Strong Bounds for Evolution in Networks

Paul G. Spirakis[1,2]

ESRC workshop on Algorithmic Game Theory
Department of Mathematics, London School of Economics

These results have been presented in:

- Theor. Comp. Science 2013: Natural Models for Evolution on Networks,
  by *G. Mertzios*[3], *S. Nikoletseas*[1], *C. Raptopoulos*[1], and *P. Spirakis*[1,2]
- SODA 2012; Algorithmica: Approximating Fixation Probabilities in the Generalized Moran Process,
  by *J. Díaz*[4], *L.A. Goldberg*[5], *G. Mertzios*[3], *D. Richerby*[5], *M. Serna*[4], and *P. Spirakis*[1,2]
- ICALP 2013: Strong Bounds for Evolution in Undirected Graphs,
  by *G. Mertzios*[3] and *P. Spirakis*[1,2]

[1]CTI & University of Patras, Greece, [2]University of Liverpool, UK, [3]Durham University, UK,
[4]Universitat Politécnica de Catalunya, Spain, [5]University of Oxford, UK

Evolutionary graph theory

- Evolution in biology / Population dynamics have been mainly traditionally in homogeneous populations
- However, in reality, the topology / structure of the population can strongly affect the output of the dynamics.
- Evolutionary graph theory has been introduced in [Lieberman, Hauert, Nowak, *Nature*, 2005]
- Main idea: arrange the population on a network (i.e. graph)
- There are two types of vertices:
  - aggressive ("mutants") $\longleftrightarrow$ fitness $r \geq 1$,
  - non-aggressive ("residents") $\longleftrightarrow$ fitness 1.

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- There are two types of vertices:
  - aggressive ("mutants") $\longleftrightarrow$ fitness $r \geq 1$,
  - non-aggressive ("residents") $\longleftrightarrow$ fitness 1.
- Time is discrete $t = 1, 2, \ldots$
- At every iteration $t \geq 1$,
  - choose a vertex u with probability proportional to its fitness;
  - choose randomly a neighbor $v \in N(u)$ (resp. an arc $\langle uv \rangle$);
  - replace v by an offspring of u.

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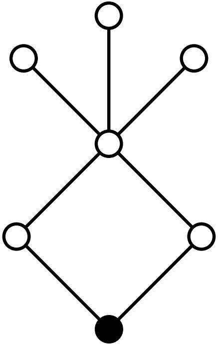
The main model in [Lieberman, Hauert, Nowak, *Nature*, 2005]:
(the "generalized Moran process")



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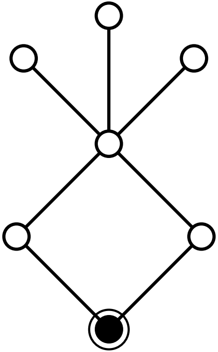

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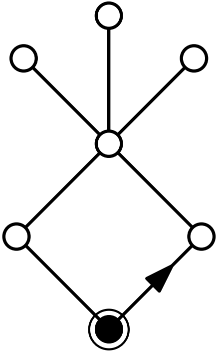

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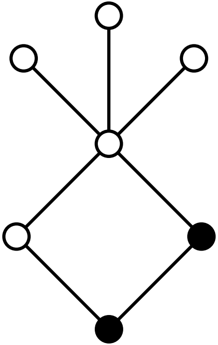

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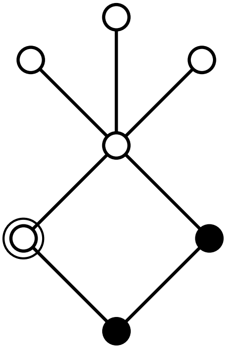

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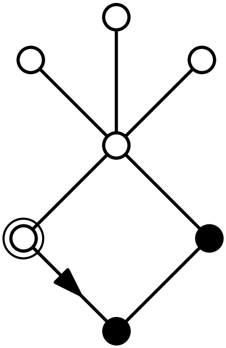

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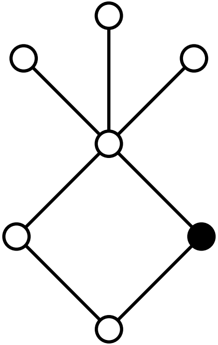

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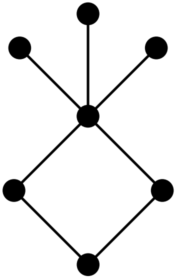

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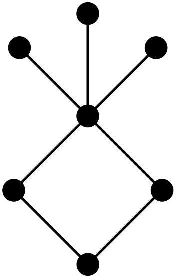

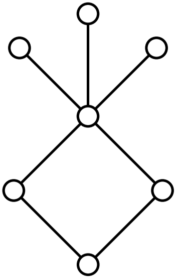

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- When the graph G is directed, extreme phenomena can occur:
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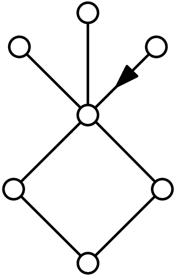

