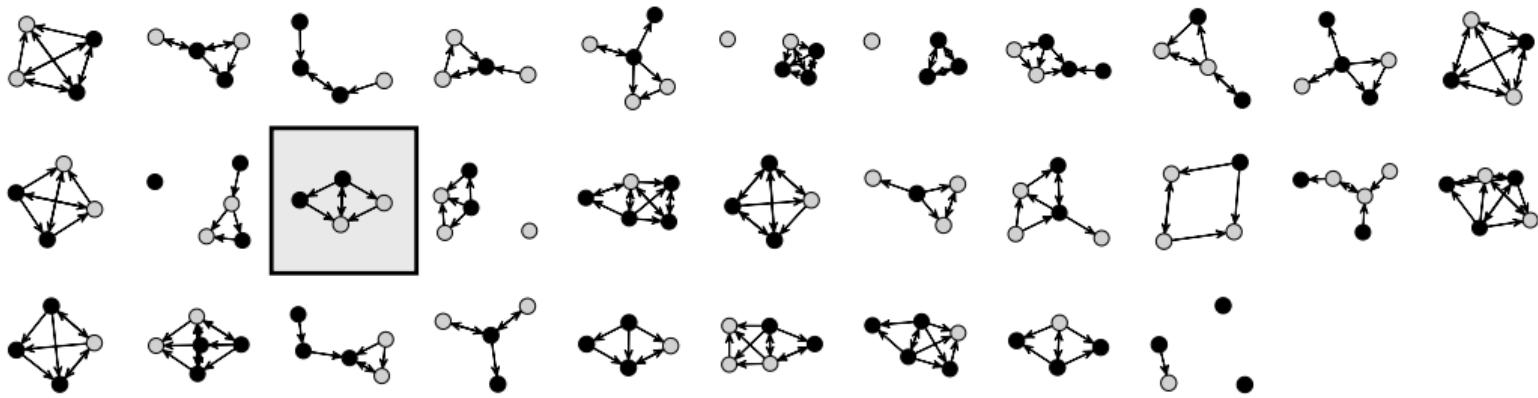


Key findings



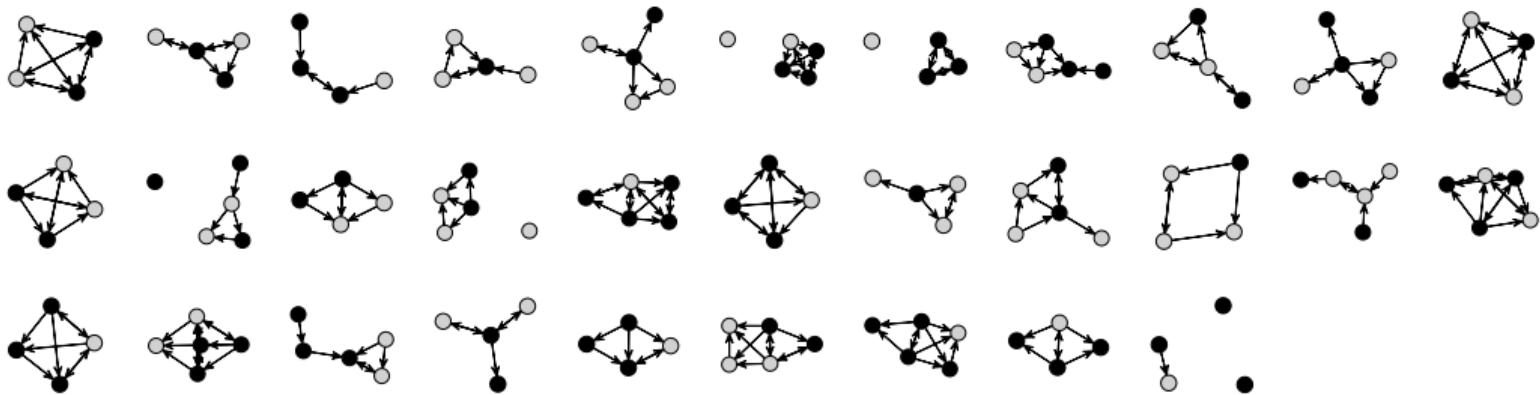
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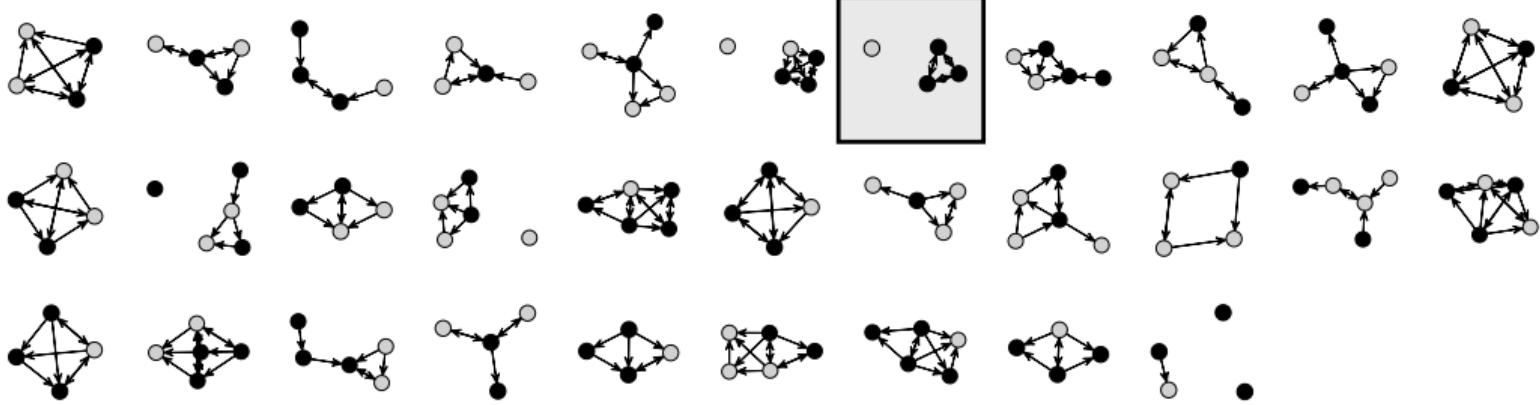
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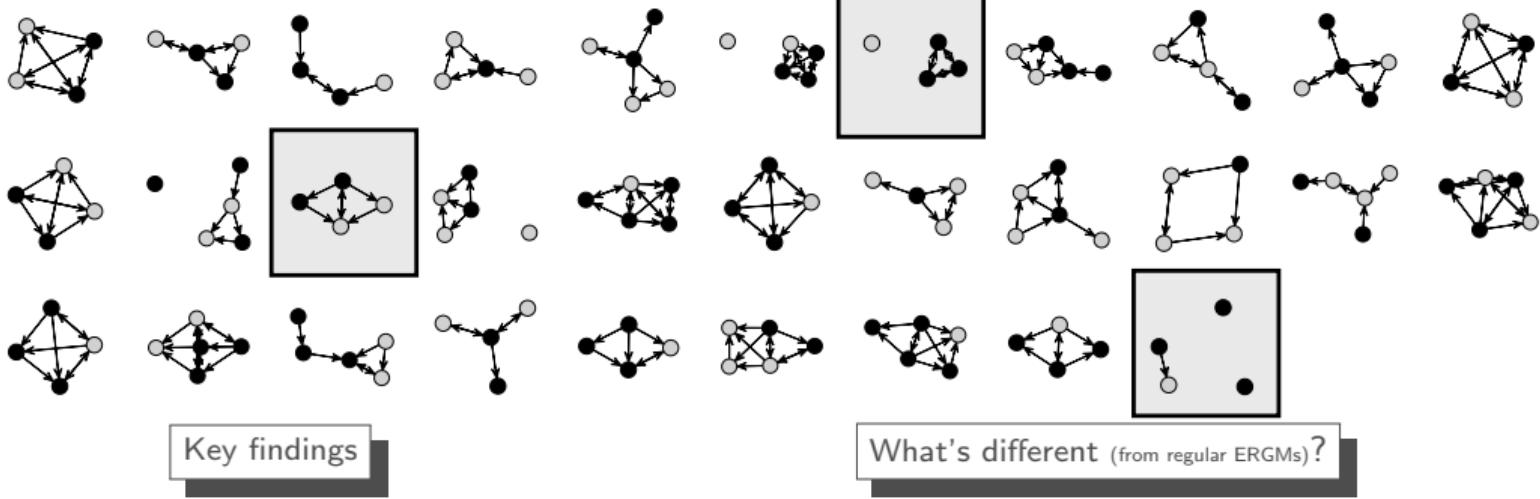
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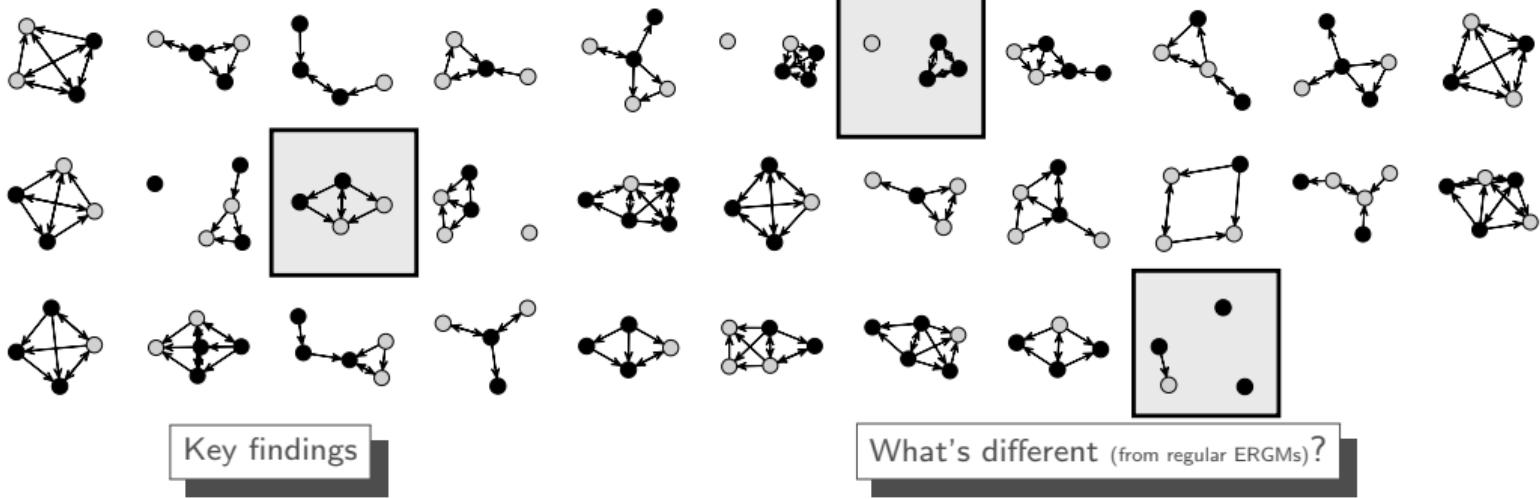


