# Influence maximization in Boolean networks

Filippo Radicchi

filiradi@indiana.edu https://cgi.luddy.indiana.edu/~filiradi

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SCHOOL OF INFORMATICS, COMPUTING, AND ENGINEERING

T. Parmer, L.M. Rocha
and F. Radicchi

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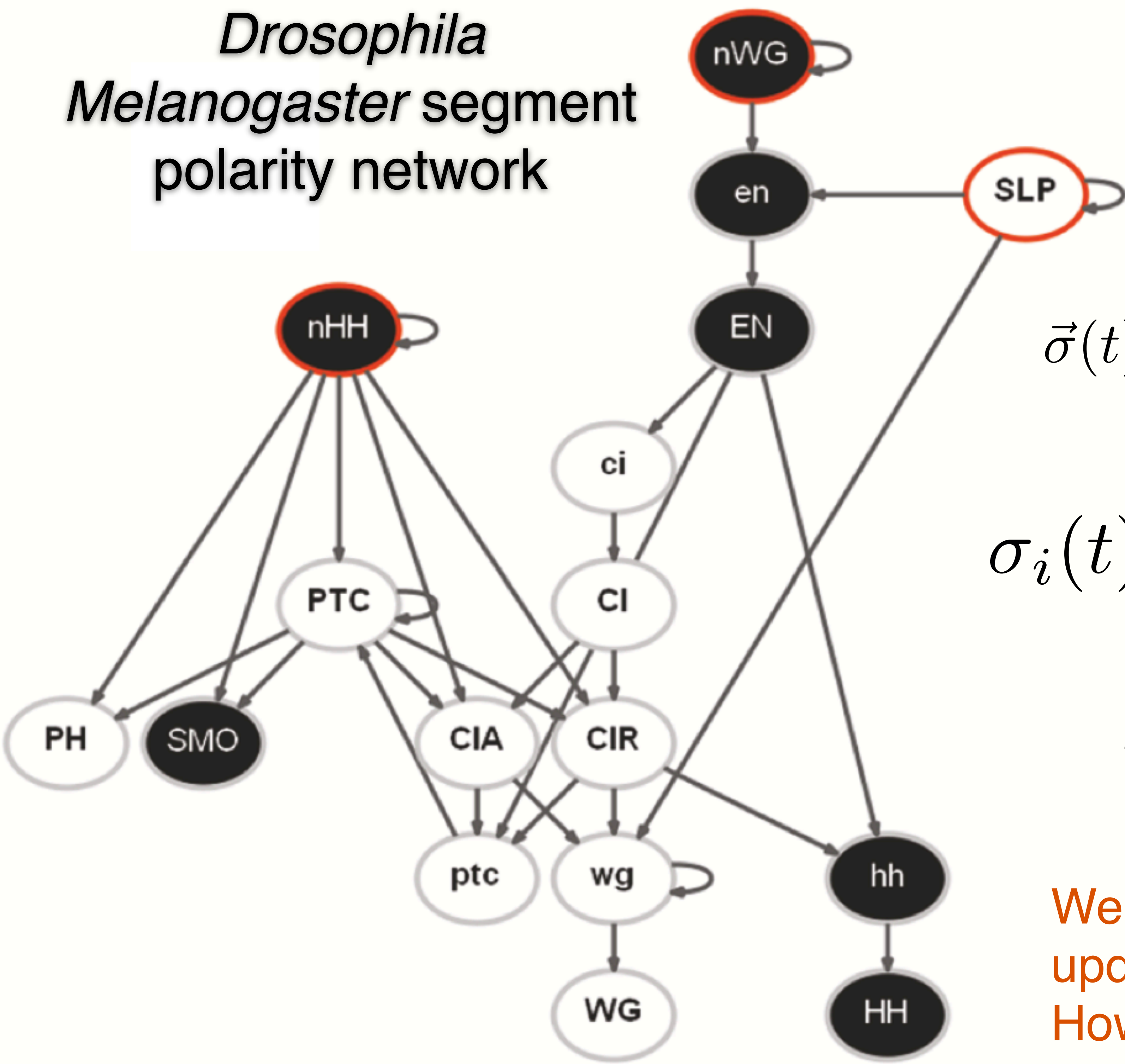
# Boolean networks