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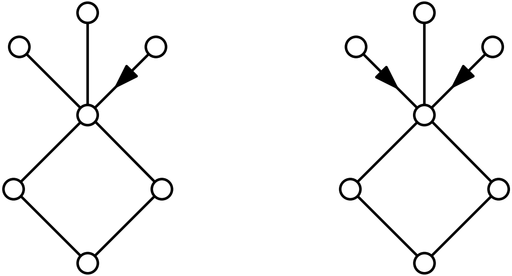

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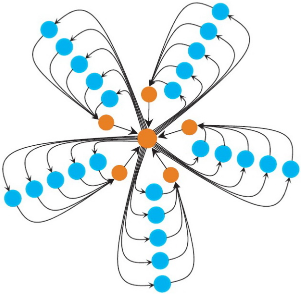

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$\Rightarrow$ We are mainly interested in undirected graphs.

Evolutionary graph theory

Theorem (Isothermal Theorem, Lieberman et al., *Nature*, 2005)

Let $G = (V, E)$ *be an undirected and regular graph (i.e.* $\deg(u) = \deg(v)$ *for every* $u, v \in V$*). If* $r > 1$*, then* $f_r(G) = \frac{1-\frac{1}{r}}{1-\frac{1}{r^n}} \approx 1 - \frac{1}{r}$.

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- The complete graph acts as a "benchmark"
- A graph G is called:
  - an amplifier if $f_r(G) > \frac{1-\frac{1}{r}}{1-\frac{1}{r^n}}$, and
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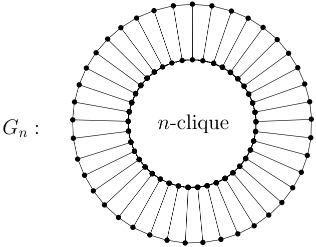
- **Question 1:** Do there exist strong undirected amplifiers / suppressors of selection?
- **Question 2:** How does the population structure affect the fixation probability?

A class of undirected suppressors of selection

- For every $n \geq 1$, we define the "clique-wheel" graph G_n with $2n$ vertices:
  - clique with n vertices
  - induced cycle with n vertices
  - perfect matching between them



Theorem (Mertzios, Nikoletseas, Raptopoulos, Spirakis, *TCS*, 2013)

For every $r \in (1, \frac{4}{3})$, the fixation probability of G_n is $f_{G_n}(r) \leq \frac{1}{2}(1 - \frac{1}{r})$, as $n \to \infty$.

Computation of fixation probabilities

Questions that were open until recently:

- How can we compute the fixation/extinction probability for a given graph?
- Can we do this efficiently?
  - the resulting Markov chain implies a system of linear equations
  - however: exponentially many equations – in general one for every vertex subset
- Does the generalized Moran process reach absorption (i.e. fixation or extinction) quickly?

Nothing is known until now, except immediate results for special cases

- e.g. expected linear time for regular graphs

Computation of fixation probabilities

Our results: [Díaz, Goldberg, Mertzios, Richerby, Spirakis, *SODA*, 2012; *Algorithmica*, to appear]

- The generalized Moran process reaches absorption (either fixation or extinction) in polynomial number of steps with high probability.
- Two FPRAS (*fully polynomial randomized approximation schemes*) for the problems of:
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Definition

An FPRAS for a function f is a randomized algorithm g that, given input X, gives an output satisfying:

$$(1-\varepsilon)f(X) \leq g(X) \leq (1+\varepsilon)f(X)$$

with probability at least $\frac{3}{4}$ and has running time polynomial in $|X|$ and $\frac{1}{\varepsilon}$.

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General approach for the FPRAS:

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The correctness of the FPRAS is based on two points:

1. expected polynomial time until absorption is reached

   $\Longrightarrow$ every simulation needs polynomial number of steps

2. the fixation probability is polynomially upper/lower bounded (i.e. not too big/small)

   $\Longrightarrow$ a polynomial number of simulations suffices to estimate the fixation/absorption probabilities.

Upper / lower bounds

So far, the only known general bounds for the fixation probability:

Lemma (Díaz, Goldberg, Mertzios, Richerby, Serna, Spirakis, *SODA*, 2012; *Algorithmica*, to appear)

Let $G = (V, E)$ be an undirected graph with n vertices. Then:

- $f_r(G) \geq \frac{1}{n}$ *for any* $r \geq 1$
- $f_r(G) \leq 1 - \frac{1}{n+r}$ *for any* $r > 0$

- Tighter upper / lower bounds $\Rightarrow$ better running time of these FPRAS.

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- We are interested in finding graphs with many strong / weak starts $f_r(v)$ for the mutant

Universal and selective amplifiers

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Our results

First result:

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For any function $g(n) = \Omega(n^{\frac{3}{4}+\varepsilon})$*, where* $\varepsilon > 0$*, there exists no class* $\mathcal{G}$ *of* $g(n)$*-universal amplifiers for any* $r > r_0 = 1$.

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Therefore:

Corollary

There exists no infinite class of strong universal amplifiers.

