SCUOLA ALTI STUDI LUCCA

Symmetry Reduction via Linear Invariant Subspaces: Exact and Approximate Methods

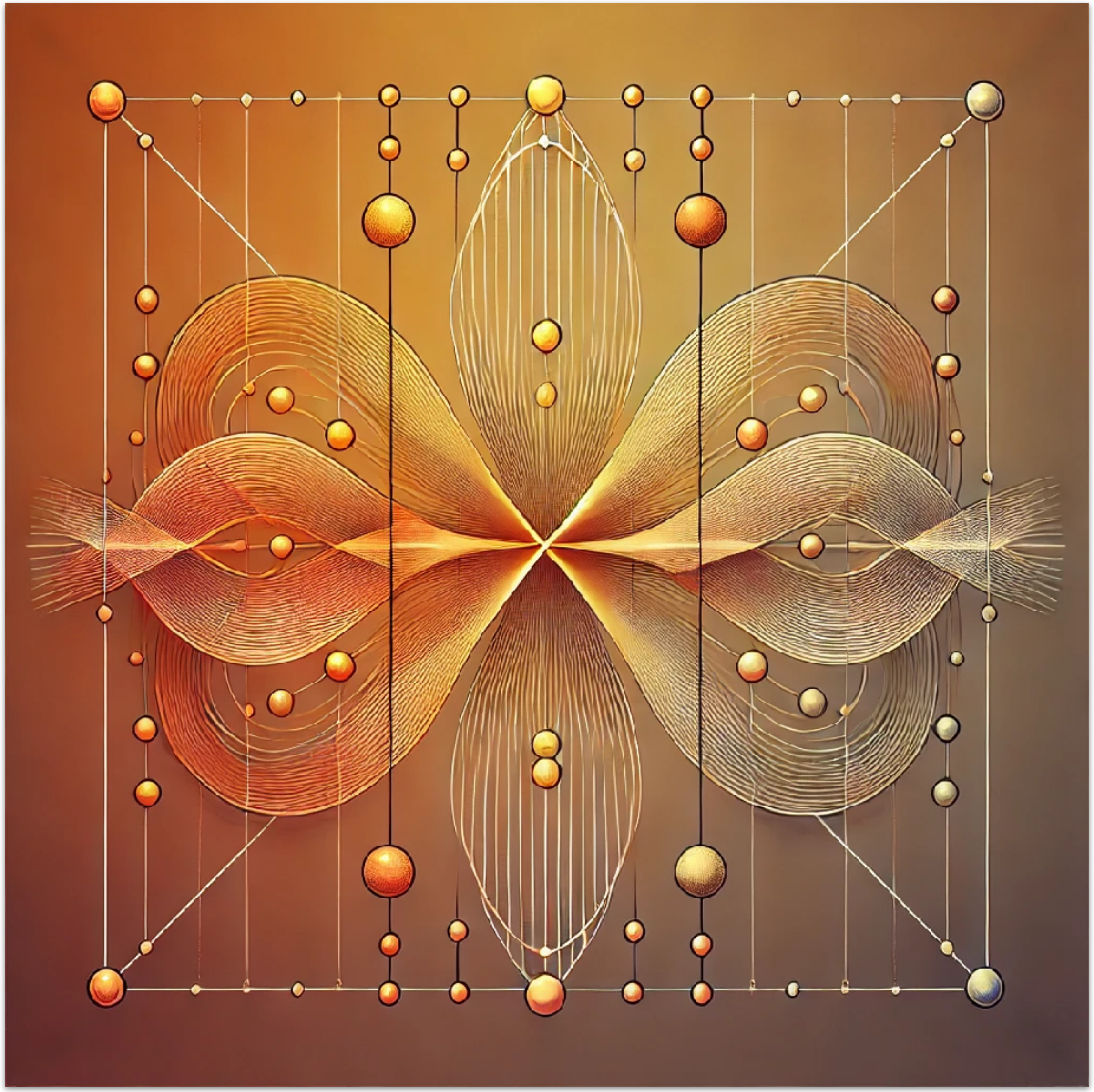
Lipari Workshop on Complex Networks

Mirco Tribastone

3 July 2024

Symmetry

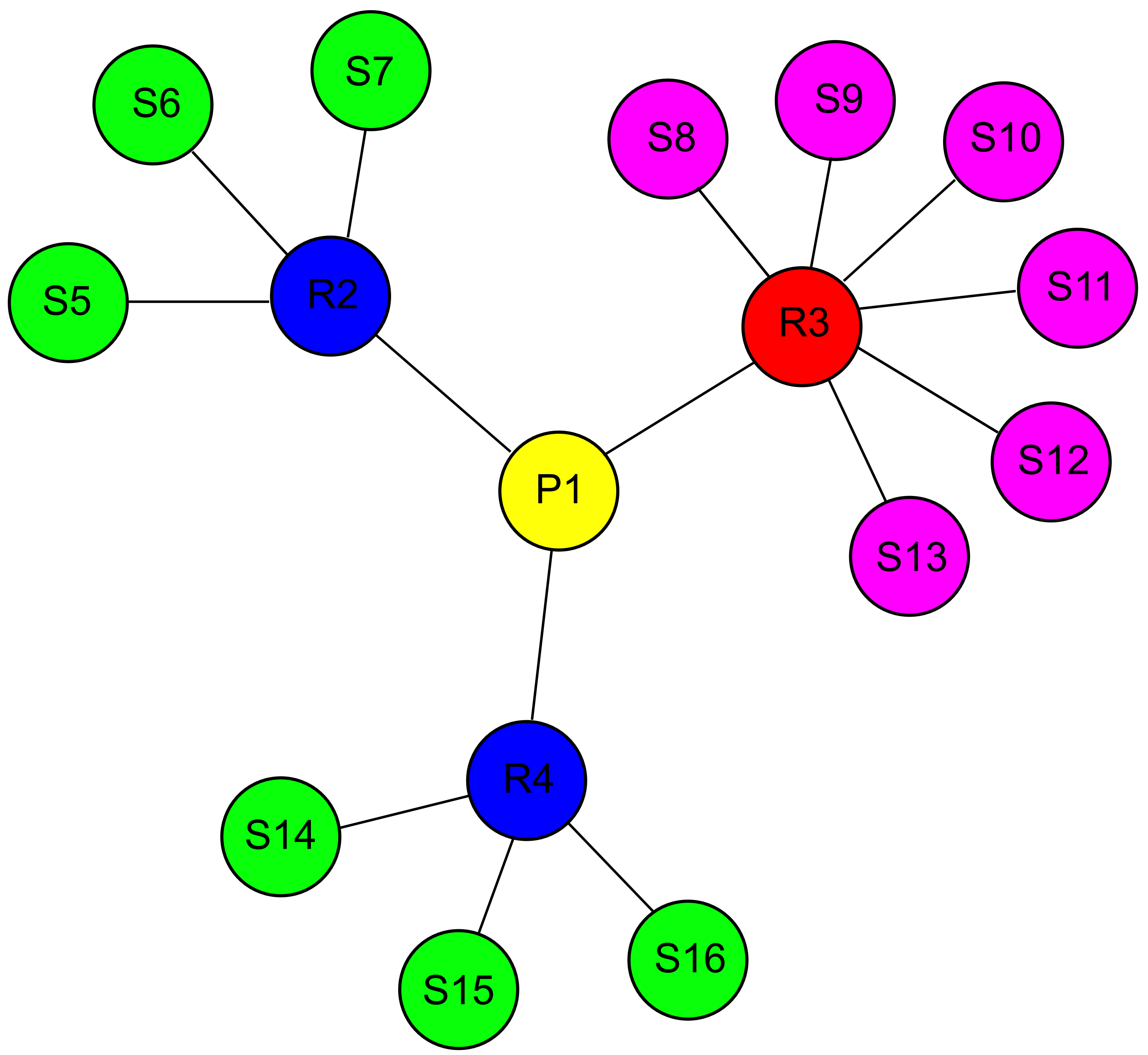
A fundamental concept across all scientific disciplines