*Drosophila Melanogaster* segment polarity network




State of node i

$$\sigma_i(t) = 0, 1$$

Network configuration

$$\vec{\sigma}(t) = (\sigma_1(t), \ldots, \sigma_i(t), \ldots, \sigma_N(t))$$

Boolean function

$$\sigma_i(t) = F_i\left(\vec{\sigma}_{\mathcal{N}_i}(t-1)\right)$$

Neighbors of node i

$$\mathcal{N}_i = \{j_1, \ldots, j_{k_i}\}$$

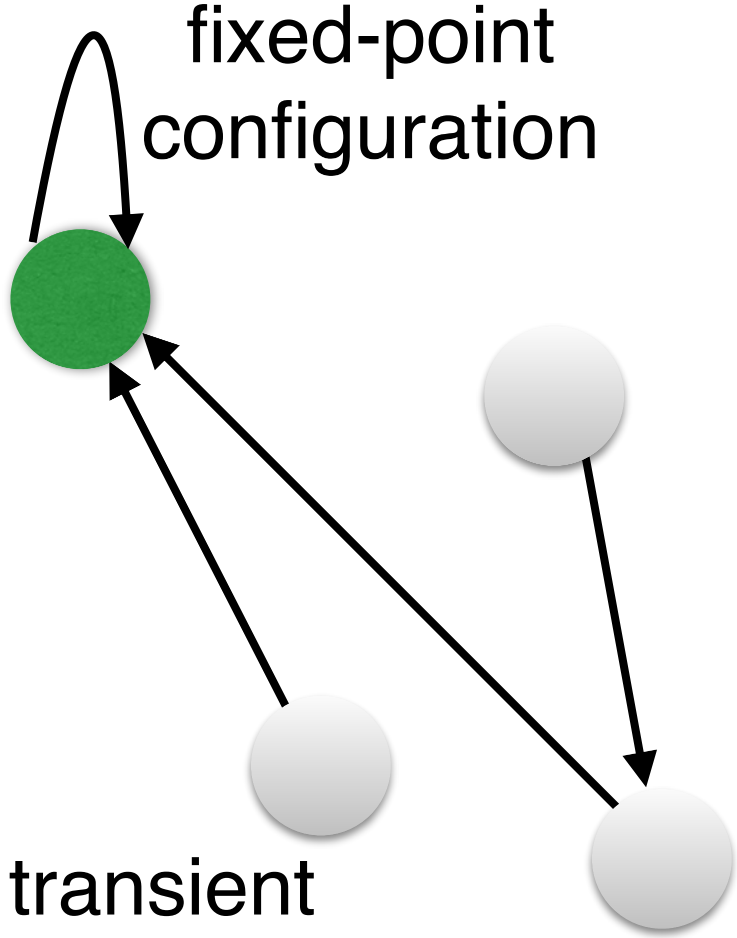
We consider the case when all nodes update synchronously their state. However, our methods can be generalized for arbitrary updating schemes.

S. Kauffman, Nature 224,177–178 (1969).

R. Albert, H.G. Othmer , J. Theor. Biol. 223, 1–18 (2003).

# Boolean networks

## State-transition graph (STG)




Each configuration corresponds to a node in the STG; transitions between configurations are determined by the Boolean rules of the dynamics

If there are N nodes in the network, the STG is composed of

$$2^N \text{ nodes}$$

# Individual-based mean-field approximation (IBMFA)

$$s_i(t) = P(\sigma_i(t) = 1)$$

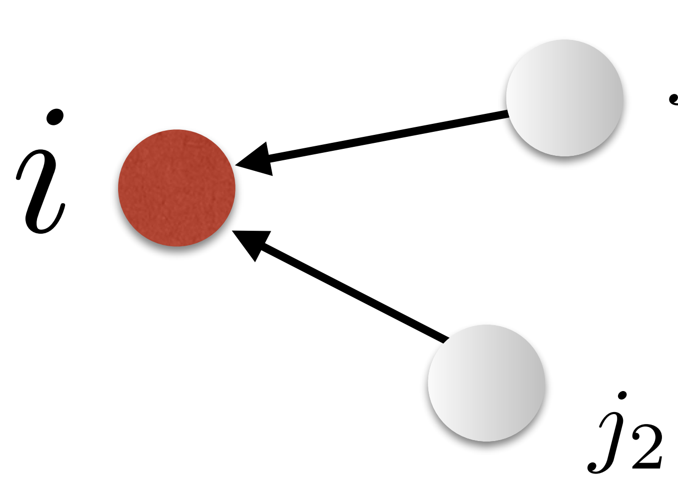
expectation value over an infinite number of realizations of the dynamics

$$P\left(\vec{\sigma}(t)|\vec{s}(t)\right) = \prod_{i=1}^{N} [s_i(t)]^{\sigma_i(t)} [1 - s_i(t)]^{1-\sigma_i(t)}.$$

state variables are assumed to be uncorrelated

the evolution of the expectation value obeys

$$s_i(t) = \sum_{\{n_j : j \in \mathcal{N}_i\}} \delta_{1,F_i(\vec{n}_{\mathcal{N}_i})} \prod_{j \in \mathcal{N}_i} [s_j(t-1)]^{n_j} [1 - s_j(t-1)]^{1-n_j}.$$