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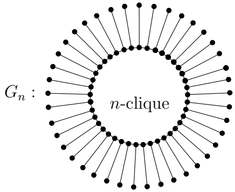
Second result:

Theorem

The class $\mathcal{G} = \{G_n : n \geq 1\}$ of urchin graphs is a class of $(\frac{n}{2}, n)$-selective amplifiers.



Our results

Second result:

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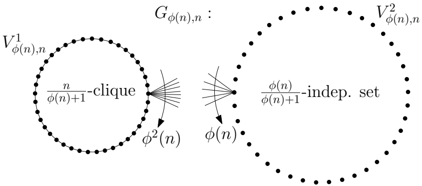

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Therefore there exist:

- strong selective amplifiers
- "quite" strong selective suppressors

Our results

Third result:

Theorem (Thermal Theorem)

Let $G = (V, E)$ be a connected undirected graph and $r > 1$.
Then $f_r(v) \geq \frac{r-1}{r+\frac{\deg v}{\deg_{\min}}}$ for every $v \in V$.

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  - for every vertex v of G
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- Almost tight bound:
  - for regular graphs: $f_r(v) \geq \frac{r-1}{r+1}$

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  - the temperature of vertex v is $\frac{1}{\deg v}$
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Corollary

In every graph G there exists at least one vertex v with $f_r(v) \geq \frac{r-1}{r+1}$ (i.e. independent of the size n).

No strong universal amplifiers

Theorem

For any function $g(n) = \Omega(n^{\frac{3}{4}+\varepsilon})$, *where* $\varepsilon > 0$, *there exists no class* $\mathcal{G}$ *of* $g(n)$*-universal amplifiers for any* $r > 1$.

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For any function $g(n) = \Omega(n^{\frac{3}{4}+\varepsilon})$, where $\varepsilon > 0$, there exists no class $\mathcal{G}$ of $g(n)$-universal amplifiers for any $r > 1$.

Proof sketch (by contradiction).

- Let $g(n) = \Omega(n^{1-\delta})$, where $\delta = \frac{1}{4} - \varepsilon < \frac{1}{4}$
- Suppose that $\mathcal{G}$ is a class of $g(n)$-universal amplifiers, i.e. for every $r > 1$ and every graph $G \in \mathcal{G}$ with $n \geq n_0$ vertices:
$$f_r(G) \geq 1 - \frac{c(r)}{g(n)} \geq 1 - \frac{c_0(r)}{n^{1-\delta}}$$
for appropriate functions $c(r)$ and $c_0(r)$.

Proof sketch (by contradiction).

- We partition the vertices of G into three subsets:

$$V_1 = \{v \in V : f_r(v) \geq 1 - \frac{c_0(r)}{n^{1-\delta}}\}$$

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  for appropriate functions $c_1(r)$ and $\phi(n,r) = \omega(1)$

- Since $\mathcal{G}$ is a class of $g(n)$-universal amplifiers $\Rightarrow$ $V_1 \neq \emptyset$

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Therefore:

- Since $\delta < \frac{1}{4} \Rightarrow 1 - \delta > 1 - 2\delta > 2\delta > \delta$

$\Rightarrow$ every neighbor of a vertex $v \in V_1 \cup V_2$ must belong to V_3

$\Rightarrow$ $V_1 \cup V_2$ is an independent set

No strong universal amplifiers

Proof sketch (by contradiction).

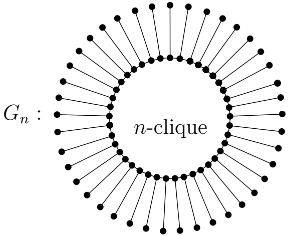
Using an upper bound from
[Mertzios, Nikoletseas, Raptopoulos, Spirakis, *Theor. Comp. Sci.*, 2013],
it follows:

- $\Omega(n^{-3\delta}) \leq \frac{c'''(r)}{n^{1-\delta}}$, for some function $c'''(r)$,
- contradiction since $\delta < \frac{1}{4}$

□

Strong selective amplifiers

- For every $n \geq 1$, we define the "urchin" graph G_n with $2n$ vertices:
  - a clique with n vertices
  - an independent set with n vertices (called "noses")
  - a perfect matching between them



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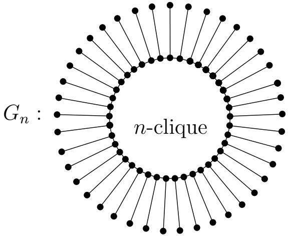


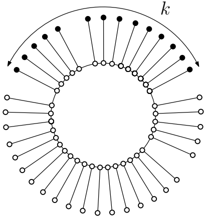
Our result:

Theorem

For every $r > 5$, the fixation probability of a nose v of G_n is $f_r(v) \geq 1 - \frac{c(r)}{n}$, where $c(r)$ is a function depending only on r.