"Generate an artistic drawing of a graph inspiring the idea of symmetry."

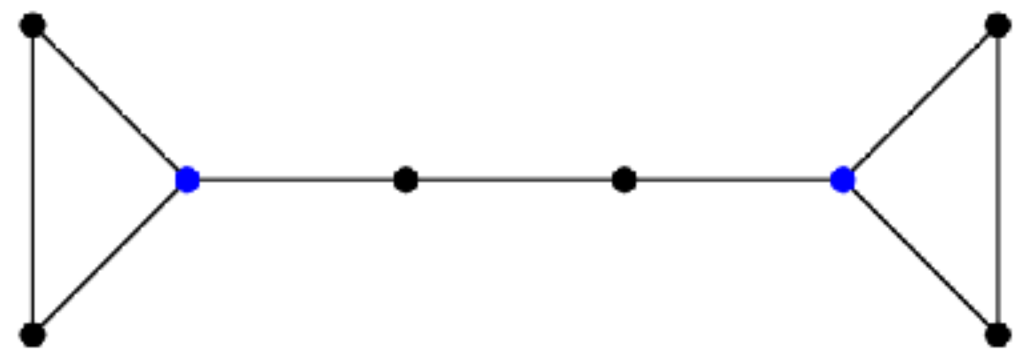
Symmetry in Graphs: Structure

Colors identify an equitable partition



Nodes of the same color are adjacent to the same number of nodes of each color

An **orbit partition is an equitable partition**, but the converse is not true in general