$$\mathcal{N}_i = \{j_1, j_2\}$$

$F_i$

| $\sigma_{j_1}$ | $\sigma_{j_2}$ | $\sigma_i$ |
|---|---|---|
| 0 | 0 | 1 |
| 0 | 1 | 0 |
| 1 | 0 | 0 |
| 1 | 1 | 1 |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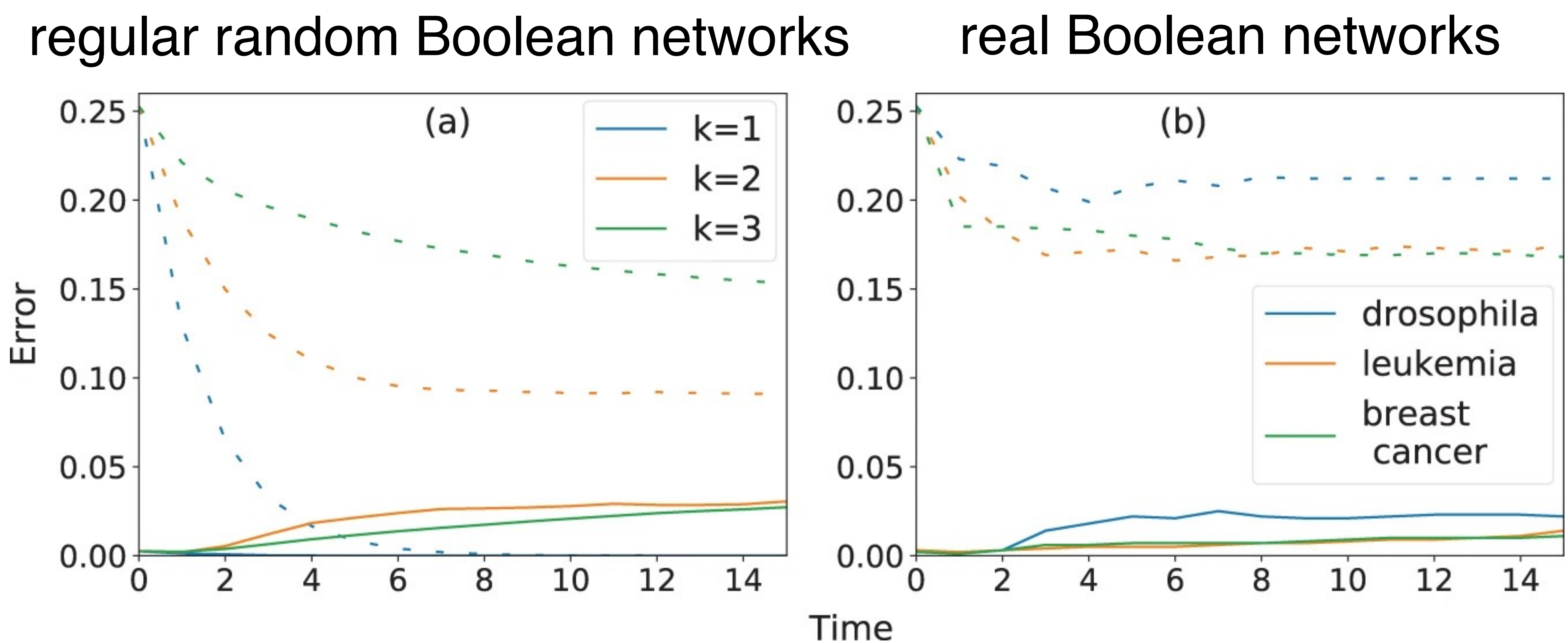
# Individual-based mean-field approximation (IBMFA)




started from random configurations $s_i(t=0) = P(\sigma_i(t=0)=1) = 1/2$

accuracy of IBMFA is tested on numerical simulations

baseline error (dashed) is given by the standard deviation of numerically simulated trajectories

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# Boolean networks

We study the dynamics of a network under a peculiar choice of its initial configuration

seed set

$$\mathcal{X} = \{(i_1, \hat{\sigma}_{i_1}), \ldots, (i_k, \hat{\sigma}_{i_k})\}$$

The state of the nodes in the seed set is pinned, i.e., does not change in time

$$\sigma_i(t) = \hat{\sigma}_i \quad \text{if } i \in \mathcal{X}$$

The initial state of all nodes outside the seed set value is maximally uncertain, i.e.,

$$s_i(t=0) = P(\sigma_i(t=0) = 1) = 1/2 \qquad \text{if } i \notin \mathcal{X}$$

subsequent values of the state variables are determined by the rules of the dynamics

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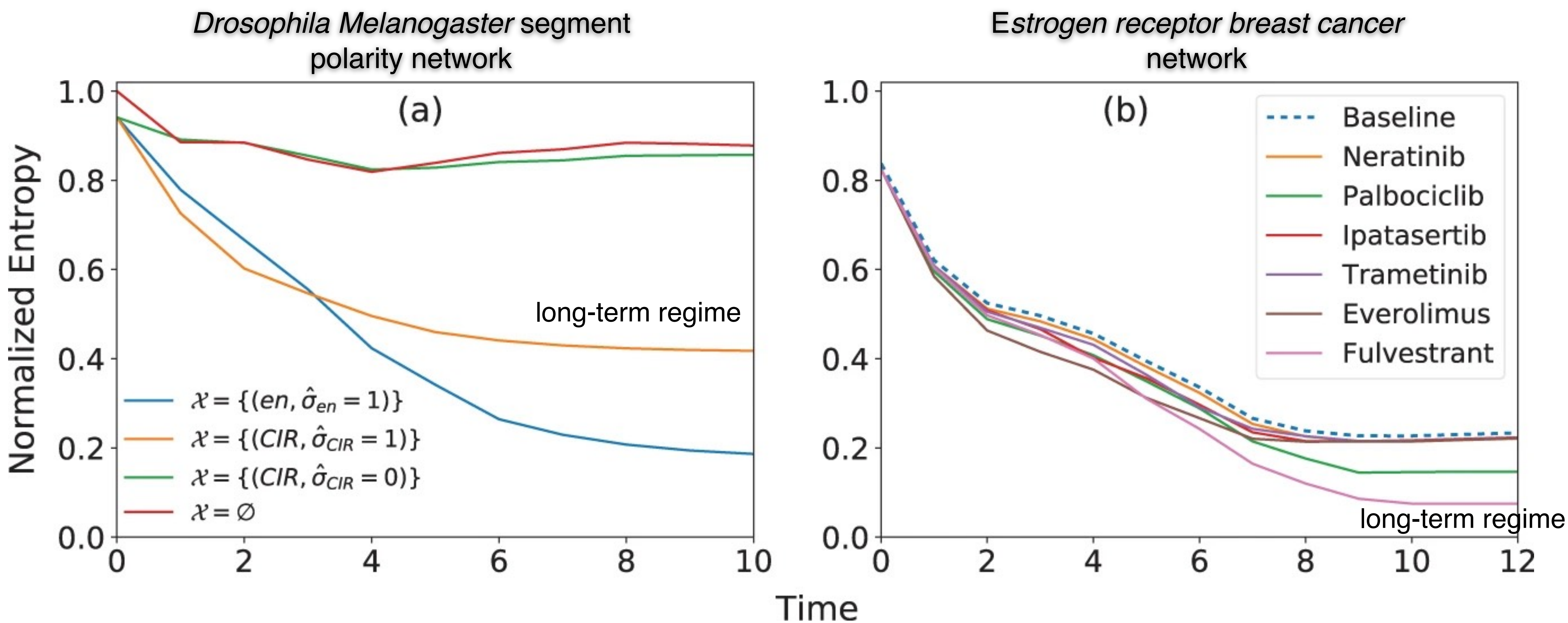
# Dynamical influence of seed sets