Strong selective amplifiers

- Consider a state with $k \in \{0, 1, \ldots, n\}$ infected noses



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- Consider a state with $k \in \{0, 1, \ldots, n\}$ infected noses
- The infected clique vertices can be allocated as follows:

$Q^k_{i,x}$: among the neighbors of the infected noses, x are not infected
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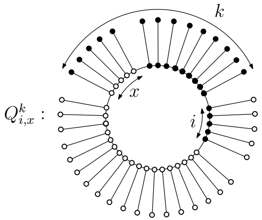

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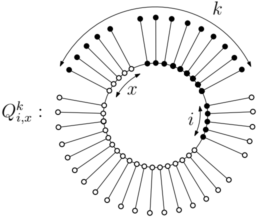

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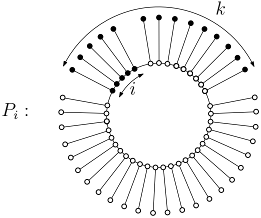

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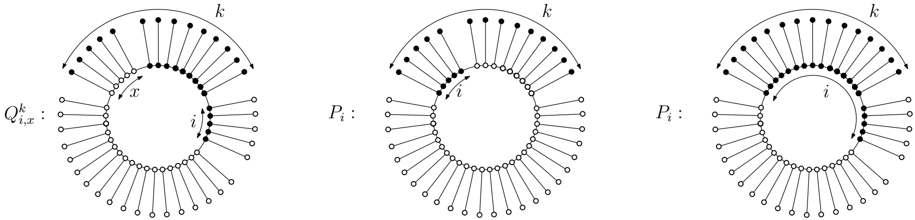

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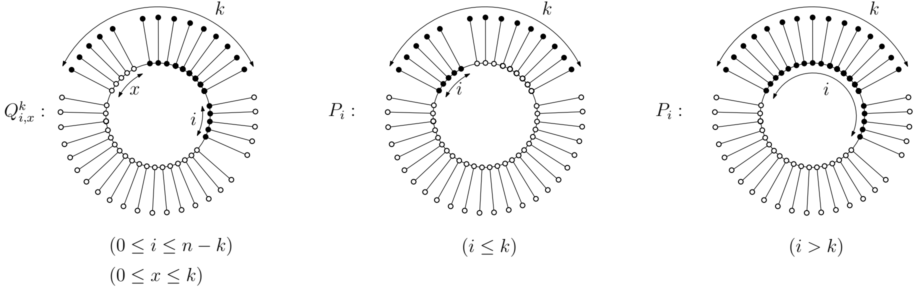
Strong selective amplifiers

- If $i = 0 \Rightarrow Q^k_{0,x} = P^k_{k-x}$



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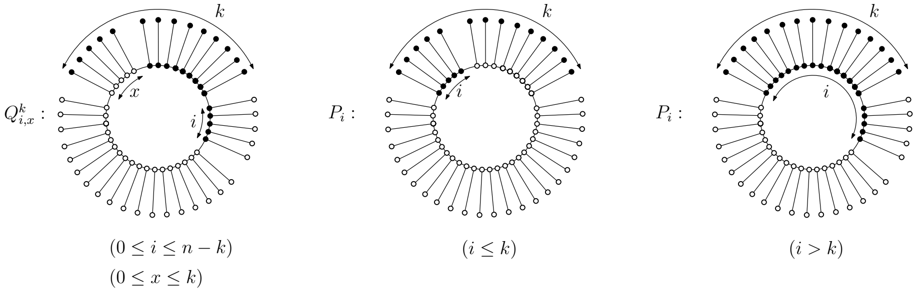

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For any i and x, denote by $q^k_{i,x}$ (resp. p^k_i) the probability that:

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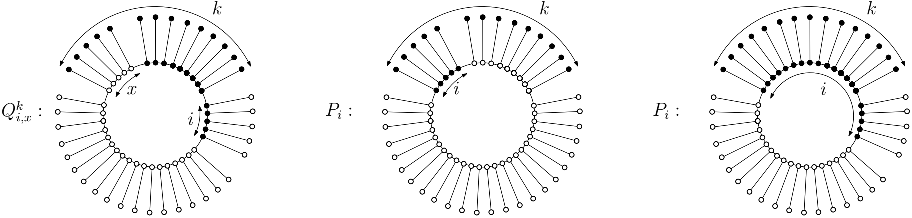

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For all appropriate values of k, i, x: $q_{i,x}^{k} > p_{k+i-x}^{k}$.

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Lemma

For all appropriate values of k, i, x: $q^k_{i,x} > p^k_{k+i-x}$.

$\Rightarrow$ to compute a lower bound on the fixation probability $f_r(v)$ of a nose v:

- whenever we have k infected noses and i infected clique vertices,
- we assume that we are at state P^k_i
- denote this relaxed Markov chain by $\mathcal{M}$

Strong selective amplifiers

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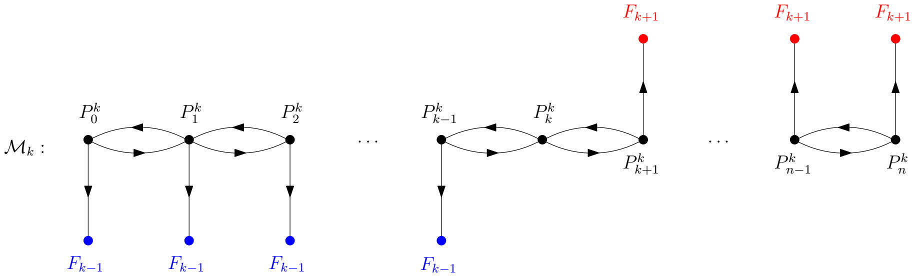

