Counting Fixed Points and Pure 2-Cycles of Tree Cellular Automata

Volker Turau

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Introduction

Discrete Synchronous Dynamical Systems (DSDS)

- Let G be a finite graph, each node has a state from a finite domain
- In discrete-time rounds, all nodes concurrently update their state based on local rule
  - Node's state in round t is determined by states of neighboring nodes in round $t-1$
- Facts
  - After a finitely many rounds a DSDS either reaches a fixed point or enters a 2-cycle
  - Finding number of fixed points of a DSDS is in general #P-complete, i.e. problems defined as counting number of accepting paths of polynomial-time non-deterministic Turing machine

Challenges

- For a given DSDS count number of
  - fixed points
  - 2-cycles
  - gardens of Eden configurations
- Give lower and upper bounds for these numbers

Known Facts

- Exact enumeration of fixed points and other types of configurations is computational hard in general
- This holds even in some severely restricted cases with respect to both network topology and update rules [*Tošić* 2010]
    - monotone update rules
    - each node has at most three neighbors
    - 2-state model

Contributions

- Model of this work
  - State of a node: 0 or 1 (called colors)
  - Local rules: Majority and minority rule
  - Finite trees
- Main contributions
  - Algorithm to determine number of fixed points of a tree T in time $O(n\Delta)$
  - Upper and lower bounds based on
    - diameter $D(T)$
    - maximal degree $\Delta(T)$

Motivation

- Boolean networks (BN) model dynamics of gene regulatory networks
- BNs are special type of DSDS for majority rule
- Number of fixed points is a measure for general memory storage capacity of BN
- BNs can solve SAT problems
- BN fixed points correspond to SAT solutions

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Definitions

Definitions

Discrete Synchronous Dynamical System (DSDS)

Let $G(V, E)$ be a finite graph and $\mathcal{C}(G)$ the set of all mappings $c : V \longrightarrow \{0, 1\}$. A **DSDS** is a mapping

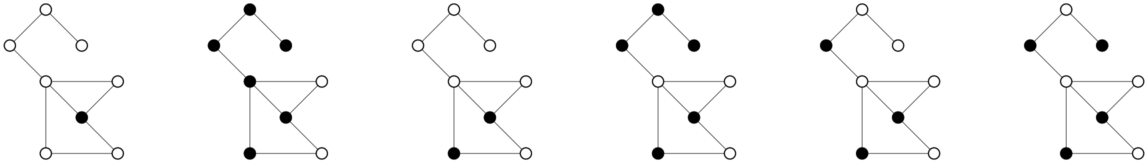
$$\mathcal{M} : \mathcal{C}(G) \longrightarrow \mathcal{C}(G)$$

For each $c \in \mathcal{C}(G)$, $\mathcal{M}$ yields a series of colorings $c, \mathcal{M}(c), \mathcal{M}(\mathcal{M}(c)), \ldots$.

Minority Process

Minority process: Each node assumes color of minority of its neighbors.

Example of Minority Process



Definitions

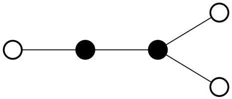
Fixed Points and 2-Cycles

$c \in \mathcal{C}(G)$ is called

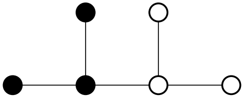
- **fixed point** if $\mathcal{M}(c) = c$
- **2-cycle** if $\mathcal{M}(c) \neq c$ and $\mathcal{M}(\mathcal{M}(c)) = c$

A 2-cycle c is called **pure** if it is $\mathcal{M}(c)(v) \neq c(v)$ for each node v of G

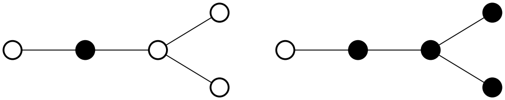
Examples



A fixed point



A pure 2-cycle



A non-pure 2-cycle

Classes

Classes

- $\mathcal{F}_{\mathcal{M}}(G)$: All $c \in \mathcal{C}(G)$ that constitute a fixed point
- $\mathcal{P}_{\mathcal{M}}(G)$: All $c \in \mathcal{C}(G)$ that constitute a pure 2-cycle