$$H(\vec{s}) = \frac{1}{N}\sum_{i=1}^{N} h_2(s_i)$$ upper bound of the ground-truth entropy

$$h_2(s) = -s\log_2(s) - (1-s)\log_2(1-s)$$

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# Influence maximization in Boolean networks

unconstrained greedy optimization

$$\mathcal{X}_v = \{(b_1, \hat{\sigma}_{b_1}), \ldots, (b_v, \hat{\sigma}_{b_v})\}$$ optimal seed set at stage v

For v=0 $\mathcal{X}_0 = \emptyset$ . Set v = 1 and iterate:

1. choose the best seed

$$(b_v, \hat{\sigma}_{b_v}) = \arg \min_{(i,\hat{\sigma}_i) \notin \mathcal{X}_{v-1}} H(\vec{s}|\mathcal{X}_{v-1} \cup (i, \hat{\sigma}_i))$$

2. the new set of seeds is

$$\mathcal{X}_v = \mathcal{X}_{v-1} \cup (b_v, \hat{\sigma}_{b_v})$$

3. increase v to v + 1

The above algorithm is iterated until $H(\vec{s}|\mathcal{X}_v) = 0$ meaning that the seed set leads to a fixed point

the entropy function is computed in the long-term regime of the dynamics

a greedy post-processing technique is applied to set of identified seeds

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# Influence maximization in Boolean networks

constrained greedy optimization towards the attractor

$$\Theta = \{(1, \tilde{\sigma}_1), \ldots, (N, \tilde{\sigma}_N)\}$$

$$\mathcal{X}_v = \{(b_1, \hat{\sigma}_{b_1}), \ldots, (b_v, \hat{\sigma}_{b_v})\}$$

optimal seed set at stage v

For v=0 $\mathcal{X}_0 = \emptyset$ . Set v = 1 and

1. choose the best seed

$$(b_v, \hat{\sigma}_{b_v}) = \arg \min_{(i,\hat{\sigma}_i) \notin \mathcal{X}_{v-1}, (i,\hat{\sigma}_i) \in \Theta} H(\vec{s} | \mathcal{X}_{v-1} \cup (i, \hat{\sigma}_i))$$

2. the new set of seeds is

$$\mathcal{X}_v = \mathcal{X}_{v-1} \cup (b_v, \hat{\sigma}_{b_v})$$

3. increase v to v + 1

The above algorithm is iterated until $H(\vec{s}|\mathcal{X}_v) = 0$ meaning that the seed set leads to a fixed point