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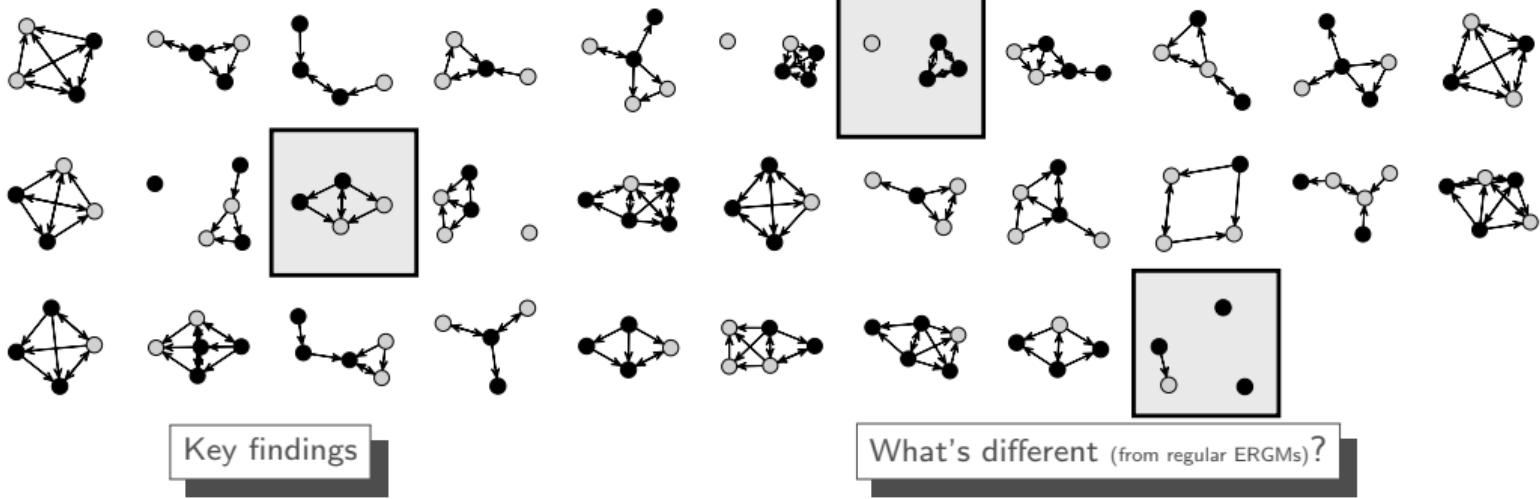
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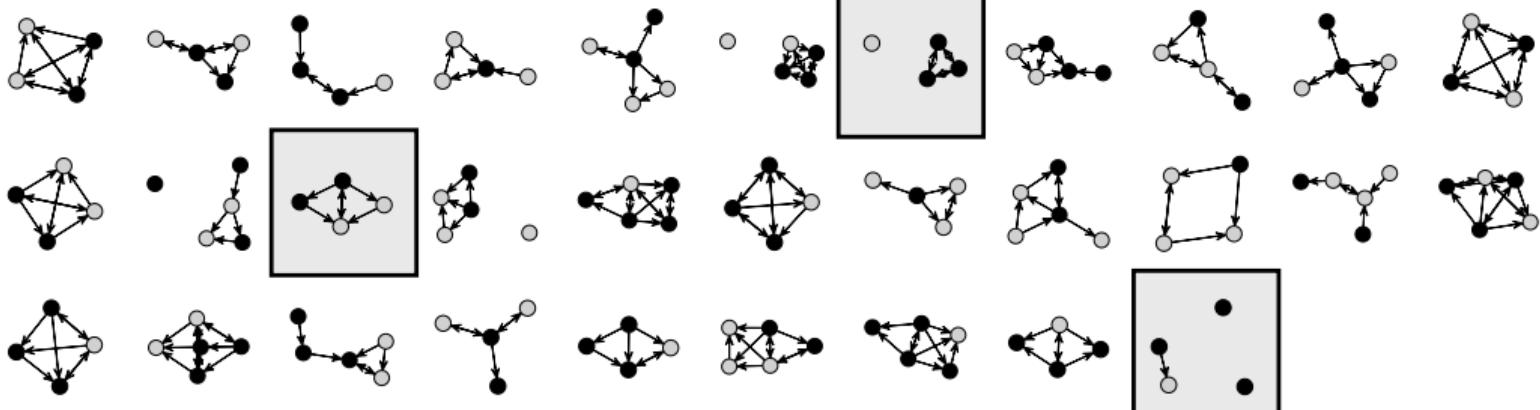
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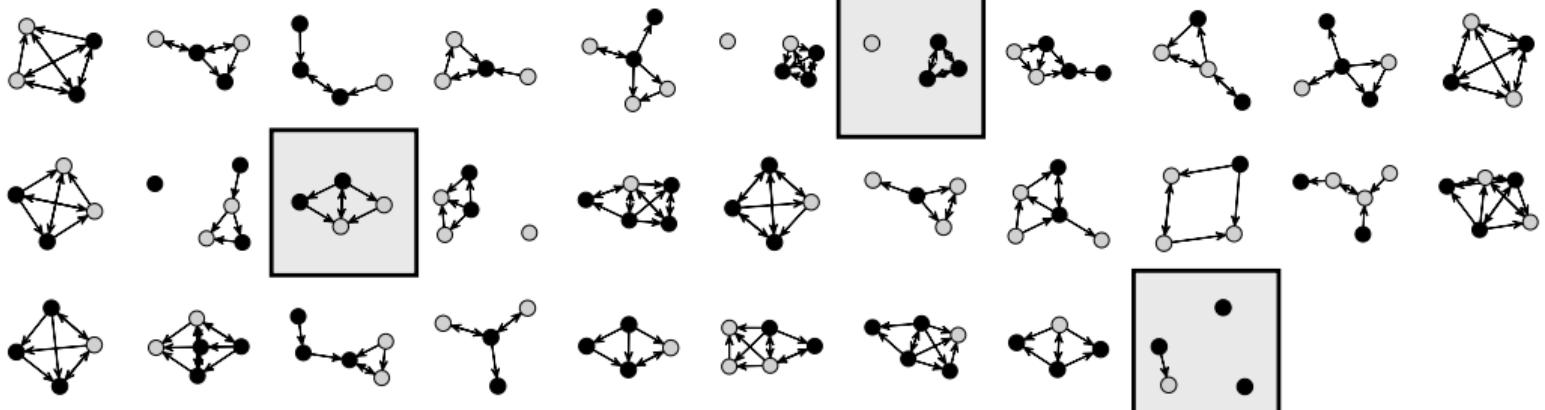