- Classes are closed with respect to complements
- Let $\mathcal{F}_{\mathcal{M}}(G)^+$ (resp. $\mathcal{P}_{\mathcal{M}}(G)^+$) be the subset of $\mathcal{F}_{\mathcal{M}}(G)$ (resp. $\mathcal{P}_{\mathcal{M}}(G)$) which a globally distinguished node v^* has state 0

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Fixed Points of Trees

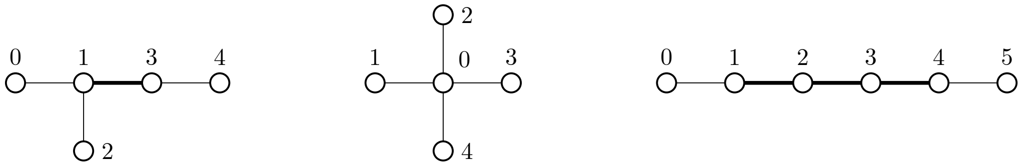
Characterizing Fixed Points

- Let $T = (V, E)$ be a tree
- $F \subseteq E$ is called $\mathcal{F}$-*legal* if $2deg_F(v) \leq deg(v)$ for each $v \in V$
- Let $E_{fix}(T)$ be the set of all $\mathcal{F}$-*legal* subsets of $E(T)$

Theorem (Turau 2022)

$|E_{fix}(T)| = |\mathcal{F}_{\mathcal{M}}(T)^+|$

$\mathcal{F}$-legal Subsets



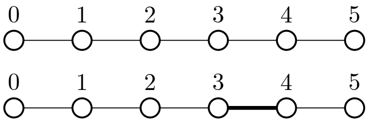
- $E_{fix}(T_1) = \{\emptyset, \{(1,3)\}\}$
- $E_{fix}(T_2) = \{\emptyset\}$
- $E_{fix}(T_3) = \{\emptyset, \{(1,2)\}, \{(2,3)\}, \{(3,4)\}, \{(1,2),(3,4)\}\}$

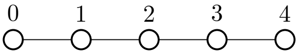
Counting Fixed Points of Paths

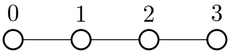
Corollary

Let P_n be a path with n nodes, then $|E_{fix}(P_n)| = \mathbb{F}_{n-1}$.

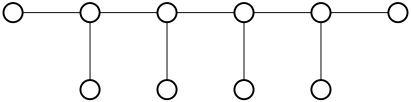
Proof by induction:

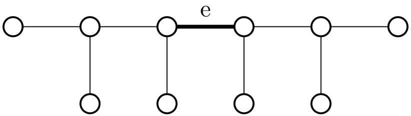


without edge $(3,4)$: 

with edge $(3,4)$: 

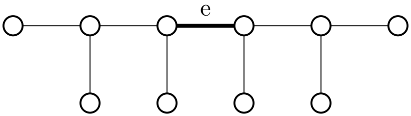
Decomposing $\mathcal{F}$-legal Subsets



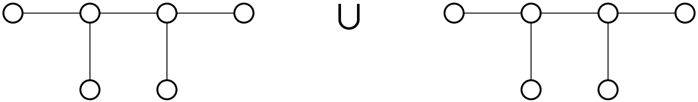


Two categories of $\mathcal{F}$-legal subsets: Without and with e

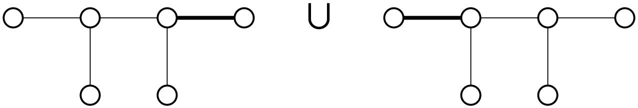
Decomposing $\mathcal{F}$-legal Subsets



Without edge *e*:



With edge *e*:



Recursively Counting Fixed Points of Trees

- For $e = (v_1, v_2) \in E$ with $deg(v_i) > 1$ let T_i be the subtree of T consisting of e and the connected component of $T \setminus e$ that contains v_i
- For $v \in V$ define $E_{fix}(T, v) = \{F \in E_{fix}(T) \mid 2deg_F(v) \leq deg(v) - 2\}$