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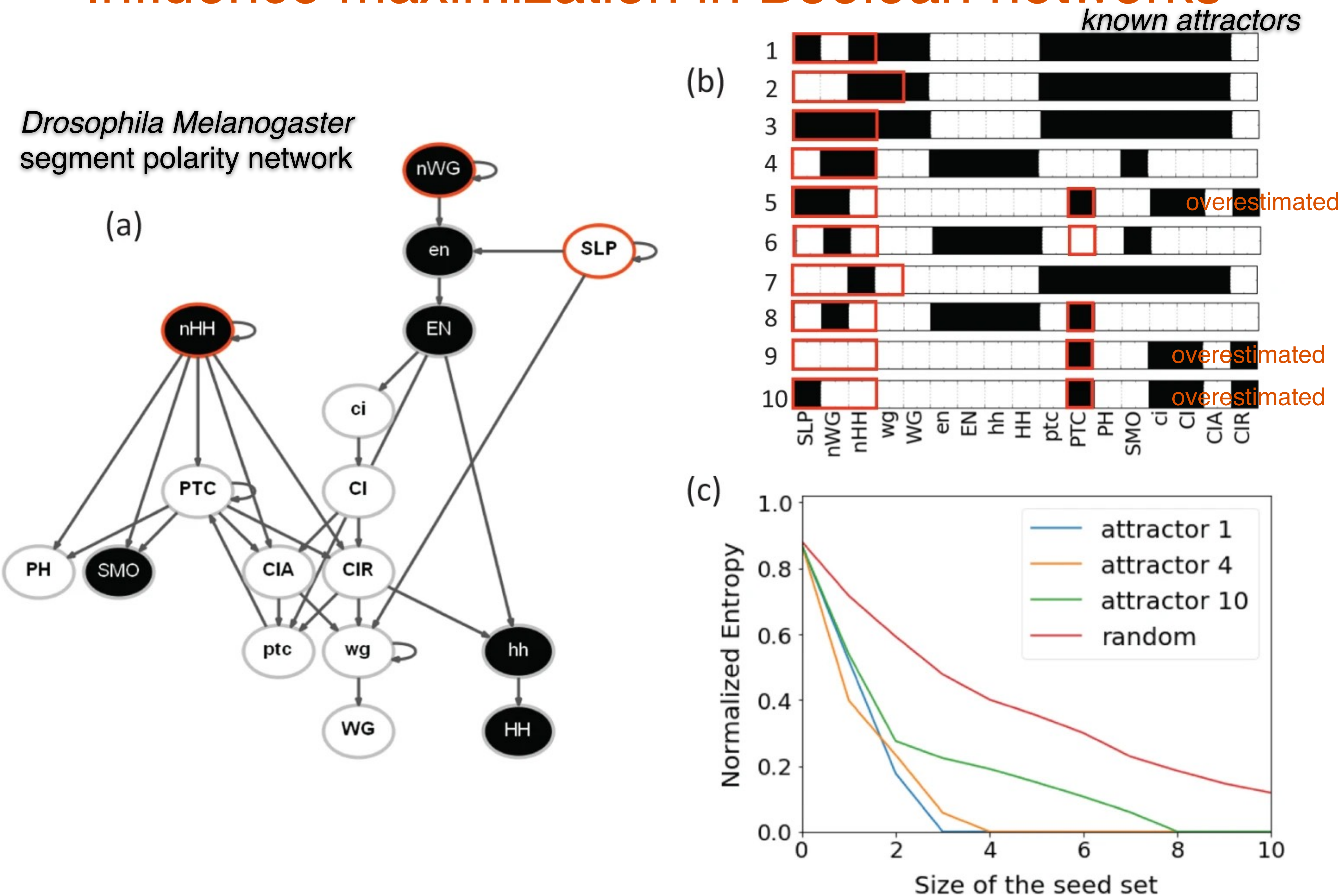


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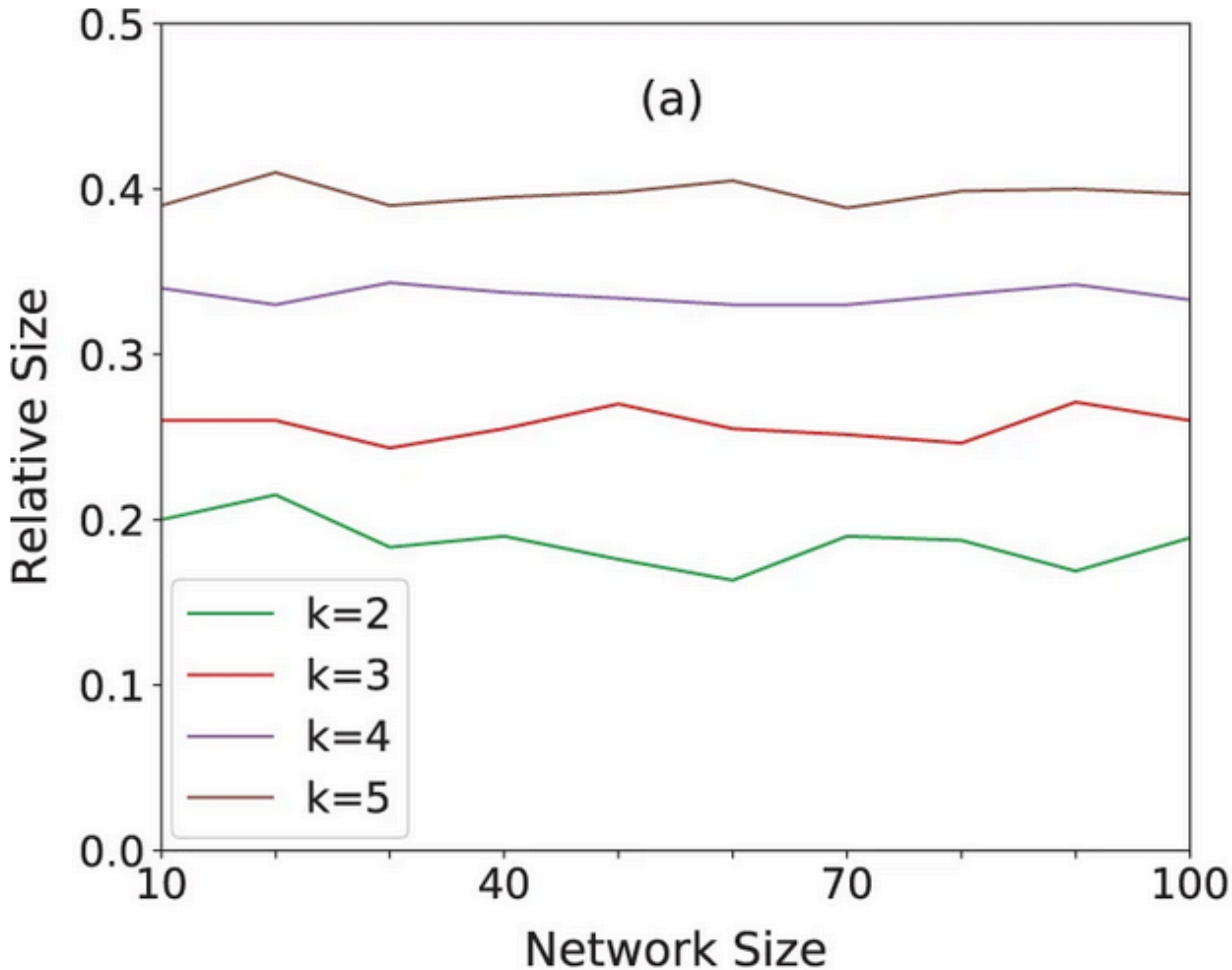
# Influence maximization in Boolean networks