Strong selective amplifiers

Since we need to compute a lower bound of the fixation probability:

- whenever we arrive at state F_{k+1} or state F_{k-1},
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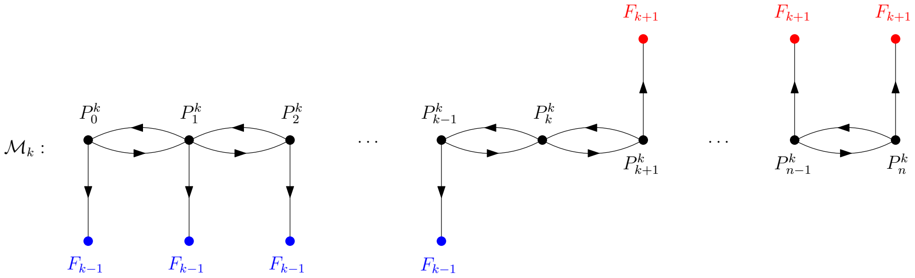
Therefore:

- $F_{k-1} = P_0^{k-1}$ (no infected clique noses)



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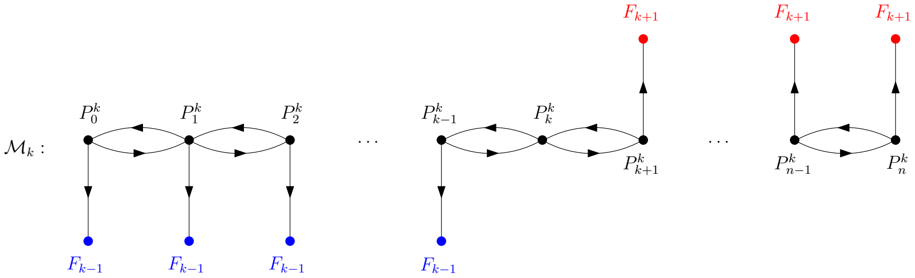

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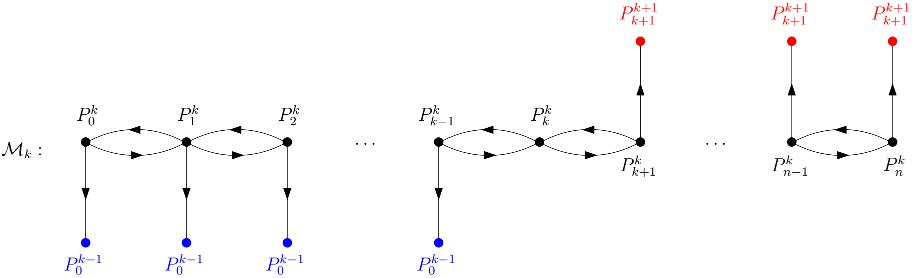

To analyze the Markov chains $\mathcal{M}_k$, $k = 1, 2, \ldots, n-1$:

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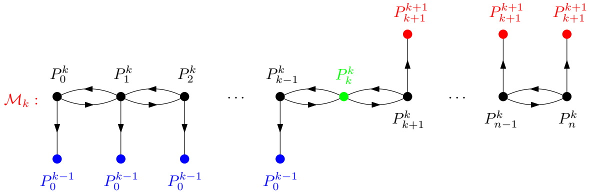

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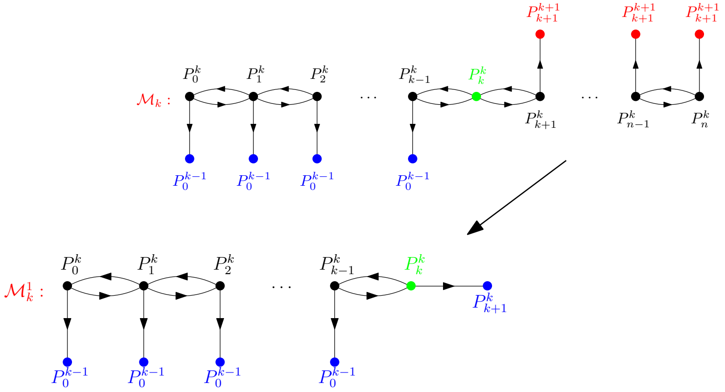