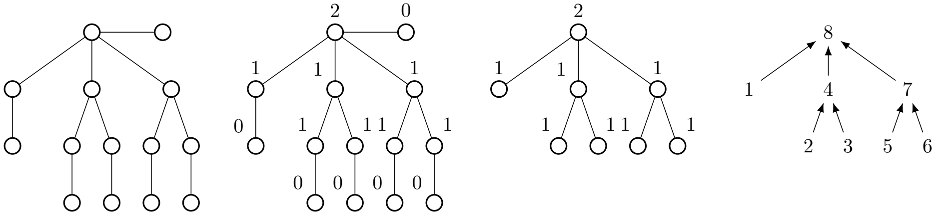
Lemma

Let $T = (V, E)$ be a tree, $e = (v_1, v_2) \in E$ with $deg(v_i) > 1$. Then

$$|E_{fix}(T)| = |E_{fix}(T_1, v_1)||E_{fix}(T_2, v_2)| + |E_{fix}(T_1)||E_{fix}(T_2)|$$

Recursively Counting Fixed Points of Trees

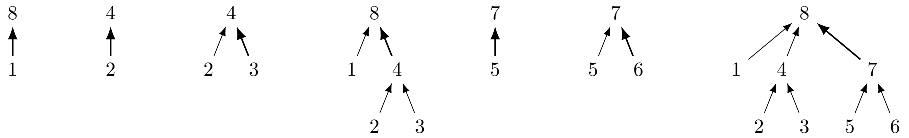
- How to compute $|E_{fix}(T_1, v_1)|$? Generalize notion of $\mathcal{F}$-legal subsets



- Select a node of T_R as a root and assign numbers $1, \ldots, t$ to nodes in T_R using a postorder depth-first search

Recursively Counting Fixed Points of Trees

- For $k = 1, \ldots, t-1$ denote by T_k the subtree of T_R consisting of k's parent together with all nodes connected to k's parent by paths using only nodes with numbers at most k
- Apply last lemma successively to all T_k



Theorem

The number of fixed points of a tree with n nodes and maximal node degree Δ can be computed in time $O(n\Delta)$.

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Upper Bounds

Bounds depending on Δ

Theorem

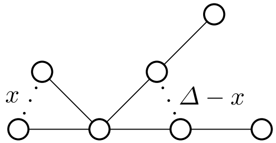
$|E_{fix}(T)| \leq 2^{n-\Delta-1}$.

Proof.

- Let $E^2(T)$ be the edges of T, where each end node has degree at least 2
- $|E_{fix}(T)| \leq 2^{|E^2(T)|}$, since $E_{fix}(T) \subseteq \mathcal{P}(E^2(T))$, the power set of $E^2(T)$
- Let l be the number of leaves of T, then $l = 2 + \sum_{j=3}^{\Delta}(j-2)\Delta_j$
- $|E^2(T)| = n - 1 - l = n - 3 - \sum_{j=3}^{\Delta}(j-2)D_j \leq n - 3 - (\Delta - 2) = n - \Delta - 1$ □

Bounds depending on Δ

- The bound is sharp for $\Delta \geq n - \lceil n/3 \rceil$



- For $x = 2\Delta - n + 1$ we have $\Delta - x \leq x$

$$E_{fix}(T_m) = \sum_{i=0}^{\Delta - x} \binom{\Delta - x}{i} = 2^{\Delta - x} = 2^{n-\Delta-1}$$

A Special Case

Lemma

Let T be a tree with a single node v that has degree larger than 2. Let $\mathcal{D}$ be the multi-set with the distances of all leaves to v. Then

$$|E_{fix}(T)| = \sum_{S \subset \mathcal{D}, |S| \leq \Delta/2} \prod_{s \in S} \mathbb{F}_s \prod_{s \in \mathcal{D} \setminus S} \mathbb{F}_{s-1}.$$

Sketch of Proof.