regular random Boolean networks

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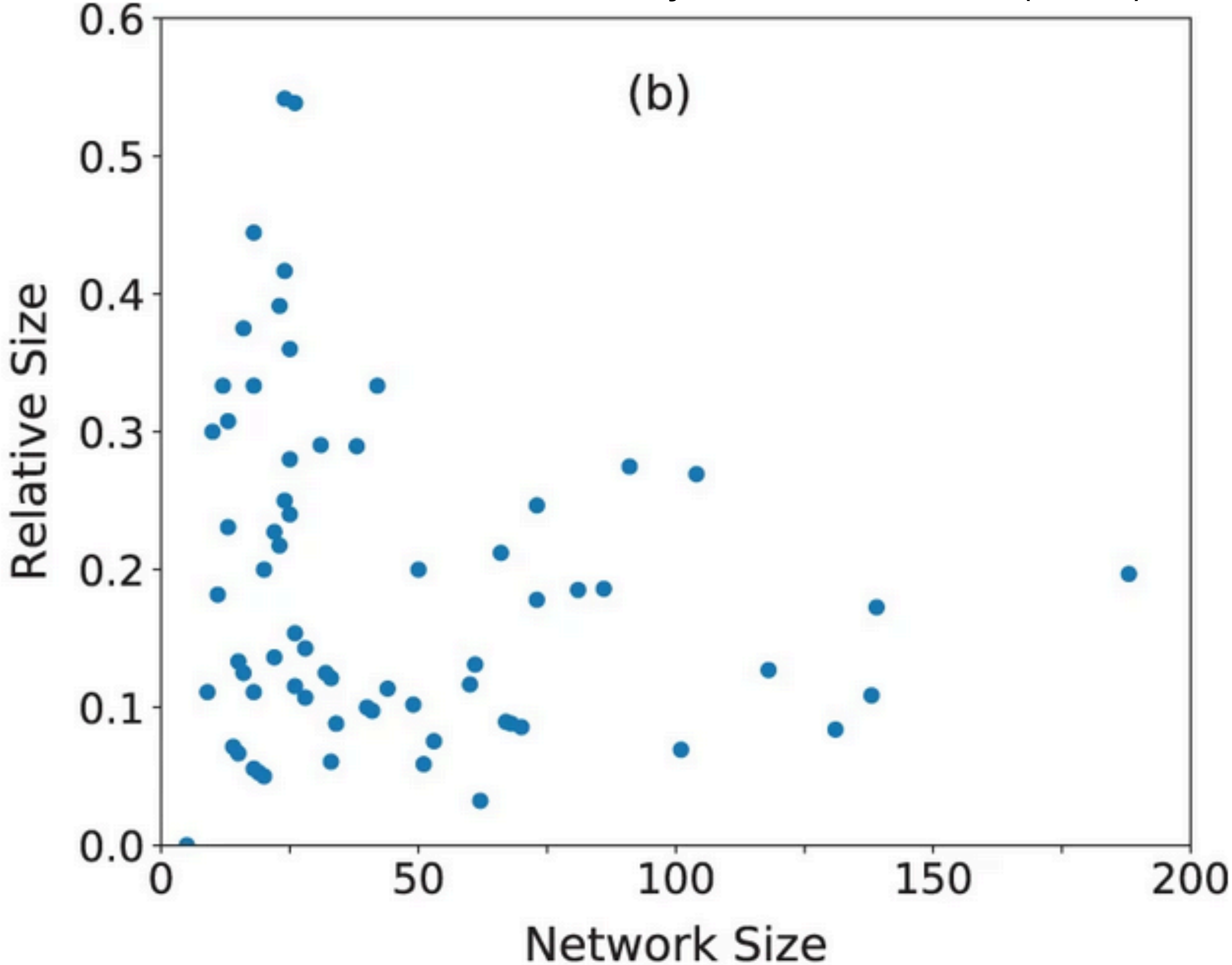
# Influence maximization in Boolean networks

Real Boolean networks from the Cell Collective repository

Helikar, T. et al. BMC Syst. Biol. 6, 1–14 (2012)

