Reachability problems for Markov chains

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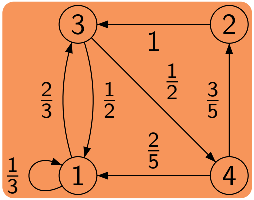
Markov chains: a basic model for probabilistic systems



M

$$\begin{pmatrix} \frac{1}{3} & 0 & \frac{2}{3} & 0 \\ 0 & 0 & 1 & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ \frac{2}{5} & \frac{3}{5} & 0 & 0 \end{pmatrix}$$

- transition system/automaton with probabilities
- stochastic transition matrix, linear algebraic properties
- distribution over states, transformer of distributions

Markov chains

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In other words,

- given a row-stochastic matrix M, $r \in \mathbb{Q}$, does there exist $n \in \mathbb{N}$, s.t., $M^n[i, j] = r$?
- That is, can you give a procedure/algorithm to check if such an n exists (Decision problem)?

Some basic UG probability theory

- If the Markov chain is irreducible and aperiodic, then from any initial state/distribution, the Markov chain will tend to a unique stationary distribution.
- In general, break into BSCCs (Bottom strongly connected components) and analyze the probabilities in the limit.

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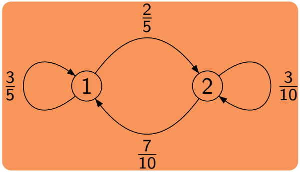

Fixpoint$= (\frac{7}{11}, \frac{4}{11})$

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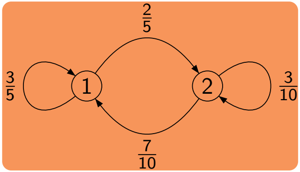

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Hard part: Is the limit point attained in finite time?!

Outline

Our goal

- To understand the source of this difficulty.
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1. Why it is important : applications to probabilistic verification
2. Another seemingly easy but hard problem: The Skolem problem
3. Links between reachability for Markov chains and Skolem problem.
4. Other related problems and applications

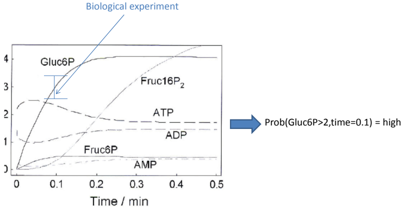
Application to verification in biopathways

Consider a Markov chain M over states $s_1, \ldots, s_t$.

Question

Starting from a given initial probability distribution $\vec{v}$, is it the case that eventually the probability of staying in state s_t will be within $[0, 1/2]$?

For e.g., states could be protein concentrations, and the Markov chain a model of biochemical reactions and we want to check for high conc.



Application to verification and related problems

Example: Consider $\vec{v} = (1/4, 1/4, 1/2)$ and

$$M = \begin{pmatrix} 0.6 & 0.1 & 0.3 \\ 0.3 & 0.6 & 0.1 \\ 0.1 & 0.3 & 0.6 \end{pmatrix}$$

- Then, does $\exists N$ s.t., for all $n > N, \vec{v} \cdot M^n \cdot (1\ 0\ 0) > 1/3$?
- Then, does $\exists n$ s.t., $\vec{v} \cdot M^n \cdot (1\ 0\ -1) = 0$?

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Theorem

All these problems are (sort of) inter-reducible:

- Reachability problem for Markov chains.
- Given stochastic vector $\vec{v}$, vector w, row-stochastic matrix M, does $\exists n$ s.t., $\vec{v} \cdot M^n \vec{w} = 1/2$
- Given stochastic vectors $\vec{v}, \vec{w}$, row-stochastic matrix M, rational r, does $\exists n$ s.t., $\vec{v} \cdot M^n \vec{w} = r$

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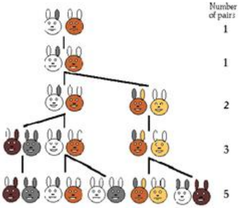
The Fibonacci Sequence