- Let $\mathcal{P}$ be the set of all Δ paths from v to a leaf of T
- For $P \in \mathcal{P}$ let $\hat{P}$ be an extension of P by one node. Let $\mathcal{P}_1 \subset \mathcal{P}$ with $|\mathcal{P}_1| \leq \Delta/2$
- Let $P_1 \in \mathcal{P}_1$ and $P_2 \in \mathcal{P} \setminus \mathcal{P}_1$. If $\hat{F}_{P_1} \in E_{fix}(\hat{P}_1)$ and $F_{P_2} \in E_{fix}(P_2)$ then $\hat{F}_{P_1} \cup F_{P_2} \in E_{fix}(T)$ and vice versa

□

A Special Case

Lemma

Let T be a 2-generalized star graph. Then $|E_{fix}(T)| \leq \mathbb{F}_{n-\lceil \Delta/2 \rceil}$.

Proof.

We use the lemma. If $\Delta \equiv 0(2)$ then

$$|E_{fix}(T)| = \sum_{i=0}^{\lfloor \Delta/2 \rfloor} \binom{\Delta}{i} = \frac{1}{2}\left(2^{\Delta} + \binom{\Delta}{\Delta/2}\right) \leq \mathbb{F}_{3\Delta/2+1} = \mathbb{F}_{n-\Delta/2},$$

otherwise $|E_{fix}(T)| = 2^{\Delta-1} \leq \mathbb{F}_{n-\lceil \Delta/2 \rceil}$. □

General Case

Theorem

$|E_{fix}(T)| \leq \mathbb{F}_{n-\lceil \Delta/2 \rceil}$ *for a tree T with n nodes.*

Sketch of Proof.

- Induction on n
- There exists edge (v, w) where v is a leaf and all neighbors of w but one are leaves
- If $deg(w) > 2$ then there exists a neighbor $u \neq v$ of w that is a leaf. Let $T_u = T \setminus u$.
- Then $|E_{fix}(T)| = |E_{fix}(T_u)|$ and since $\Delta(T_u) \geq \Delta(T) - 1$ we have by induction

$$|E_{fix}(T)| = |E_{fix}(T_u)| \leq \mathbb{F}_{n-1-\lceil \Delta(T_u)/2 \rceil} \leq \mathbb{F}_{n-\lceil \Delta(T)/2 \rceil}$$

Hence, we assume $deg(w) = 2$

General Case

Proof contd.

- Let $u \neq v$ be 2^{nd} neighbor of w. Denote by T_v (resp. T_w) the tree $T \setminus v$ (resp. $T \setminus \{v, w\}$)
- Then $|E_{fix}(T)| \leq |E_{fix}(T_v)| + |E_{fix}(T_w)|$
- If there exists a node different from u with degree Δ then by induction

$$|E_{fix}(T)| \leq \mathbb{F}_{n-1-\lceil \Delta/2 \rceil} + \mathbb{F}_{n-2-\lceil \Delta/2 \rceil} = \mathbb{F}_{n-\lceil \Delta/2 \rceil}$$

- Assume that u is the only node with degree Δ. Repeating above argument shows that T is 2-generalized star graph
- Hence, $|E_{fix}(T)| \leq \mathbb{F}_{n-\lceil \Delta/2 \rceil}$ by above Lemma

□

Conjecture

- Let $\tau_{n,\Delta} := \max\{|E_{fix}(T)| \mid T \text{ is a tree with } n \text{ nodes and maximal degree } \Delta\}$

Conjecture 1

$\tau_{n,\Delta} = \tau_{n-1,\Delta} + \tau_{n-2,\Delta}$ for $\Delta < (n-1)/2$.