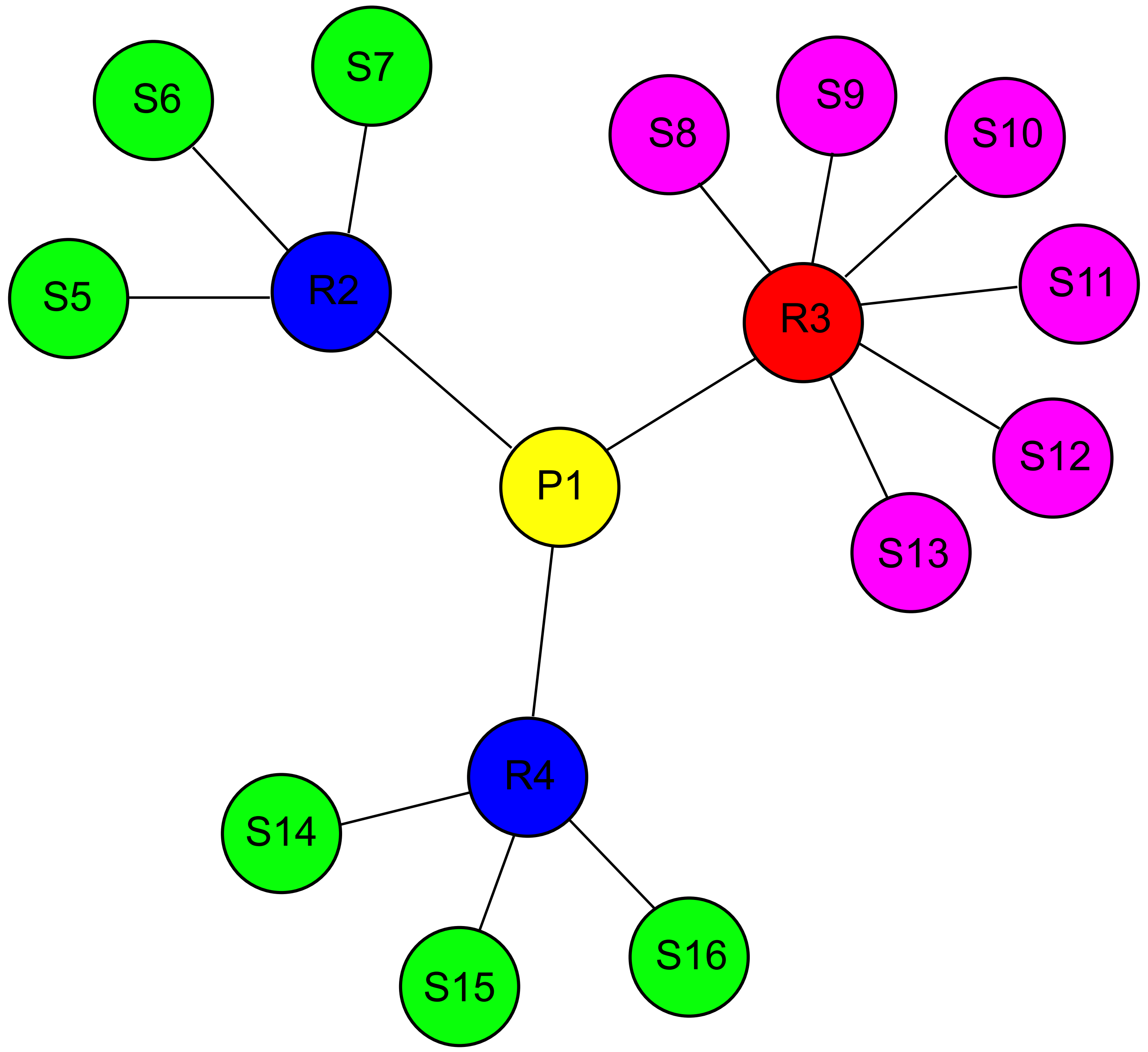


This fact finds its use in practical tools for graph isomorphism

The coarsest equitable partition that refines an initial coloring can be computed in $O(m \log n)$ time (n is the number of nodes, m is the edgeds) by partition refinement [Cardon and Crochemore (1982)]

Equitable partitions preserve a subset of the spectrum of the graph and (some) centralities

Symmetry in Graphs: Dynamics



Simple dynamics on a graph

Consider a dynamical system involving its adjacency matrix *A*

$$\dot{x} = Ax$$

For all colors C, C',
for all nodes i,i' in C

$$\sum_{k \in C'} a_{ik} = \sum_{k \in C'} a_{i'k}$$

$$x_i(0) = x_{i'}(0) \implies x_i(t) = x_{i'}(t)$$

Synchronization/dynamical symmetry

Dynamical Symmetry in Graphs: Properties

Coincides with the notion of equitable partition for undirected/binary graphs (and can be generalized to arbitrary graphs by considering outdegrees)

The partition induces a "uniform" linear subspace *U* where coordinates of the same color have the same values

Dynamical symmetry is the property of *U* being invariant under *A*

An equitable partition is a necessary and sufficient condition for dynamical symmetry [Cardelli et al. (2017), but I guess it has been found several times for linear models]

$$\dot{x} = Ax$$

For all colors C, C',
for all nodes i,i' in C

$$\sum_{k \in C'} a_{ik} = \sum_{k \in C'} a_{i'k}$$

$$x_i(0) = x_{i'}(0) \implies x_i(t) = x_{i'}(t)$$

Synchronization/dynamical symmetry

Dynamical Symmetry: Related Work

Markov chain lumping

$$\dot{\pi} = \pi Q \qquad \pi(k+1) = \pi(k)P$$

Known as **exact lumpability** [Buchholz (1994)]

It is the dual notion of **ordinary lumpability** (defined on the transpose matrix), known since Kemeny and Snell (1969)

N-ODE “backward” lumping

$$\dot{x}_1 = -\min(x_1 + x_2, K) + x_3$$
$$\dot{x}_2 = -\min(x_1 + x_2, K) + x_3$$
$$\dot{x}_3 = +x_1 x_2$$

Extension for a class of nonlinear ODEs [Cardelli et al., (2016)]

NP-complete, but effective tools exist (Z3 SMT)

P-ODE “backward” lumping

$$\dot{x}_1 = -x_1 x_2 + x_3$$
$$\dot{x}_2 = -x_1 x_2 + x_3$$
$$\dot{x}_3 = +x_1 x_2$$
$$(A_1 + A_2 \leftrightarrow A_3)$$