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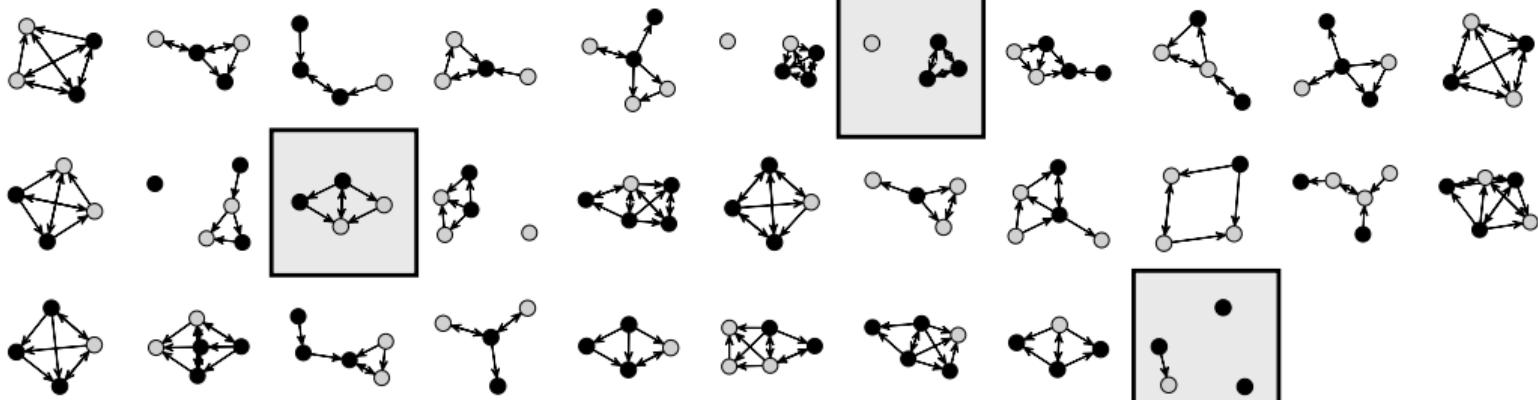


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- ▶ Transformed variables: $(\text{Homophily})^{1/2}$.
- ▶ Bootstrapping: 1,000 replicates in less than 1.5 minutes...
... if you are lucky, using “regular” ERGMs would take you about 5 hours.

▶ details ▶ gof ▶ data

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?”

Goodness-of-fit: Conditional Distributions

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

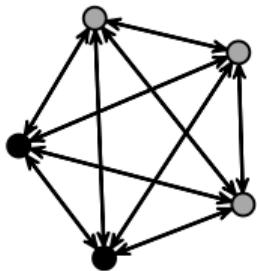
Goodness-of-fit: Conditional Distributions

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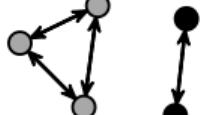
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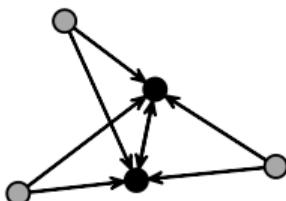
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(a) Mutual Ties and
Transitive Triads



(b) Homophilic
Ties



(c) Attribute
Receiver Effect

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

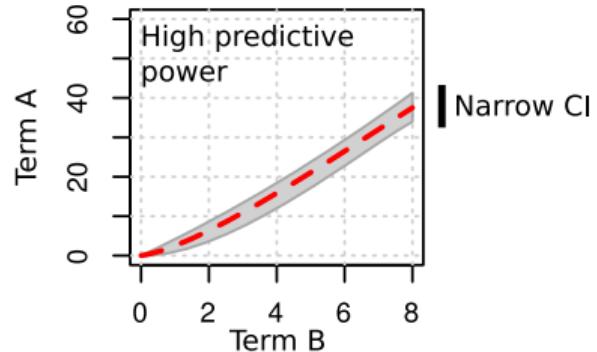
How much does *Term B* can tell us about
Term A?

- ▶ 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*?

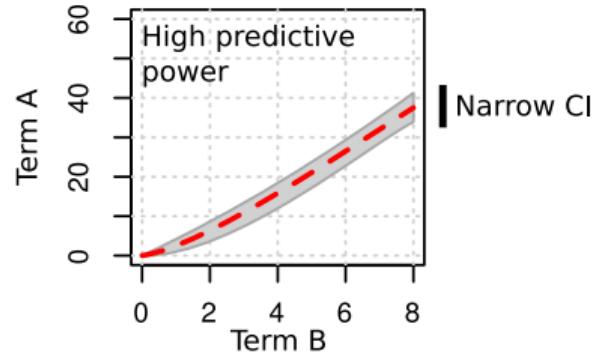
- ▶ High predictive power ($\text{Term A} \mid \text{Term B}$):
 - ▶ Stepped slope.
 - ▶ Narrow Confidence Interval (CI).



(All this is based on Chapters 3 and 6)

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

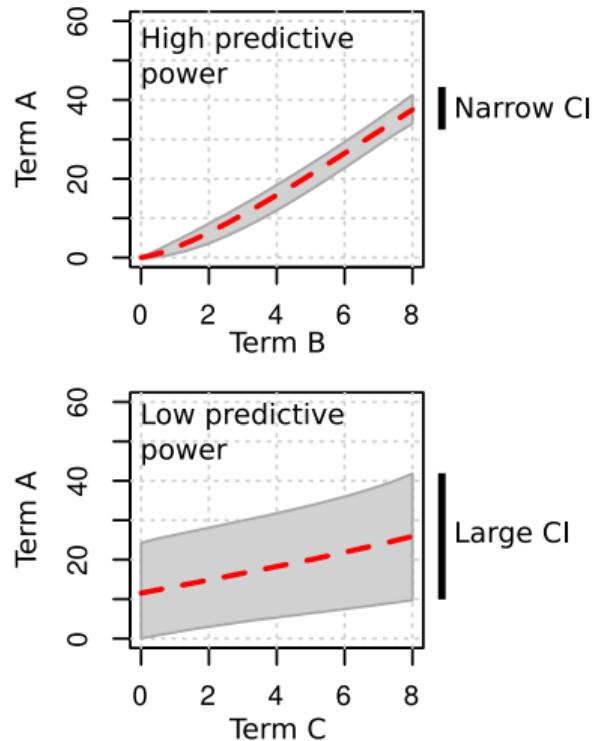
- ▶ High predictive power (*Term A* | *Term B*):
 - ▶ Stepped slope.
 - ▶ Narrow Confidence Interval (CI).
- ▶ Low predictive power (*Term A* | *Term C*):



(All this is based on Chapters 3 and 6)

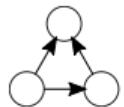
How much does *Term B* can tell us about *Term A*?

- ▶ High predictive power (*Term A* | *Term B*):
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- ▶ 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)

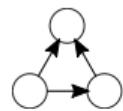
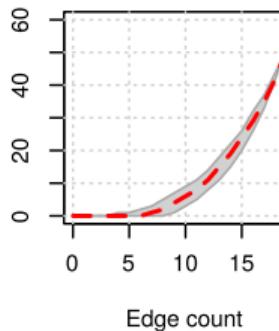
Conditional Distribution: Transitive Triads



▶ more examples

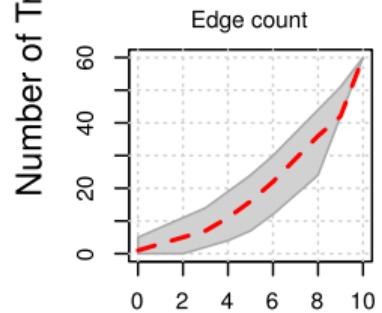
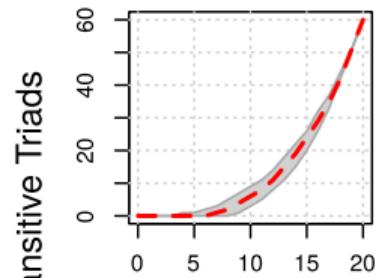
Conditional Distribution: Transitive Triads

Number of Transitive Triads

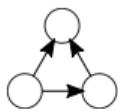


▶ more examples

Conditional Distribution: Transitive Triads

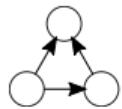
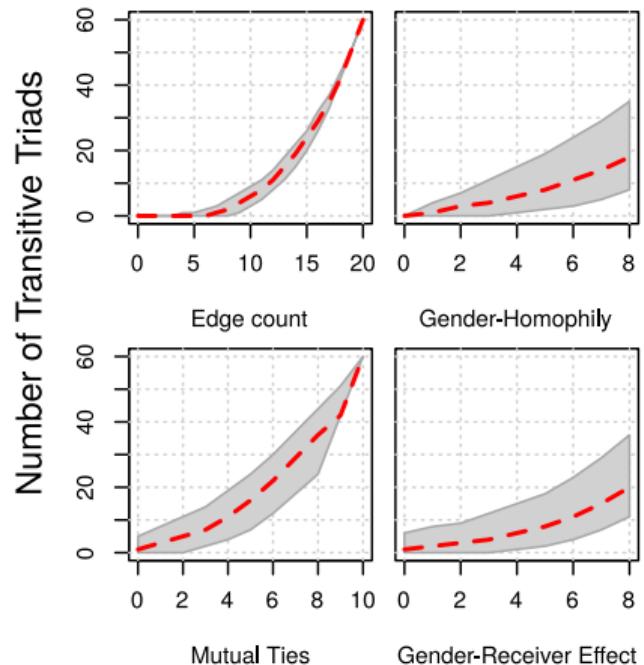