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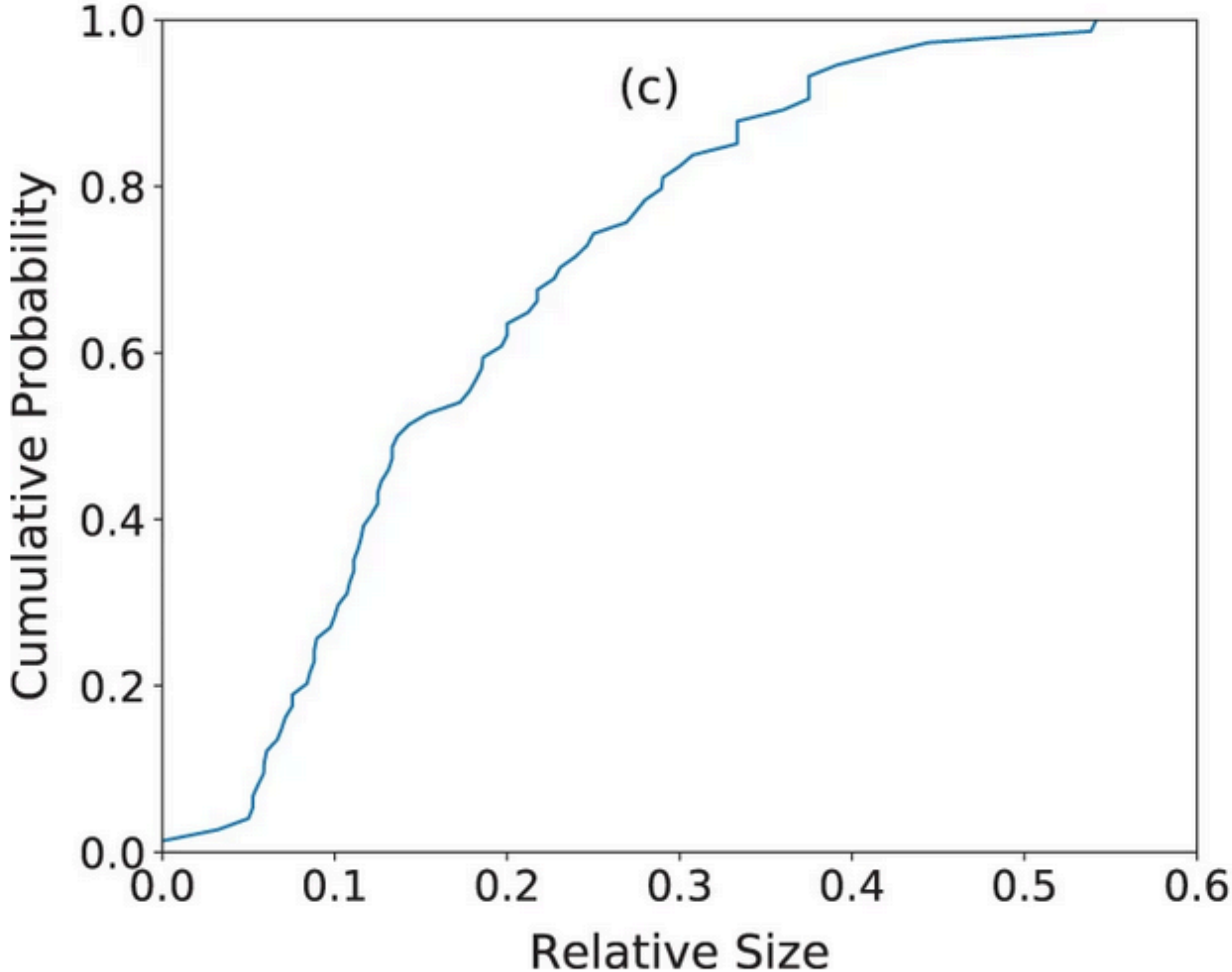


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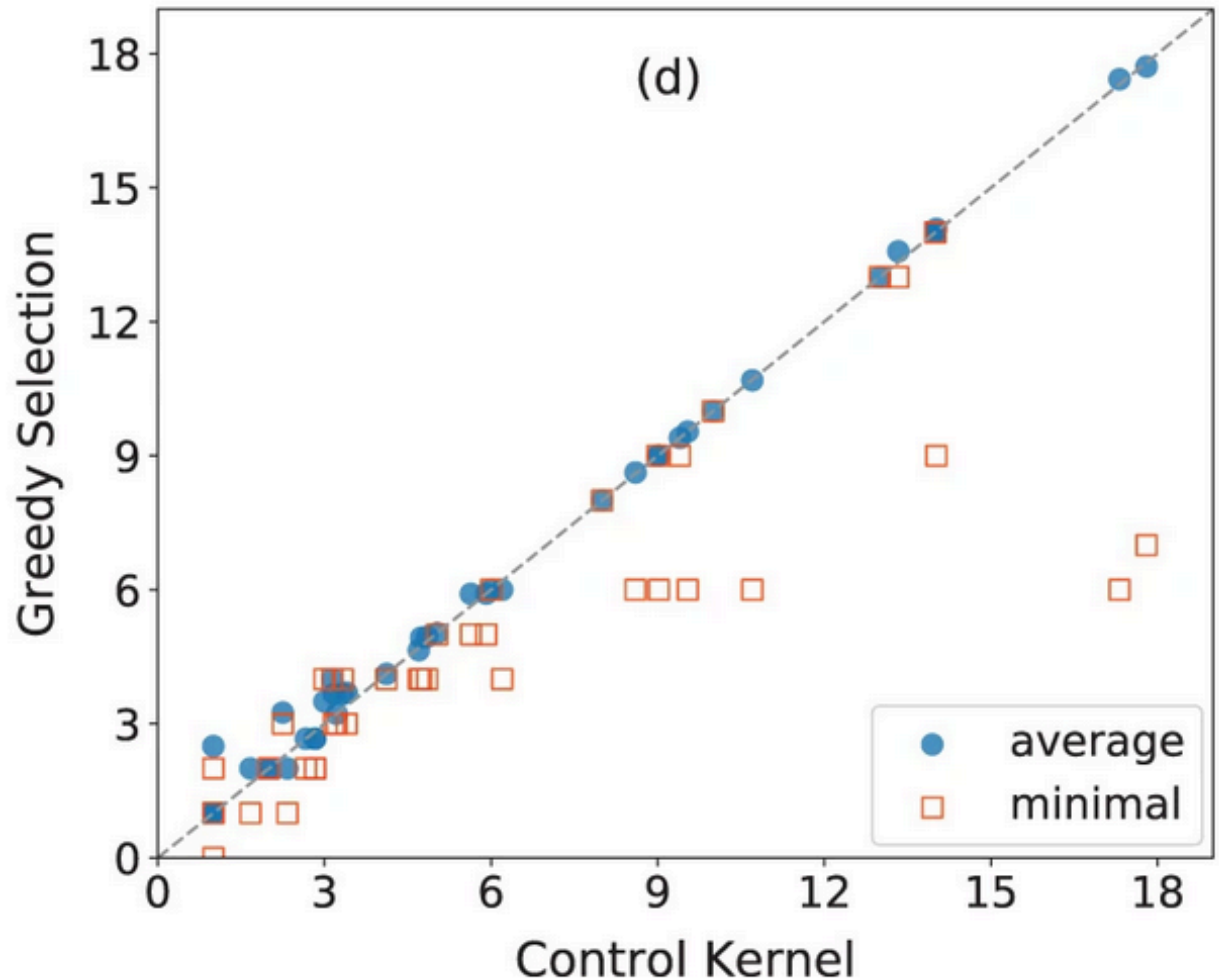
Borriello, E. & Daniels, B. C. Nat. Commun. 12, 1–15 (2021).