Extension for polynomial differential equations [Cardelli et al., (2017)]

Still polynomial running time

Boolean “backward” equivalence

$$x_1(t+1) = \neg x_3(t) \vee x_1(t)$$
$$x_2(t+1) = x_1(t) \vee x_2(t) \vee \neg x_3(t)$$
$$x_3(t+1) = x_2(t) \wedge \neq x_3(t)$$

Symmetry for a classic model for gene regulation networks [Argyris et al., (2023)]

Exact Symmetry Reduction

Building a coarse-grained model that preserves the dynamics

Original model

$$\dot{x} = Ax$$

$$\dot{x}_1 = -x_1 x_2 + x_3$$
$$\dot{x}_2 = -x_1 x_2 + x_3$$
$$\dot{x}_3 = +x_1 x_2$$

$$\dot{x}_1 = -\min(x_1 + x_2, K) + x_3$$
$$\dot{x}_2 = -\min(x_1 + x_2, K) + x_3$$
$$\dot{x}_3 = +x_1 x_2$$

Symmetry

$$\sum_{k \in C'} a_{ik} = \sum_{k \in C'} a_{i'k}$$

$$x_1 = x_2$$

---

one supernode per color

one equation per representative

Reduced model

$$\dot{X} = \hat{A} X$$

$$\hat{A}_{C,C'} = \sum_{k \in C'} a_{ik}$$

$$(\text{for any } i \in C)$$

$$\dot{X}_1 = -X_1^2 + X_2$$
$$\dot{X}_2 = +X_1^2$$

$$\dot{X}_1 = -\min(2X_1, K) + X_2$$
$$\dot{X}_2 = +X_1^2$$

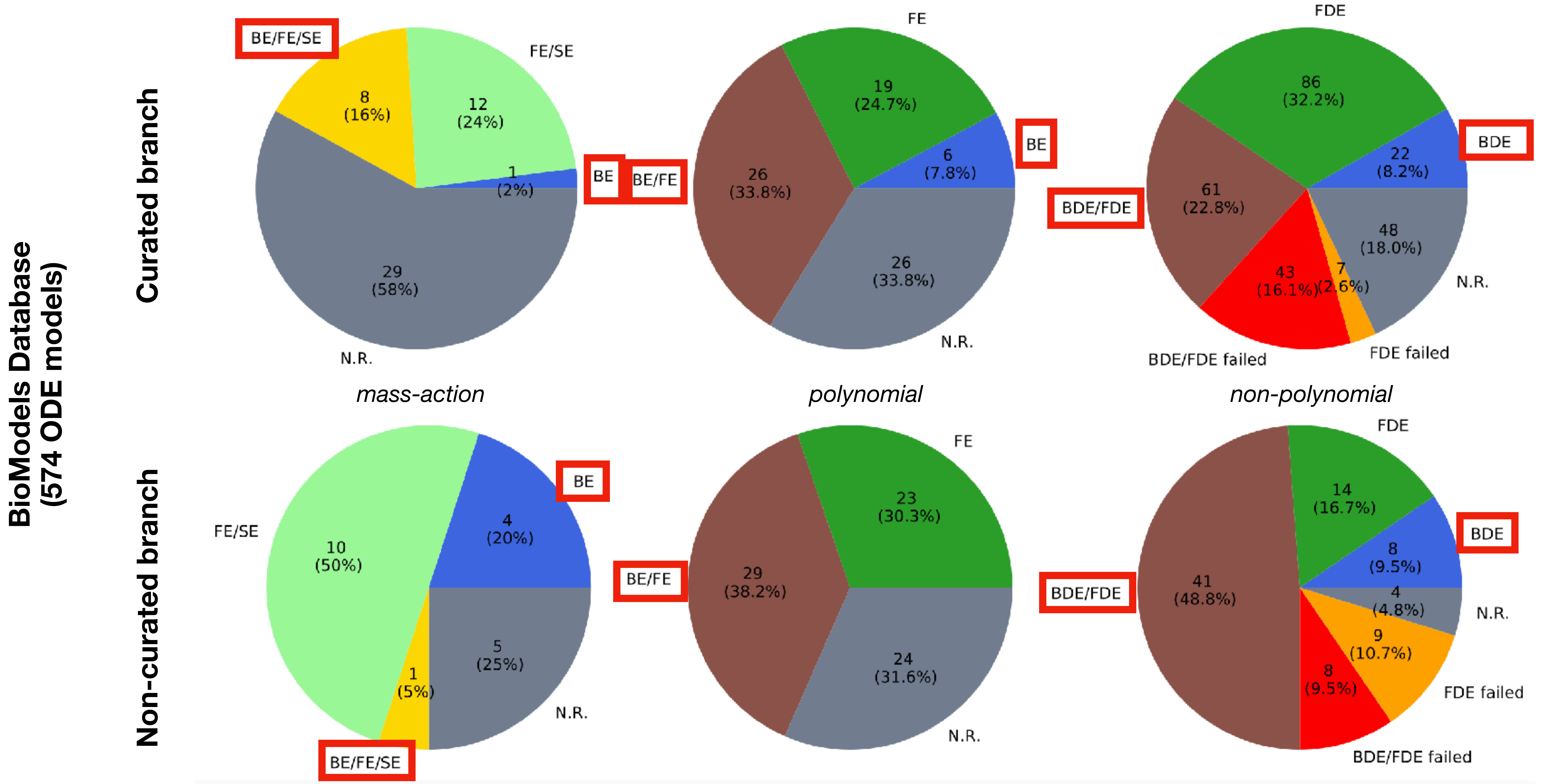
Exact Symmetry in Practice: Benchmarks

Undirected Graphs			
Instance	Original size	Reduced size	Reduction ratio
GD06-Theory	102	3	2.94 %
Yeast protein interaction network	1871	1091	58.31 %
Collaborations in General Relativity	5243	3394	64.73 %
Erdős collaboration network	5535	1902	34.36 %
Autonomous system (SNAP)	6475	3691	57.00 %
Oregon routing network	10671	5484	51.39 %
Autonomous system (Florida)	22964	11935	51.97 %
Enron email network	36693	20418	55.65 %
Dictionary	39328	26994	68.64 %
Caida routers	192245	150463	78.27 %
Citeseer coauthorship network	227321	155593	68.45 %
Citeseer copaper network	434103	150316	34.63 %
YouTube	1134891	684011	60.27 %