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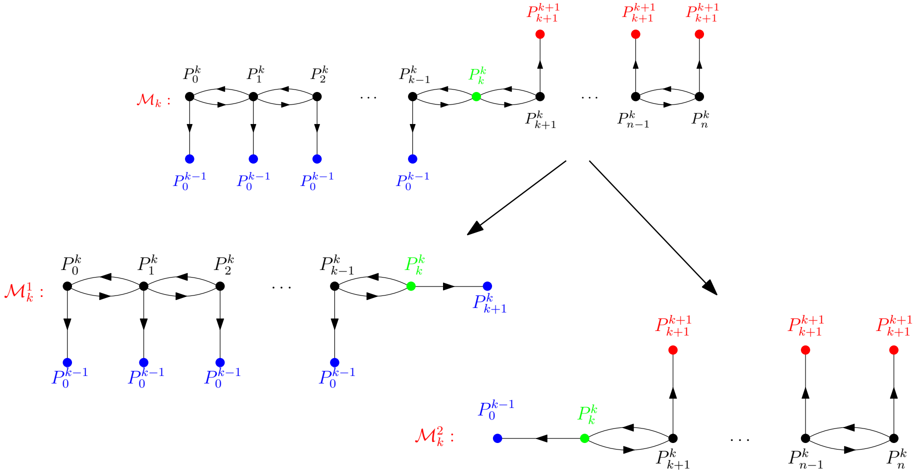
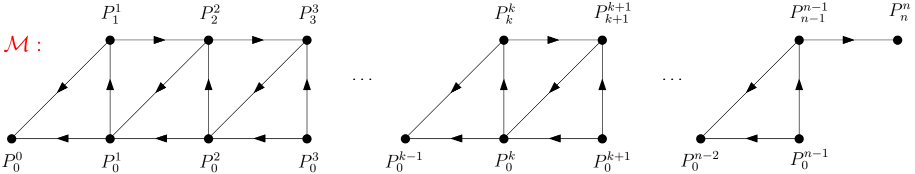


Strong selective amplifiers

Using this decomposition of the chain $\mathcal{M}$ into the chains $\{\mathcal{M}_k^1, \mathcal{M}_k^2\}_{k=1}^{n-1}$:



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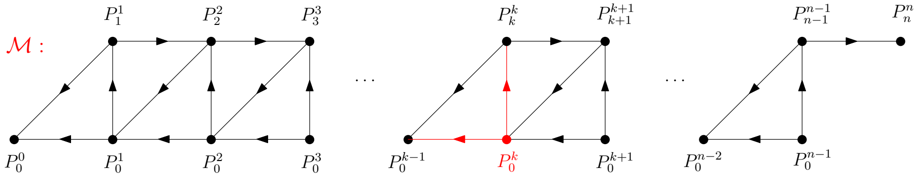

transitions from P_0^k: through the Markov chain $\mathcal{M}_1$

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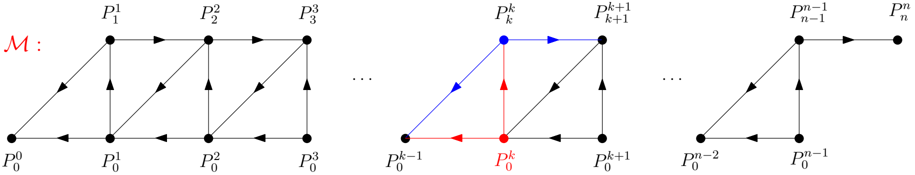

transitions from P_0^k: through the Markov chain $\mathcal{M}_1$

transitions from P_k^k: through the Markov chain $\mathcal{M}_2$

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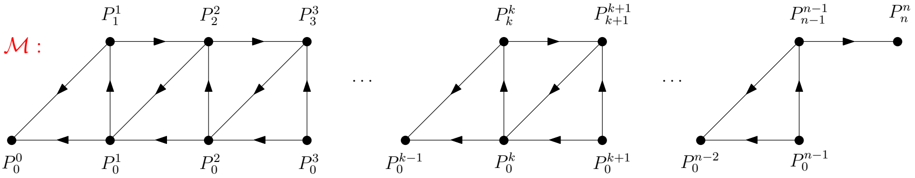
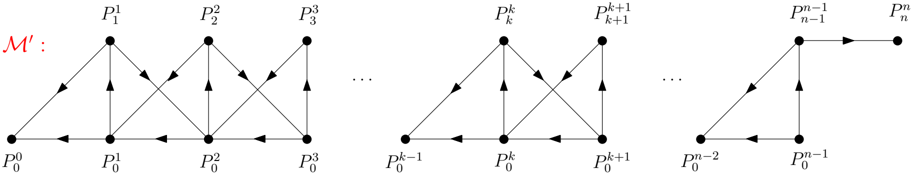


Relax $\mathcal{M}$ further: the infected vertices at P_0^k are a subset of those at P_k^k



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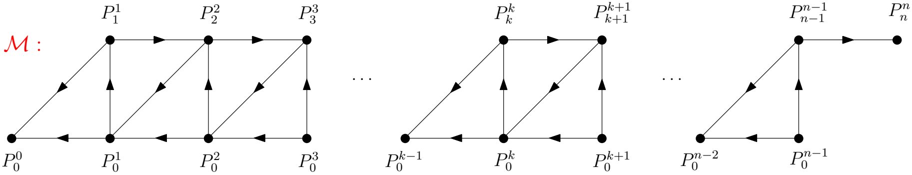

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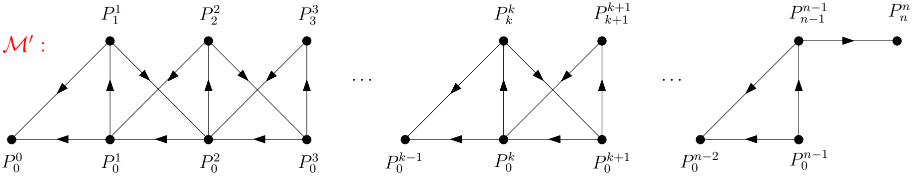