Mutual Ties



▶ more examples

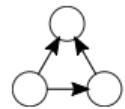
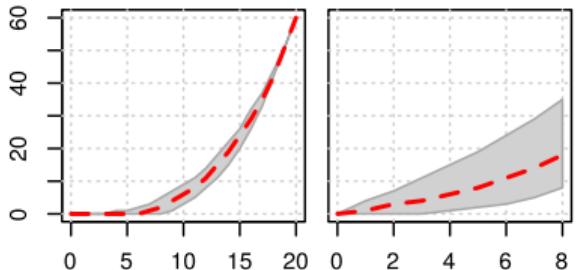
Conditional Distribution: Transitive Triads



Conditional Distribution: Transitive Triads

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

Number of Transitive Triads



Edge count

Gender-Homophily

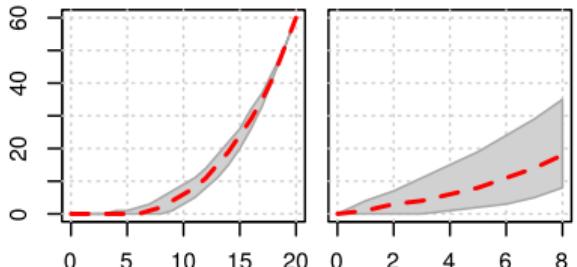
Mutual Ties

Gender-Receiver Effect

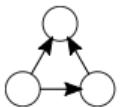
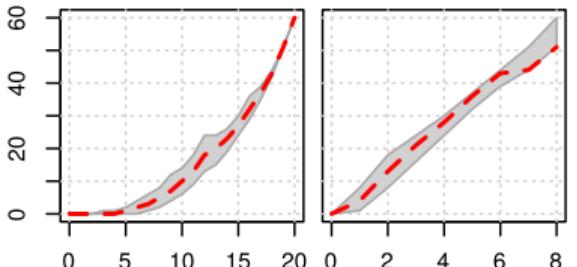
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$$\theta_{\text{triads}} = 1$$



Edge count

Gender-Homophily

Mutual Ties

Gender-Receiver Effect

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Mutual Ties

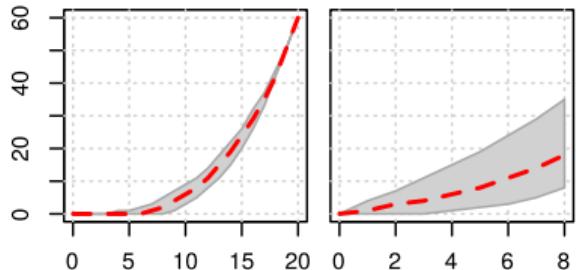
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▶ more examples

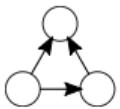
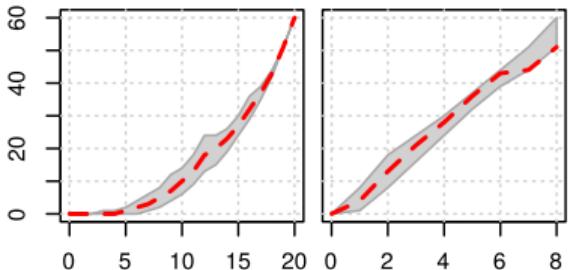
Conditional Distribution: Transitive Triads

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

Number of Transitive Triads

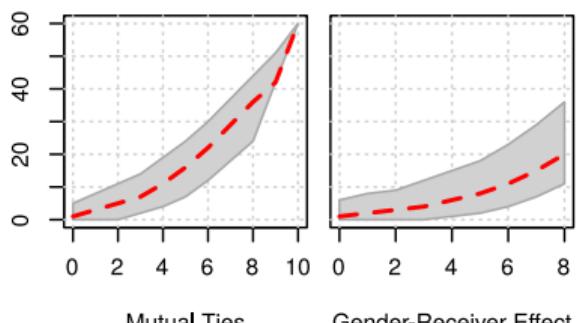


$$\theta_{\text{triads}} = 1$$

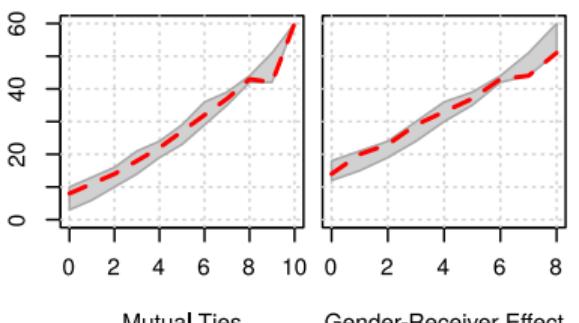


- ▶ Edge count and mutuality are good predictors of transitivity.

Edge count



Edge count



Mutual Ties

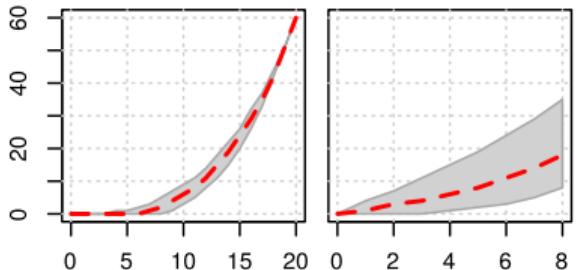
Gender-Receiver Effect

▶ more examples

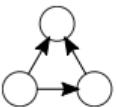
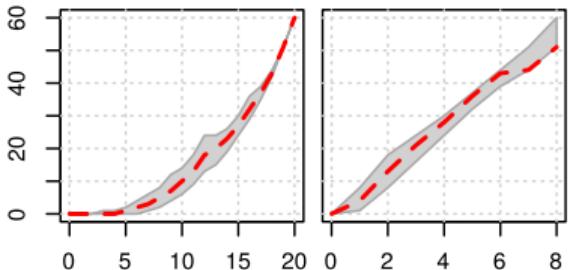
Conditional Distribution: Transitive Triads

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

Number of Transitive Triads



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



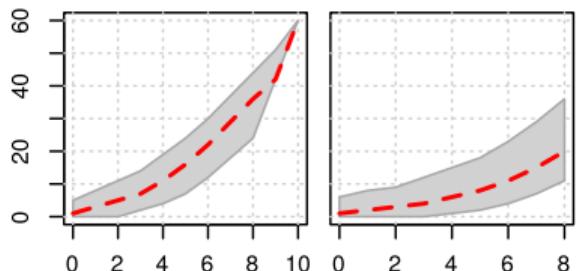
- ▶ Edge count and mutuality are good predictors of transitivity.
- ▶ Prevalence (θ_{triads}) narrows the confidence intervals.

Edge count

Gender-Homophily

Mutual Ties

Gender-Receiver Effect



Edge count

Gender-Homophily

Mutual Ties

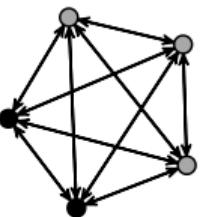
Gender-Receiver Effect

▶ more examples

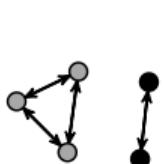
GOF for Small Networks

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

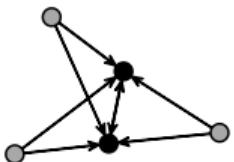
1. Markov structures (involve two or more ties) are better predictors of each other.
2. *Miopic* terms: fast saturation implies poor information, e.g. homophily and receiver effect
saturate at 8/20 ties:



(a) Mutual Ties and
Transitive Triads

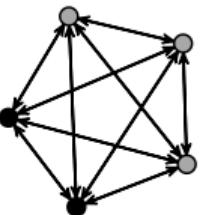


(b) Homophilic
Ties

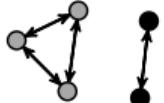


(c) Attribute
Receiver Effect

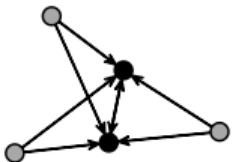
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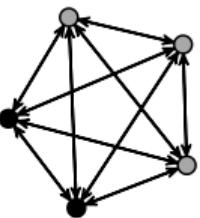
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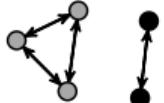
(c) Attribute
Receiver Effect

3. Not only GOF:

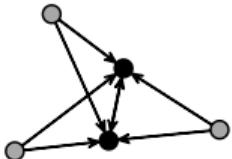
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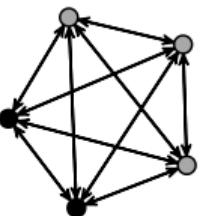
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Ties



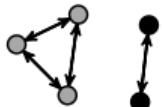
(c) Attribute
Receiver Effect

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

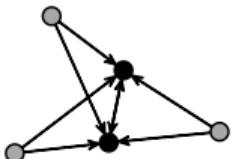
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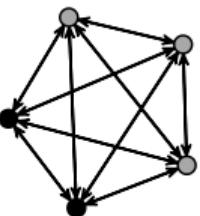
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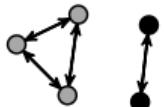
(c) Attribute
Receiver Effect

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

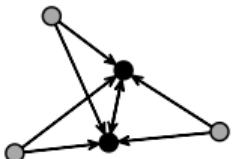
1. Markov structures (involve two or more ties) are better predictors of each other.
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Ties



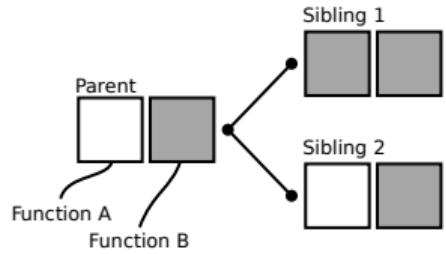
(c) Attribute
Receiver Effect

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.