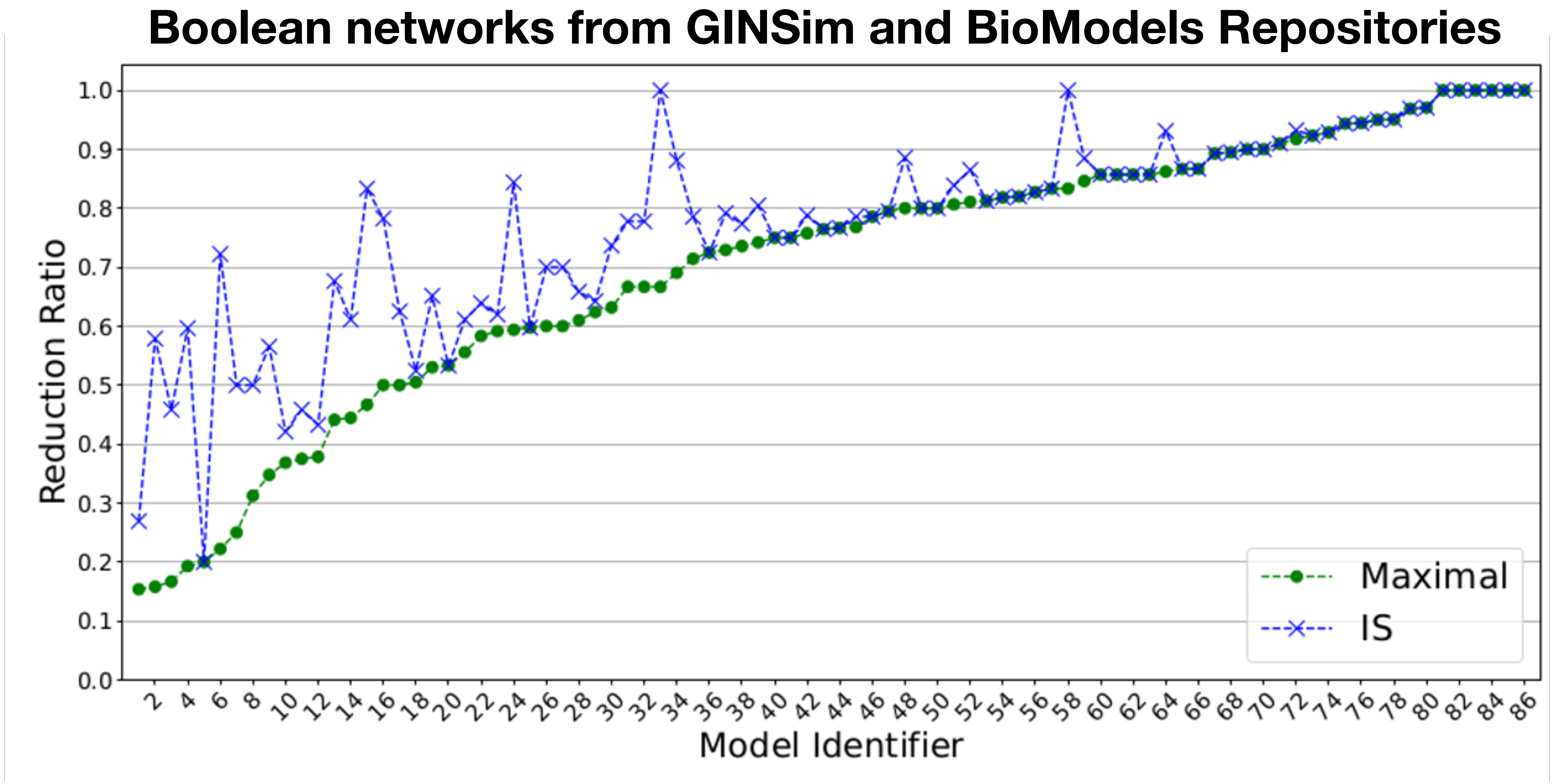
Exact Symmetry in Practice: Benchmarks

Directed Graphs			
Instance	Original size	Reduced size	Reduction ratio
Glossary	73	41	56.16 %
Graph Design ’96	112	6	5.36 %
PhDs in computer science	1883	225	11.95 %
Kohonen citation network	4471	766	17.13 %
EPA web pages	4733	598	12.63 %
Gnutella p2p network	6302	2208	35.04 %
Wikipedia who-votes-on-whom	8299	4216	50.80 %
EVA corporate inter-relationships	8498	215	2.53 %
California web search	9665	1817	18.80 %
Stanford CS web	9915	3657	36.88 %
Gnutella p2p network (I)	10880	4340	39.89 %
Gnutella p2p network (II)	26519	6741	25.42 %
Enron email traffic	69245	7437	10.74 %
Epinions trust network	75889	41055	54.10 %