Attractors are found via brute-force search

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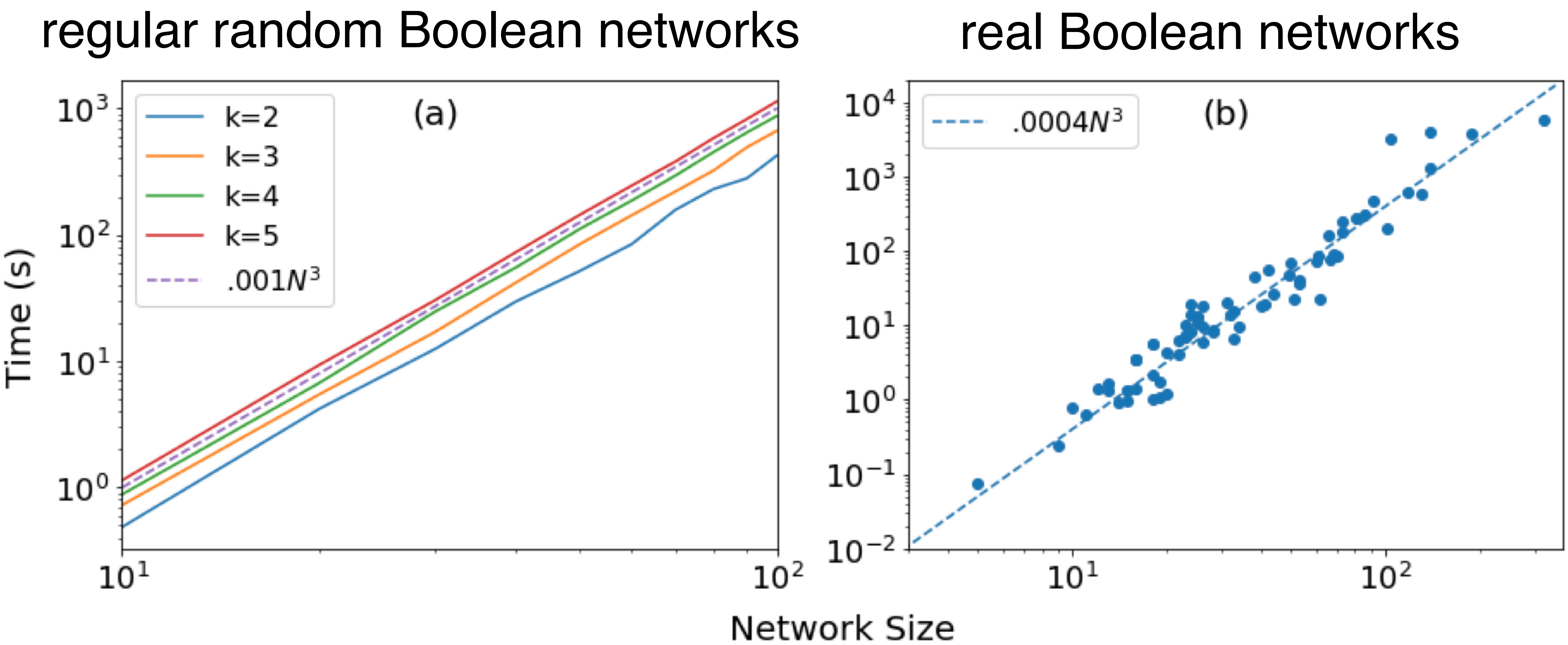
# Computational time

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