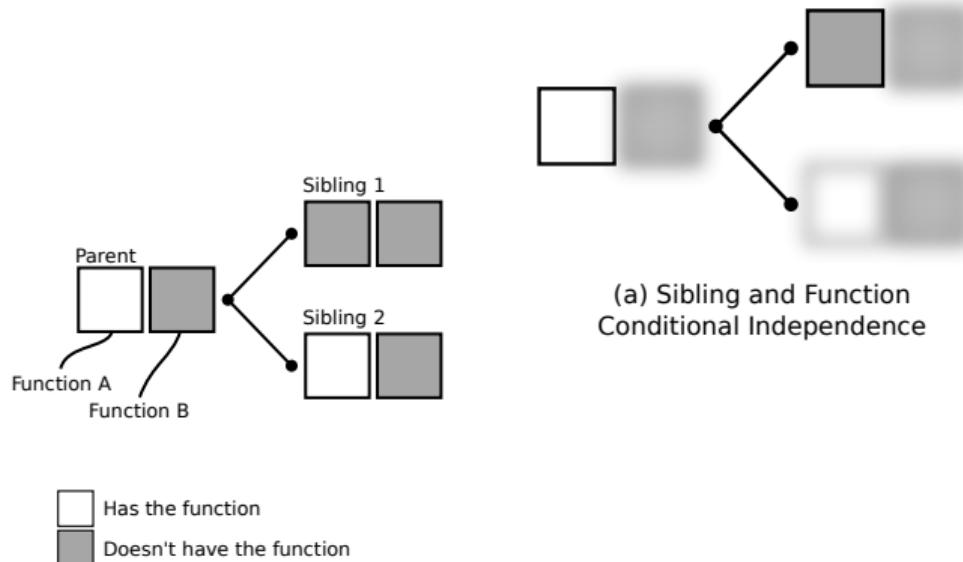
Connecting the Dots: Phylogenetic Modeling with ERGMs

(Chapter 4)

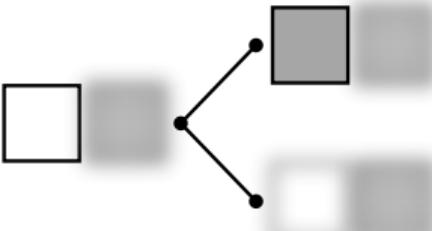
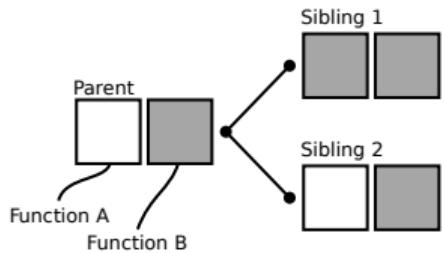
Phylogenetics Modeling Strategies



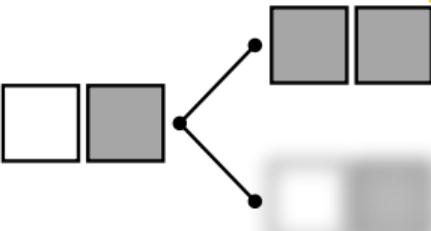
Phylogenetics Modeling Strategies



Phylogenetics Modeling Strategies

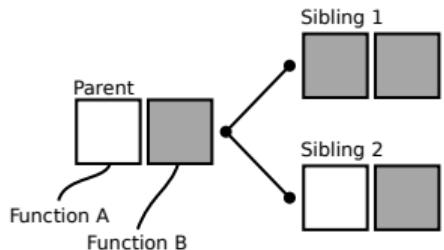


(a) Sibling and Function Conditional Independence



(b) Sibling Conditional Independence

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

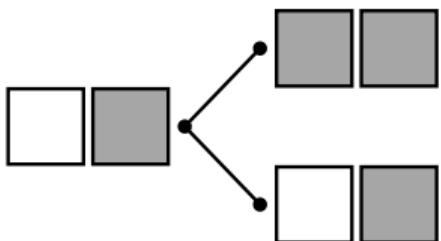


Has the function
 Doesn't have the function



(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

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Sufficient statistics

What Drives Evolution

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Sufficient statistics

# Gains	1	1
---------	---	---

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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)

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# Gains	1	1
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# Changes (gain+loss)	2	3

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

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		Case 1	Case 2
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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:

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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: $2^3 \times 2^6 = 512$

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 - Pairwise co-evolution: 3 terms,

 - Pairwise Neofunctionalization: 3 terms,

What Drives Evolution: a game changer

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

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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:

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 - 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,

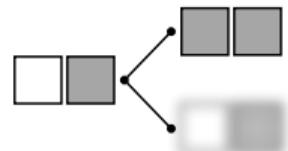
Function specific loss: 3 terms,

Total: 15 parameters.

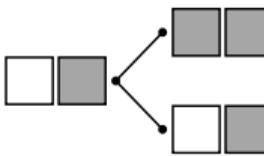
- ▶ Easier to fit and interpret.



(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).
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Barry: your go-to *motif* accountant

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

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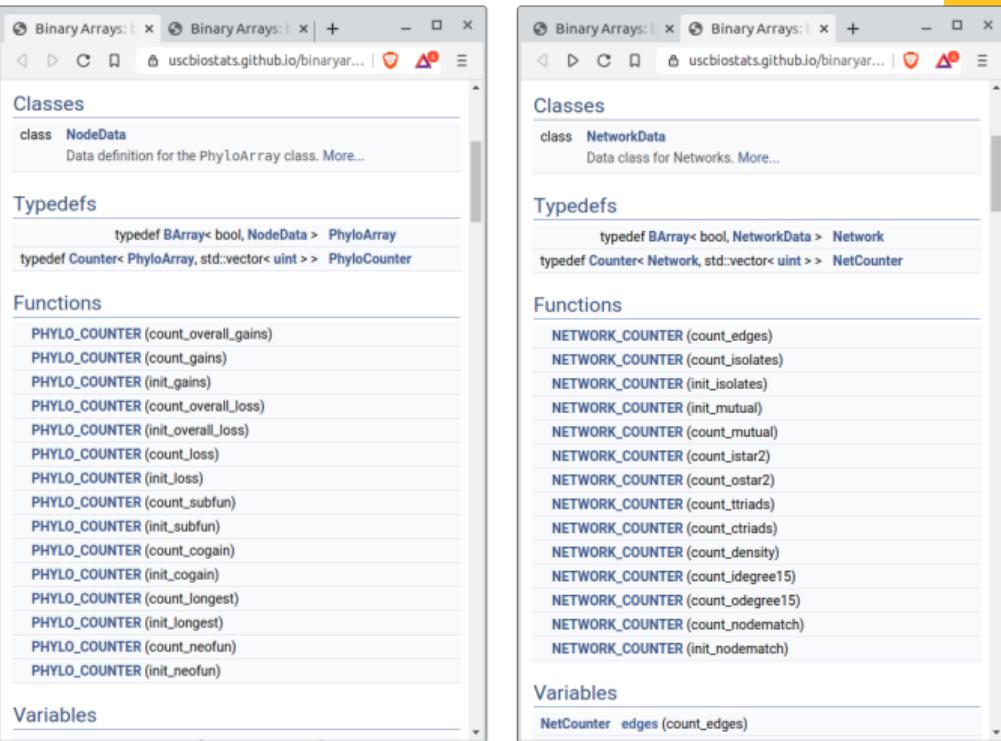


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Concluding Remarks

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Before my dissertation

Predicting gene functions

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

Concluding Remarks

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

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

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- ▶ 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!