Slashdot social network	82169	57561	70.05 %
Stanford web graph	281905	129335	45.88 %
CNR web crawl	325558	85419	26.24 %
Notre Dame web graph	325730	49952	15.34 %
Berkely.edu + stanford.edu web	685252	292492	42.68 %
Flickr web crawl	820879	370145	45.09 %
.eu domain web crawl	862665	341687	39.60 %
Google web graph	916429	354624	38.70 %
.in domain web crawl	1382909	333283	24.10 %
Wikipedia pages	1634990	1116472	68.29 %

Exact Symmetry in Practice: Benchmarks



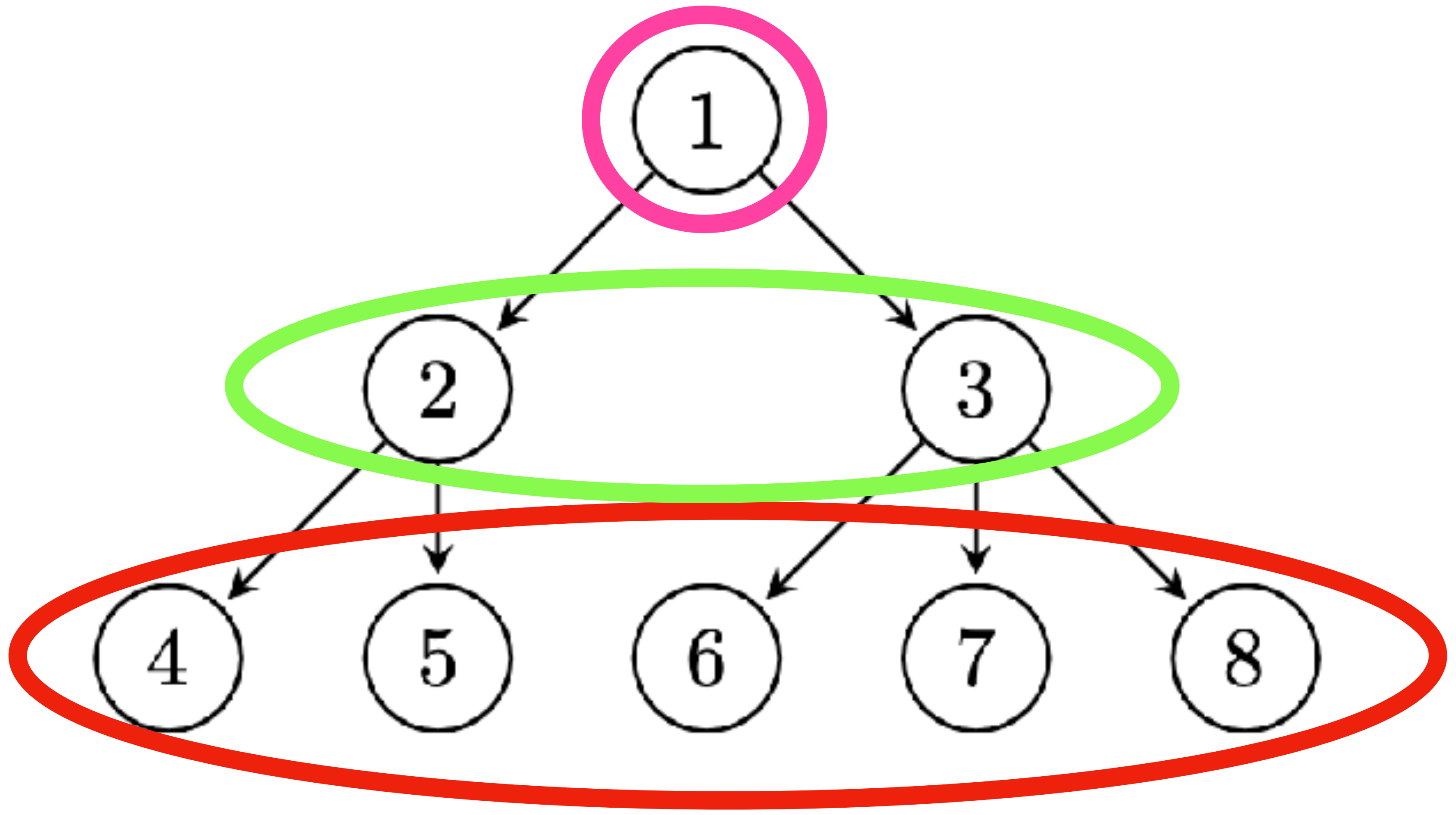
Exact Symmetry in Practice: Benchmarks



Maximal reduction = initial partition containing all variables
IS = initial partition isolates all “input” variables from each other (ensures models can be reused for any input values)