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Lower Bounds

Theorem

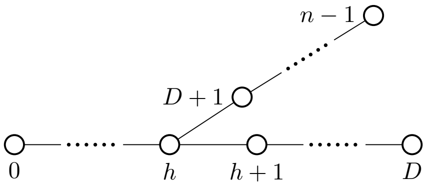
Let T be a tree. If the tree obtained from T by removing all leaves has r inner nodes, then

$$|E_{fix}(T)| \geq 2^{r/2}.$$

If T has diameter D, then

$$|E_{fix}(T)| \geq \mathbb{F}_D.$$

There are trees for which $|E_{fix}(T)|$ is much larger than $\mathbb{F}_D$

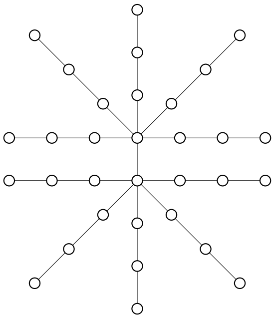


$$|E_{fix}(T)| = \mathbb{F}_D \mathbb{F}_{n-D-1} + \mathbb{F}_h \mathbb{F}_{D-h} \mathbb{F}_{n-D-2}$$

Conjecture

Conjecture 2

Except for a finite number of cases for each combination of n and D there exists a star-like graph that maximizes the number of fixed points



A tree with 32 nodes and diameter 7 with 181376 fixed points. All other trees with 32 nodes and diameter 7 have less fixed points.

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Pure 2-Cycles

Characterizing Pure 2-Cycles

- Let $T = (V, E)$ be a tree
- $F \subseteq E$ is called $\mathcal{P}$-*legal* if $2deg_F(v) < deg(v)$ for each $v \in V$
- Let $E_{pure}(T)$ be the set of all $\mathcal{P}$-*legal* subsets of $E(T)$

Theorem (Turau 2022)

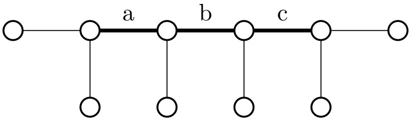
$|E_{pure}(T)| = |\mathcal{P}_{\mathcal{M}}(T)^+|$

Since $E_{pure}(T) \subseteq E_{fix}(T)$ we have $|\mathcal{P}_{\mathcal{M}}(T)| \leq |\mathcal{F}_{\mathcal{M}}(T)| \leq 2\mathbb{F}_{n-\lceil \Delta/2 \rceil}$

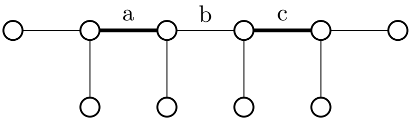
Theorem

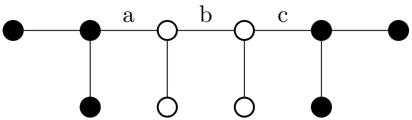
The number of pure 2-cycles of a tree with n nodes and maximal node degree Δ can be computed in time $O(n\Delta)$.

Example



- $E_{pure}(T_2) = \{\emptyset, \{a\}, \{b\}, \{c\}, \{a, c\}\}$
- Pure 2-cycle for $F = \{a, c\}$





Counting Pure 2-cycles of Trees

Theorem

A tree with maximal degree Δ *has at most* $\min\left(2^{n-\Delta}, 2\mathbb{F}_{\lfloor n/2 \rfloor}\right)$ *pure 2-cycles.*

Theorem

Let T a tree with n nodes, diameter D, and maximal degree Δ*.*

1. *If* $2D \geq n$ *then* $|E_{pure}(T)| \leq \mathbb{F}_{n-D}$
2. *If* $n < 2\Delta + 1$ *then* $|E_{pure}(T)| \leq 2^{\lfloor \frac{n-\Delta-1}{2} \rfloor}$

These bound are sharp.

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Conclusion

Conclusion & Outlook

- Contributions
  - Counting fixed points for general cellular automata is #P-complete
  - For tree cellular automata based on minority/majority rule problem solvable in time $O(\Delta n)$
  - Upper and lower bounds for number of fixed points and pure 2-cycles
- Open problems
  - Other classes of graphs for which problem solvable in polynomial time
  - Counting configurations with no predecessor (garden of Eden)

Counting Fixed Points and Pure 2-Cycles of Tree Cellular Automata

LATIN

Volker Turau
Professor

Phone +49 / (0)40 428 78 3530
e-Mail turau@tuhh.de

http://www.ti5.tu-harburg.de/staff/turau