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-  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

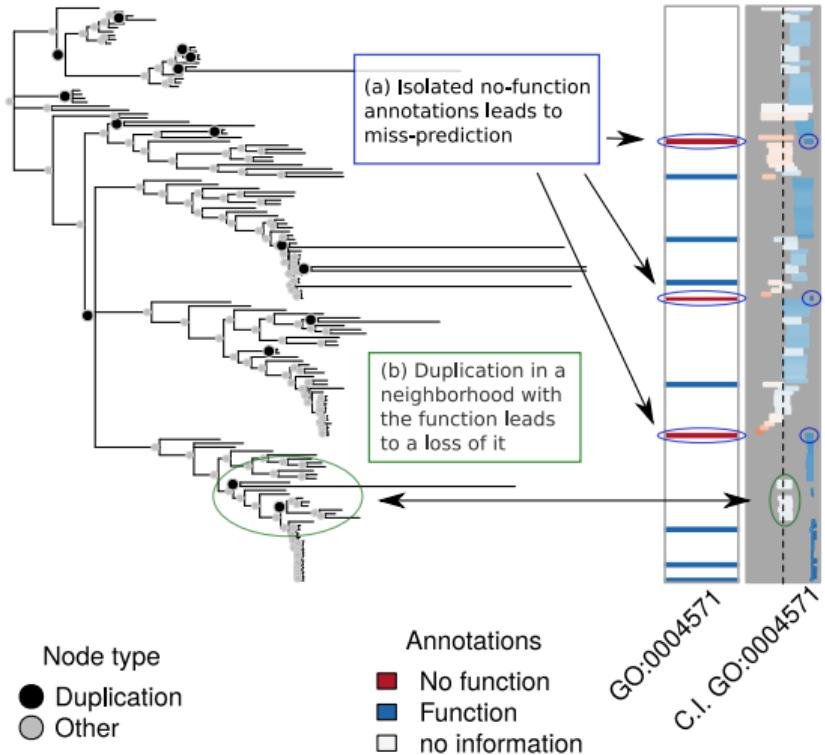
◀ go back

Example 2: Bad quality prediction

MAE: 0.52

AUC: 0.33

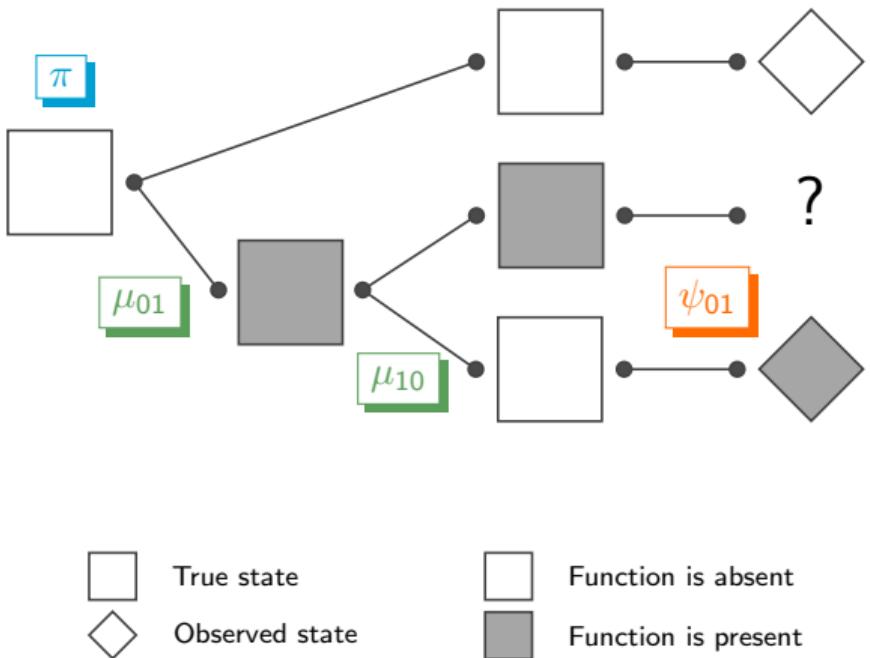
Type: Molecular Function

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](#)

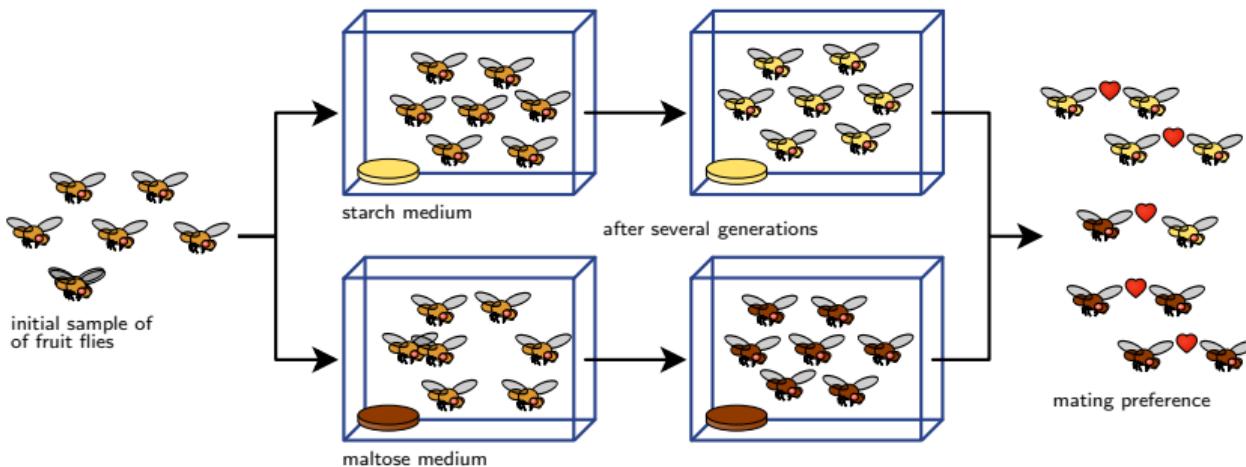


Figure 3 Dodd 1989: After one year of isolation, flies showed a significant level of assortativity in mating (wikimedia)

◀ go back

Duplication

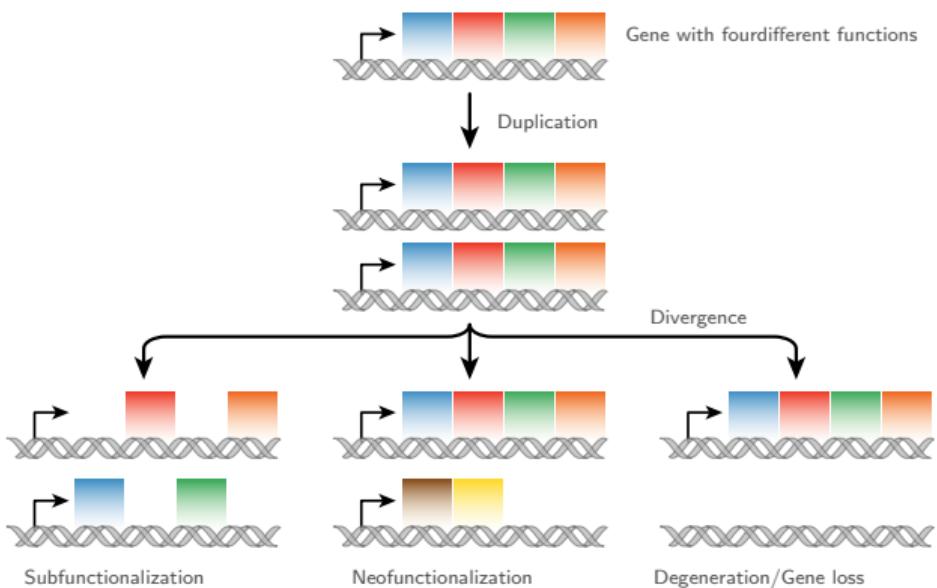


Figure 4 A key part of molecular innovation, gene duplication provides opportunity for new functions to emerge
(wikimedia)