Approximate Structural Symmetry Reduction

An asymmetric graph



Intuition: allow some tolerance ε when counting the number of neighbors

For example, setting $\varepsilon = 1$ recognizes approximate symmetries

Approximate symmetry

$$\sum_{k \in C'} a_{ik} = \sum_{k \in C'} a_{i'k} \Longrightarrow \left| \sum_{k \in C'} a_{ik} - \sum_{k \in C'} a_{i'k} \right| \leq \varepsilon$$

It is still defined as an equivalence relation/partition which can be computed in polynomial time

Graph embedding

$$E \in \mathbb{R}^{n \times N}, \quad E_{iC} = \sum_{k \in C} a_{ik}$$

Brazil			
Method	EIG	CLO	BET
ε-BE	**8.47E-05**	**5.35E-04**	**2.79E-02**
Graphwave	5.30E-04	1.51E-03	4.08E-02
SEGK	4.90E-03	1.40E-03	6.17E-02
DRNE	3.41E-03	1.23E-03	4.81E-02
struc2vec	3.68E-03	1.11E-03	4.57E-02
GAS	7.88E-02	2.70E-02	4.19E-01
RIDεRs	6.01E-03	2.64E-03	5.03E-02

Film			
Method	EIG	CLO	BET
ε-BE	**2.30E-03**	5.26E-03	**8.10E-03**
Graphwave	*TO*	*TO*	*TO*
SEGK	*TO*	*TO*	*TO*
DRNE	1.02E-02	6.01E-03	1.30E-02
struc2vec	*TO*	*TO*	*TO*
GAS	1.04E-02	**2.39E-03**	1.25E-02
RIDεRs	8.21E-3	2.64E-03	1.10E-02

Method	*Networks*				
	Brazil	*USA*	*BlogCatalog*	*Brightkite*	*GitHub*
	$n = 131$	1190	10312	58689	177316
ε-BE	**2.94E-1**	**6.49E-1**	**6.24E+0**	**7.68E+1**	**4.81E+2**
Graphwave	2.52E+0	1.03E+1	1.47E+3	*TO*	*TO*
SEGK	1.92E+1	4.58E+3	*TO*	*TO*	*TO*
DRNE	1.07E+1	2.50E+1	1.96E+2	1.26E+3	*TO*
struc2vec	1.83E+1	9.93E+3	*TO*	*TO*	*TO*
GAS	2.30E+0	7.95E+0	4.90E+2	4.98E+2	2.65E+3
RIDεRs	3.51E+1	2.73E+2	3.96E+2	7.38E+3	*TO*

Runtime comparison against state-of-the-art methods for graph embedding

Approximate Dynamical Symmetry Reduction

An asymmetric linear ODE

$$x_1(t+1) = \frac{6}{10}x_1(t) - \frac{2}{10}x_2(t) + \frac{2}{10}x_3(t)$$

$$x_2(t+1) = \left(\frac{2}{10} - \varepsilon\right)x_1(t) + \frac{8}{10}x_2(t) + \frac{1}{5}$$

$$x_3(t+1) = \frac{2}{10}x_1(t) + \frac{8}{10}x_3(t) + \frac{1}{5}$$

$\varepsilon = 0$

No reduction for $0 < \varepsilon \leq 2/10$

Idea: transform the equality between trajectories of variables into a **similarity measure**

$$\bigwedge_{(i,j)\in R} (x_i = x_j) \implies \bigwedge_{(i,j)\in R} \left(A_i x + b_i = A_j x + b_j\right)$$

(R is the equivalence relation)

becomes

$$\bigwedge_{1\leq i,j\leq n} \left(|x_i(t) - x_j(t)| \leq D_{ij}\right) \implies \bigwedge_{1\leq i,j\leq n} \left(|x_i(t+1) - x_j(t+1)| \leq D_{ij}\right)$$

(D_{ij} to be found, for a given set of initial conditions)

Can be framed as optimal transportation problem; iterative algorithm takes $O(n^5 \log n)$ time per iteration

"Backward" Dissimilarity: Intuition

$$|A_2 x(t) - A_3 x(t)| = |\tfrac{1}{10}(x_1(t) - x_1(t)) + \tfrac{8}{10}(x_2(t) - x_3(t)) + \tfrac{1}{10}\, x_1(t)|$$
$$\leq \tfrac{8}{10}|x_2(t) - x_3(t)| + \tfrac{1}{10}\,|x_1(t)|$$
$$\leq \tfrac{8}{10}|x_2(t) - x_3(t)| + \tfrac{1}{10}\lambda\,.$$

(λ is a bound on the solution norm; if $\lambda = 2$ then $D_{ij} = 1$)