Eliminate from $\mathcal{M}'$ the states P_k^k $\Rightarrow$ a birth-death process $\mathcal{B}$

Strong selective amplifiers

In the birth-death process $\mathcal{B}$:

- we can compute a lower bound for the probability that, starting at P_0^1, we arrive at P_n^n before arriving at P_0^0

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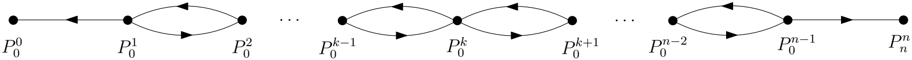

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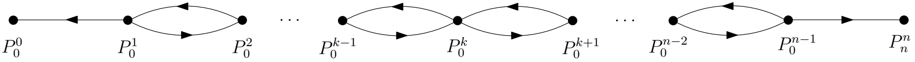

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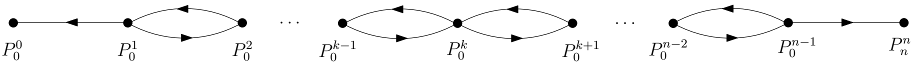

Using these decompositions, we prove that:

Theorem

For every $r > 5$, the fixation probability of a nose v of G_n is $f_r(v) \geq 1 - \frac{c(r)}{n}$, where $c(r)$ is a function depending only on r.

$\Rightarrow$ urchin graphs are $(\frac{n}{2}, n)$-amplifiers

The Thermal Theorem

Theorem (Thermal Theorem)

Let $G = (V, E)$ *be a connected undirected graph and* $r > 1$.
Then $f_r(v) \geq \frac{r-1}{r+\frac{\deg v}{\deg_{\min}}}$ *for every* $v \in V$.

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- modify $\mathcal{M}_0$ into the chain $\mathcal{M}_0^*$
- for every $i = 1, 2, \ldots, n-1$: relax $\mathcal{M}_{i-1}^*$ into the chain $\mathcal{M}_i^*$
- $\mathcal{M}_{n-1}^*$ provides the desired lower bound

The Thermal Theorem

For every vertex subset $S \subseteq V$:

- the fixation probability $f_r(S)$ of S is computed by:

$$f_r(S) = \frac{\sum_{xy \in E,\ x \in S,\ y \notin S} \left(r \frac{1}{\deg x} f_r(S+y) + \frac{1}{\deg y} f_r(S-x) \right)}{\sum_{xy \in E,\ x \in S,\ y \notin S} \left(\frac{r}{\deg x} + \frac{1}{\deg y} \right)}$$

where $f_r(\emptyset) = 0$ and $f_r(V) = 1$ (boundary conditions)

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For every such edge $xy \in E$ (where $x \in S$ and $y \notin S$):

- x "infects" y with probability proportional to $\frac{1}{\deg x}$
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$\Rightarrow$ for every vertex $v \in V$:

- we define $\frac{1}{\deg v}$ as the temperature of v
- a "hot" vertex affects more often its neighbors than a "cold" vertex

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Furthermore:

- for every set $S \notin \{\emptyset, V\}$ there exists a vertex $x(S) \in S$ and a vertex $y(S) \notin S$ such that $x(S)y(S) \in E$ and:

$$f_r(S) \geq \frac{\left(r \frac{1}{\deg x(S)} f_r(S + y(S)) + \frac{1}{\deg y(S)} f_r(S - x(S)) \right)}{\left(\frac{r}{\deg x(S)} + \frac{1}{\deg y(S)} \right)}$$

The Thermal Theorem

Therefore:

- by replacing all "$\geq$" with "$=$", we obtain a lower bound for all $f_r(S)$

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Definition (the linear system L_0)

Let $G = (V, E)$ be a graph and $r > 1$. Every vertex $v \in V$ has a weight (temperature) $d_v > 0$. The linear system L_0 on the variables $p_r(S)$, where $\emptyset \subset S \subset V$, is:

$$p_r(S) = \frac{r \cdot d_{x(S)} \cdot p_r(S + y(S)) + d_{y(S)} \cdot p_r(S - x(S))}{r \cdot d_{x(S)} + d_{y(S)}}$$

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The system L_0 defines naturally the Markov chain $\mathcal{M}_0$:

- one state for every vertex subset $S \subseteq V$
- states $\emptyset$ and V are absorbing
- every non-absorbing state S has exactly two transitions to the states $S + y(S)$ and $S - x(S)$, with transition probabilities $q_S = \frac{rd_{x(S)}}{rd_{x(S)} + d_{y(S)}}$ and $1 - q_S$, respectively

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Observation

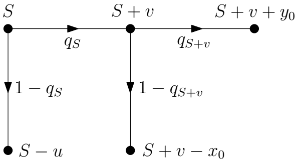
By setting $d_v = \frac{1}{\deg v}$ *for every* $v \in V$, *it follows that* $f_r(S) \geq p_r(S)$ *for every set* $S \subseteq V$.