◀ go back

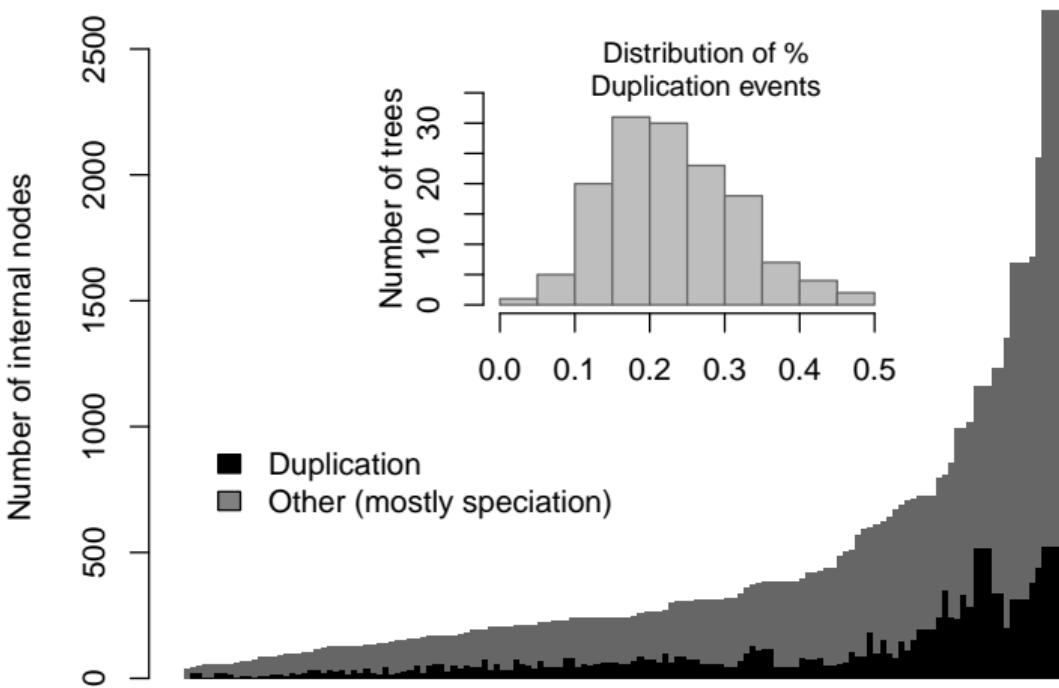
Data: Phylogenetic trees

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

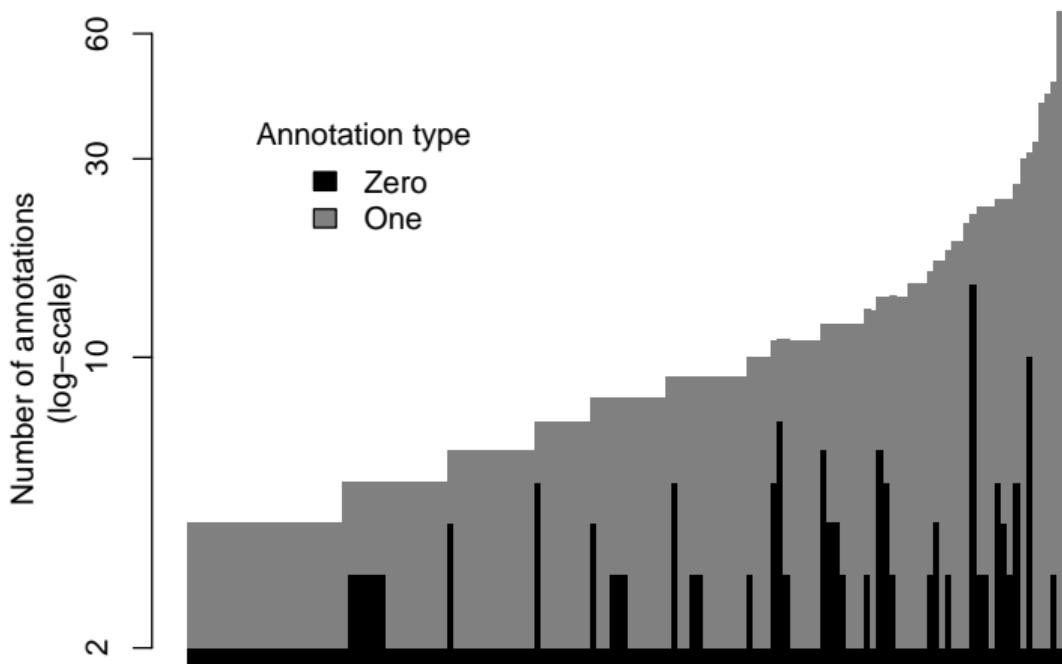
Data: Annotations (example)

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

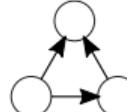
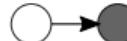
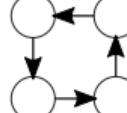
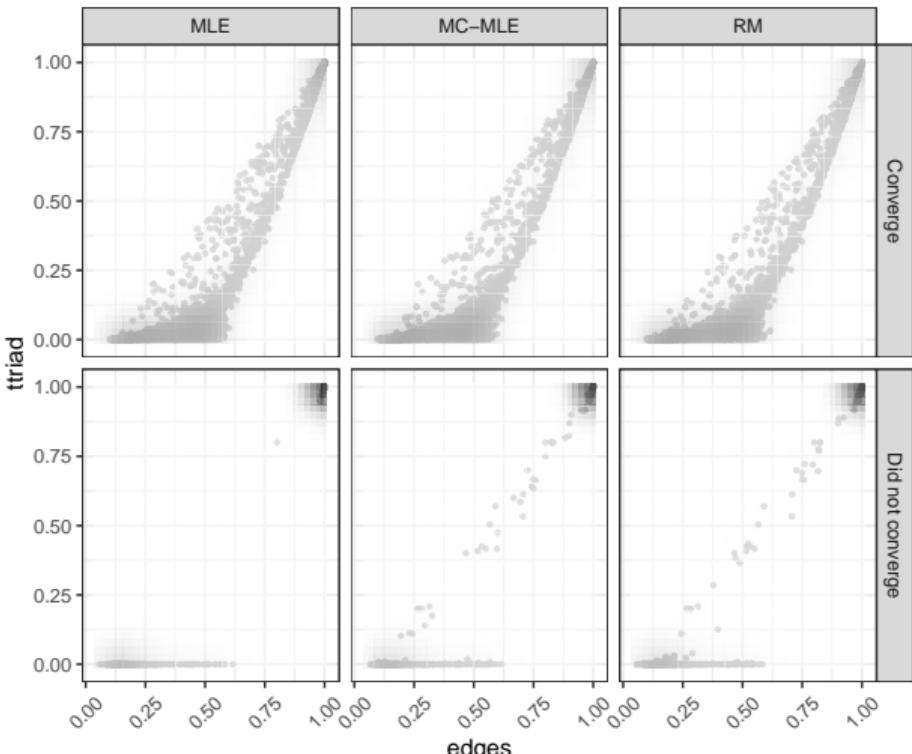
Representation	Description
	Mutual Ties (Reciprocity) $\sum_{i \neq j} y_{ij} y_{ji}$
	Transitive Triad (Balance) $\sum_{i \neq j \neq k} y_{ij} y_{jk} y_{ik}$
	Homophily $\sum_{i \neq j} y_{ij} \mathbf{1}(x_i = x_j)$
	Attribute-receiver effect $\sum_{i \neq j} y_{ij} x_j$
	Four Cycle $\sum_{i \neq j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

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

1. Higher convergence rate

◀ return



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]

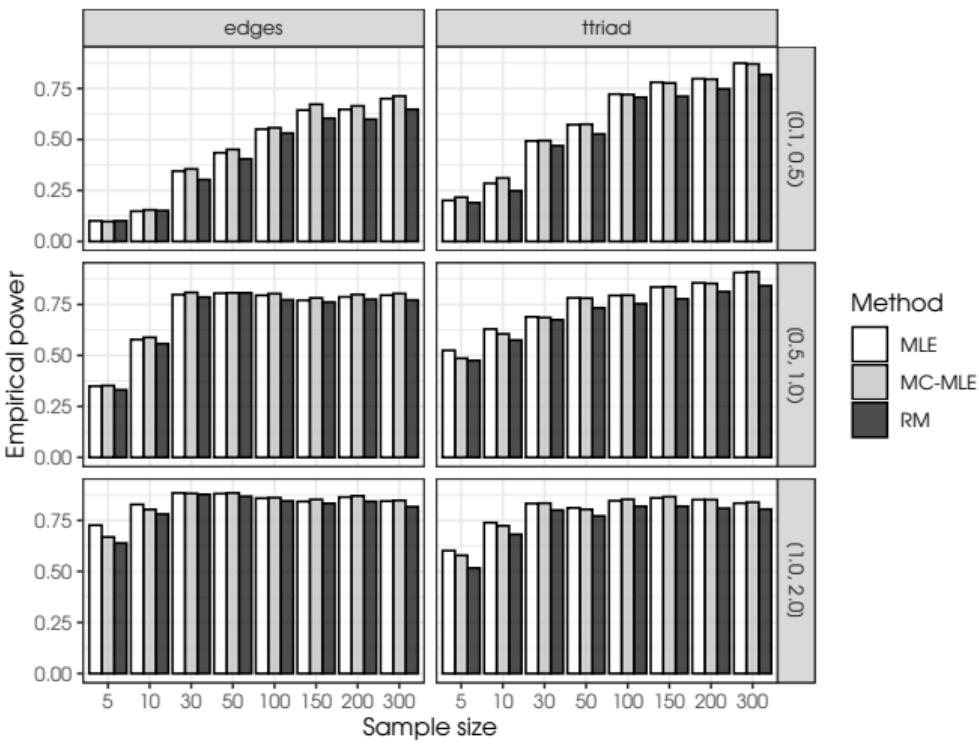
Table 3 Empirical bias. Each cell shows the 95% confidence interval of each methods' empirical bias.

▶ alt take

Simulation Study

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

◀ return



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

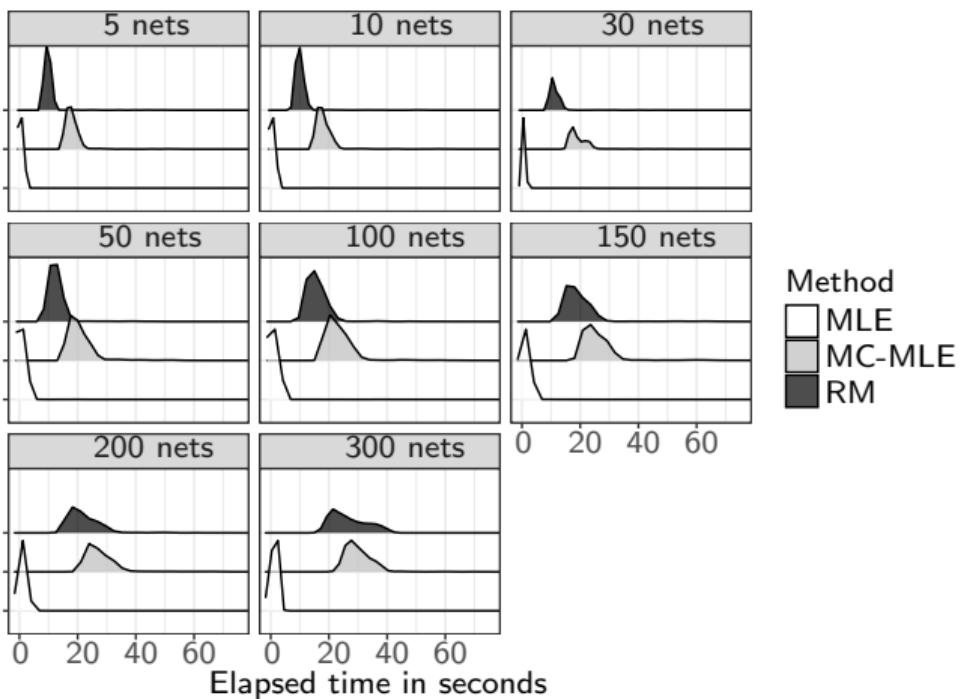
	Sample size	N. Sims.	P(Type I error)		χ^2 (vs MLE)	
			MLE	MC-MLE	RM	MC-MLE
5	4,325	0.066	0.086	0.086	11.36 ***	11.36 ***
10	4,677	0.063	0.078	0.073	8.44 ***	3.73 *
15	4,818	0.060	0.072	0.063	5.50 **	0.41
20	4,889	0.054	0.065	0.061	5.30 **	2.05
30	4,946	0.053	0.059	0.055	1.60	0.07
50	4,987	0.053	0.055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