Model		*LCS bisim.*		*BD*			*Ratios LCS bisim. / BD*			
Name	*n*	*Time*	*Iter.*	*Time*	*Iter.*	*0*	*Min*	*Avg low*	*Avg up*	*Max*
			DTMCs	`https://qcomp.org/benchmarks/`						
haddad	11	11.8	12	3.0	3	2	4.60E−2	4.79E−1	4.99E+0	7.37E+1
brp	25	866.9	10	13.8	3	2	7.71E−2	2.71E+2	3.51E+3	3.07E+5
herman	32	4095.6	8	61.3	2	136	2.41E−1	5.50E−1	2.85E+0	5.47E+0
			MOVIEGALAXIES	`https://networks.skewed.de/net/moviegalaxies`						
328	9	2.3	9	4.2	4	0	1.58E+0	6.37E+0	8.57E+0	8.19E+1
293	13	17.2	9	15.8	4	0	1.73E+0	4.29E+0	5.81E+0	2.54E+1
347	15	23.6	9	24.4	4	9	2.64E+0	1.48E+1	2.02E+1	2.85E+2
17	22	252.0	9	146.4	5	16	1.41E+0	6.00E+0	8.09E+0	6.23E+1
33	25	407.1	9	904.8	6	3	1.06E+0	3.41E+0	4.66E+0	1.91E+1
804	29	761.6	9	804.6	5	15	8.13E−1	4.38E+0	5.93E+0	6.08E+1
			DOM	`https://networks.skewed.de/net/dom`						
Cor	6	0.8	8	2.5	4	0	2.86E+0	2.17E+1	3.31E+1	1.89E+2
DMas	13	16.1	10	6.9	4	3	1.92E−1	5.26E−1	1.49E+0	5.46E+0
Mwa	19	108.5	12	18.3	4	0	2.27E−1	2.45E−1	6.06E−1	1.41E+0
			AMBASSADOR	`https://networks.skewed.de/net/ambassador`						
2000	16	26.3	9	34.7	5	2	3.41E+0	9.33E+0	1.27E+1	3.10E+1
2005	16	28.9	10	3.1	2	92	2.57E+0	2.57E+0	3.49E+0	3.49E+0
1990 1994	16	25.8	9	27.6	5	2	2.13E+0	5.49E+0	7.49E+0	1.45E+1

Conclusion

- Equitable partitioning is a simple concept that finds applications across a variety of models
  - **Many more** in addition to those seen in the talk: chemistry, logics, machine learning (graph kernels and graph neural networks), linear optimization
- Equitable partitions are “easy” to compute and **characterize** symmetric dynamics in many cases (while they are only necessary conditions for structural symmetry)
- Approximate variants become more challenging:
  - computation cost: but it is **competitive** with respect to the state of the art
  - Availability of error bounds with respect to asymmetries in the initial conditions and/or parameters: **more research needed**, bounds for specific models?

Acknowledgements

- Georgios Argyris (DTU Denmark)
- Giorgio and Giovanni Bacci (Aalborg)
- Luca Cardelli (Oxford)
- Radu Grosu (TU Wien)
- Alberto Lluch Lafuente (DTU Denmark)
- Kim Larsen (Aalborg)
- Isabel Cristina Perez Verona (IMT)
- Giuseppe Squillace (IMT)
- Stefano Tognazzi (IMT)
- Max Tschaikowski (Aalborg)
- Andrea Vandin (Scuola Sant'Anna Pisa)

Finanziato dall'Unione europea
NextGenerationEU

Italiadomani
PIANO NAZIONALE DI RIPRESA E RESILIENZA

THE Tuscany Health Ecosystem


Thanks!

References

- Giorgio Bacci, Giovanni Bacci, Kim G. Larsen, Giuseppe Squillace, Mirco Tribastone, Max Tschaikowski, and Andrea Vandin: Dissimilarity for Linear Dynamical Systems, to appear in QEST (2024)
- Luca Cardelli, Giuseppe Squillace, Mirco Tribastone, Max Tschaikowski, Andrea Vandin: Formal lumping of polynomial differential equations through approximate equivalences. J. Log. Algebraic Methods Program. 134: 100876 (2023)
- Antonio Jiménez-Pastor, Kim G. Larsen, Mirco Tribastone, Max Tschaikowski: Forward and Backward Constrained Bisimulations for Quantum Circuits. TACAS (2) 2024: 343-362
- Luca Cardelli, Radu Grosu, Kim Guldstrand Larsen, Mirco Tribastone, Max Tschaikowski, Andrea Vandin: Algorithmic Minimization of Uncertain Continuous-Time Markov Chains. IEEE Trans. Autom. Control. 68(11): 6557-6572 (2023)
- Georgios Argyris, Alberto Lluch-Lafuente, Mirco Tribastone, Max Tschaikowski, Andrea Vandin: Reducing Boolean networks with backward equivalence. BMC Bioinform. 24(1): 212 (2023)
- Stefano Tognazzi, Mirco Tribastone, Max Tschaikowski, Andrea Vandin: Differential Equivalence for Linear Differential Algebraic Equations. IEEE Trans. Autom. Control. 67(7): 3484-3493 (2022)
- Luca Cardelli, Mirco Tribastone, Max Tschaikowski, Andrea Vandin. Symbolic computation of differential equivalences. Theoretical Computer Science 777, 132-154
- Isabel Cristina Pérez-Verona, Mirco Tribastone, Andrea Vandin: A large-scale assessment of exact lumping of quantitative models in the BioModels repository. Theor. Comput. Sci. 893: 41-59 (2021)
- Luca Cardelli, Mirco Tribastone, Max Tschaikowski, Andrea Vandin: Guaranteed Error Bounds on Approximate Model Abstractions Through Reachability Analysis. QEST 2018: 104-121
- Luca Cardelli, Mirco Tribastone, Max Tschaikowski, Andrea Vandin: ERODE: A Tool for the Evaluation and Reduction of Ordinary Differential Equations. TACAS (2) 2017: 310-328
- Luca Cardelli, Mirco Tribastone, Max Tschaikowski, Andrea Vandin: Efficient Syntax-Driven Lumping of Differential Equations. TACAS 2016