The Thermal Theorem

We construct now the chain $\mathcal{M}_0^*$ from the chain $\mathcal{M}_0$ as follows:

- for every set S in $\mathcal{M}_0$:

in $\mathcal{M}_0$:



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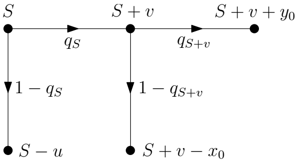

- we add a new dummy state X_S:

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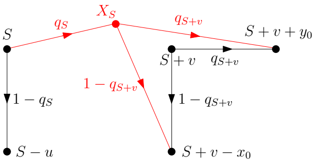

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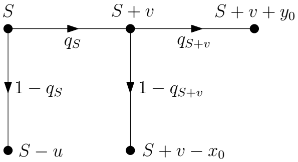

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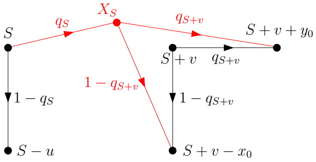
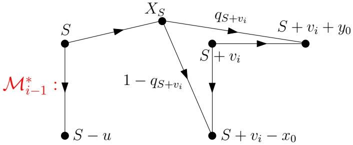


$\Rightarrow$ All values of $p_r(S)$ in $\mathcal{M}_0^*$ remain the same as in $\mathcal{M}_0$

- Consider an arbitrary numbering $v_0, v_1, \ldots, v_{n-1}$ of the vertices of G
- For every $i = 1, 2, \ldots, n-1$, construct from $\mathcal{M}^*_{i-1}$ the chain $\mathcal{M}^*_i$ as follows:
  1. for all sets $S \subset V$ with $y(S) = v_i$, change the transitions from X_S:



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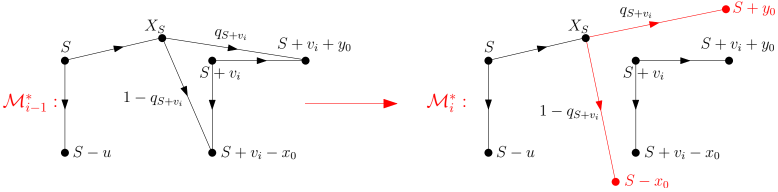

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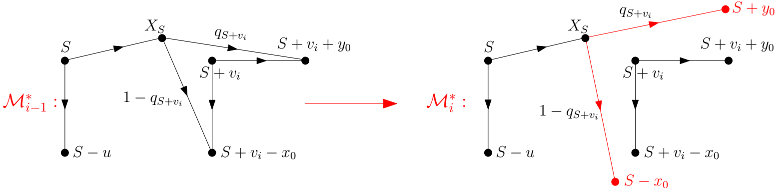

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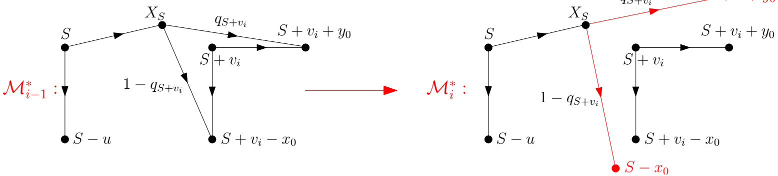

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$\Rightarrow$ the values of $p_r(S)$ do not decrease in $\mathcal{M}^*_i$

Lemma

For all these states S, the forward probability of S in $\mathcal{M}^*_i$ is a monotone decreasing function of the temperature d_{v_i} of v_i.

The Thermal Theorem

- We increase the temperature d_{v_i} in $\mathcal{M}_i^*$ to $d_{\max}$

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At the end, in the chain $\mathcal{M}_{n-1}^*$:

- $d_{v_1} = d_{v_2} = \ldots = d_{v_{n-1}} = d_{\max} = \frac{1}{\deg_{\min}}$
- $d_{v_0} = \frac{1}{\deg_{v_0}}$
- for every set S, the values of $p_r(S)$ are not larger than in $\mathcal{M}_0^*$

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- for every set S, the values of $p_r(S)$ are not larger than in $\mathcal{M}_0^*$
- We use techniques similar to the Isothermal Theorem in [Lieberman et al., *Nature*, 2005] to prove that:

$$f_r(v_0) \geq \frac{(r-1)}{r + \frac{d_{\max}}{d_{v_0}}} = \frac{(r-1)}{r + \frac{\deg v_0}{\deg_{\min}}}$$

- v_0 is chosen arbitrarily $\Rightarrow$ the Thermal Theorem

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- We refined the notion of fixation probability to specific vertices v
- We proved:
    - there exist no strong universal amplifiers
    - there exist strong selective amplifiers
    - there exist "quite" strong selective suppressors
    - the Thermal Theorem (lower bound)

Summary and open problems

- Do there exist stronger suppressors / amplifiers of selection?
  - the fixation probability of the strongest known amplifiers of natural selection is $1 - \frac{1}{r^2}$ ("star")
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- More types of mutants (many colors)?

Thank you for your attention!