◀ return

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	

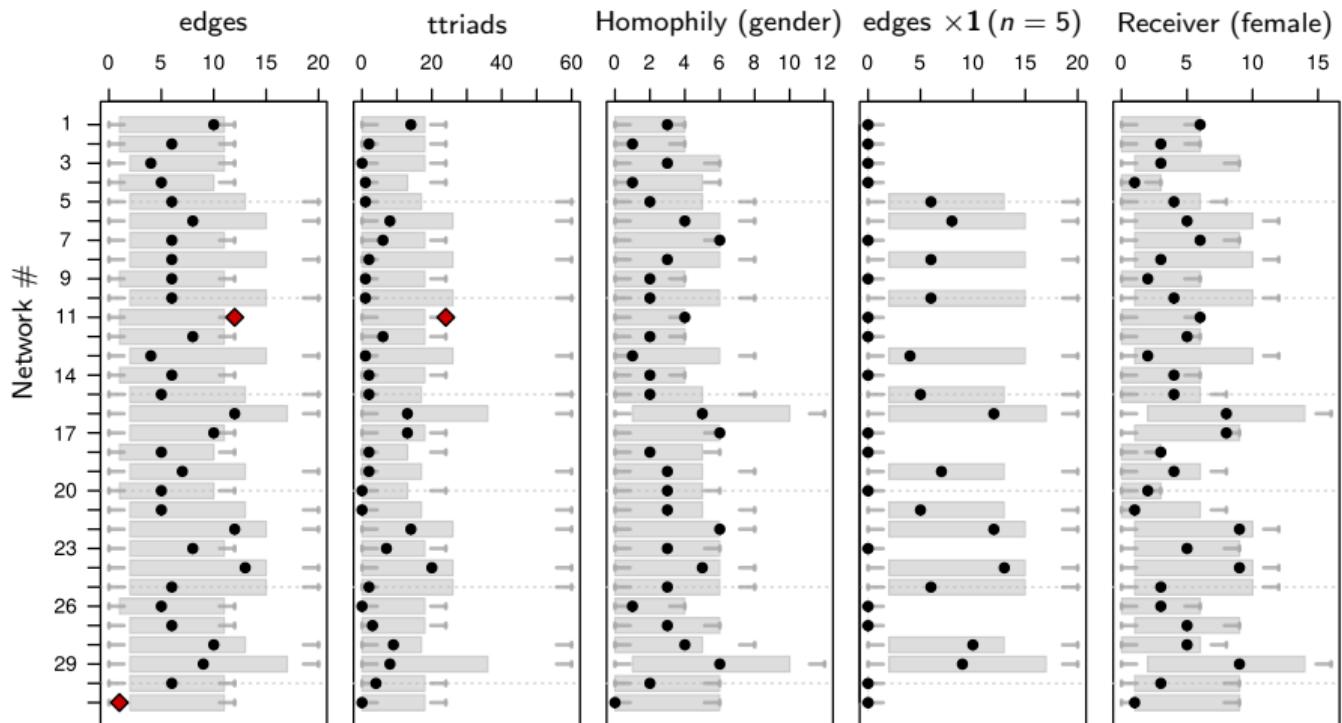
*** $p < 0.001$, ** $p < 0.01$, * $p < 0.05$

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?

◀ go back

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...					

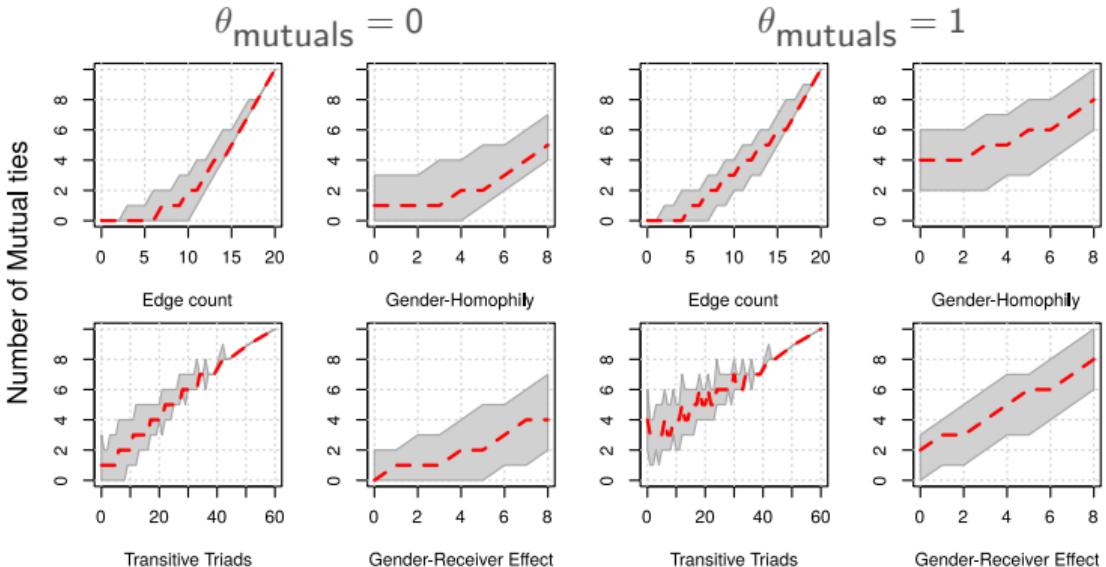
Table 4 Example of observed sufficient statistics for the team advice networks. Pooled-data ERGMs have multiple observed sufficient statistics (also known as target statistics). Furthermore, as shown here, we can manipulate common statistics as *edges* (2) and *ttriads* (3) to include, e.g. interaction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

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Conditional Distribution: Mutual Ties

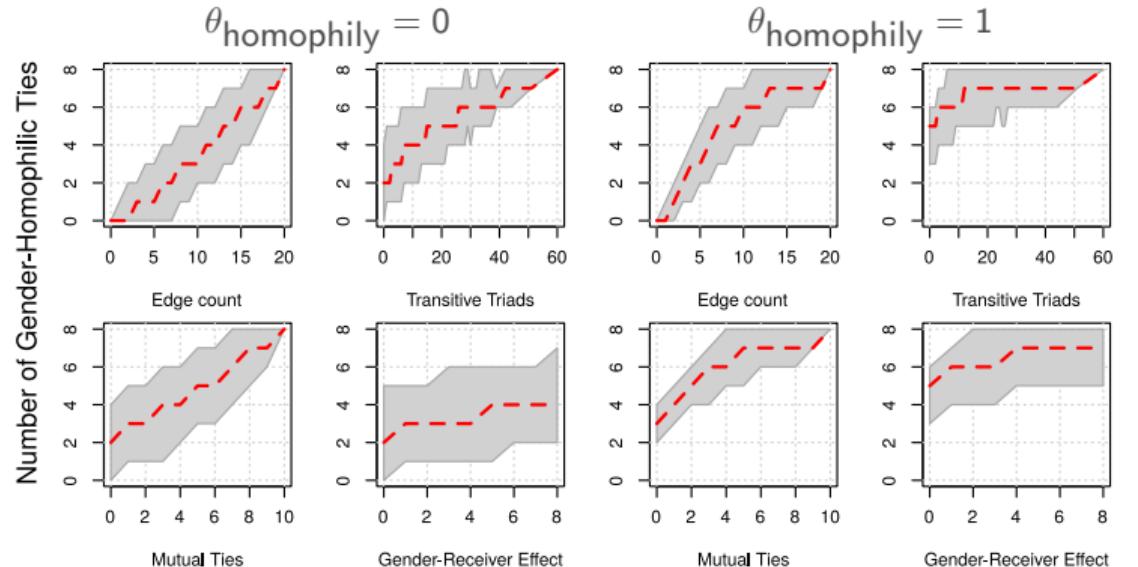


- ▶ Better predicted by other Markov structures.
- ▶ Non-Markov structures = poor prediction.
- ▶ No big impact of prevalence (θ_{mutual}).



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Conditional Distribution: Homophily



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