- Fibonacci sequence: $1, 1, 2, 3, 5, 8, 13, 21, \ldots$
- Fibonacci sequence: $u_n = u_{n-1} + u_{n-2}$ where $u_1 = u_0 = 1$

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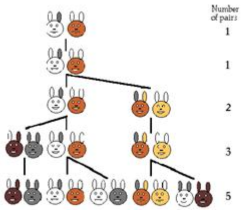

- Fibonacci sequence: $1, 1, 2, 3, 5, 8, 13, 21, \ldots$
- Fibonacci sequence: $u_n = u_{n-1} + u_{n-2}$ where $u_1 = u_0 = 1$
- But rabbits die! So, $u_n = u_{n-1} + u_{n-2} - u_{n-3}$ where $u_2 = 2, u_1 = u_0 = 1$ Question: Can they ever die out?

Linear Recurrence Sequences (LRS)

Definition

A sequence $\langle u_0, u_1, \ldots \rangle$ of numbers is called an LRS if there exists $k \in \mathbb{N}$ and constants $a_0, \ldots, a_{k-1}$ s.t., for all $n \geq k$,

$$u_n = a_{k-1} u_{n-1} + \ldots + a_1 u_{n-k+1} + a_0 u_{n-k}$$

- k is called the order/depth of the sequence.
- The first k elements $u_0, \ldots, u_{k-1}$ are called initial conditions and they determine the whole sequence.
- We can define the sequences and constants to be over integers or rationals or reals.

The Skolem Problem

Skolem 1934: Also called the Skolem Pisot problem

Given a linear recurrence sequence (with initial conditions) over integers, does it have a zero? Does $\exists n$ such that $u_n = 0$?

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Variant: (Ultimate) Positivity Problem

Given an LRS $\langle u_1, u_2, \ldots \rangle$, $\forall n$, $(n \geq T)$ is $u_n \geq 0$?

Equivalent formulations of the Skolem Problem

Linear recurrence sequence form

Given an LRS $\langle u_1, u_2, \ldots \rangle$ (with initial conditions), does $\exists n$ s.t., $u_n = 0$?

Matrix Form

Given a $k \times k$ matrix M, does $\exists n$ s.t., $M^n(1, k) = 0$?

Dot Product Form

Given a $k \times k$ matrix M, k-dim vectors $\vec{v}, \vec{w}$, does $\exists n$ s.t., $\vec{v} \cdot M^n \cdot \vec{w}^T = 0$?

Results on Skolem/Positivity problems

- Skolem-Mahler-Lech Theorem (1934, 1935, 1953)

Theorem

The set of zeros of any LRS is the union of a finite set and a finite number of arithmetic progressions (periodic sets). Further, it is decidable to check whether or not the set of zeros is infinite!

In other words, the hardness is in characterizing the finite set. All known proofs use p-adic numbers.

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  - Several of these proofs use results on linear logarithms by Baker and van der Poorten.
  - This theory fetched Baker the Field's medal in 1970!

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- Recently Ouaknine, Worrell from Oxford have published several new results - SODA'14, ICALP'14 (best paper).
  1. positivity for LRS of order ≤ 5 is decidable with complexity $coNP^{PP^{PP^{PP}}}$.
  2. ultimate positivity for LRS of order 5 or less is decidable in P and decidable in general for "simple" LRS.
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The general problem is still open!

Links between Skolem and Markov reachability

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Recall:

Markov Reachability. *Given a finite stochastic matrix M with rational entries and a rational number r, does there exist $n \in \mathbb{N}$ such that $(M^n)_{1,2} = r$?*

Skolem Problem. *Given a $k \times k$ integer matrix M, does there exist n such that $(M^n)_{1,2} = 0$?*

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Theorem [A., Antonopoulos, Ouaknine, Worrell'14.]

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In particular, we show that the Skolem problem can be reduced to the reachability problem for Markov chains in polynomial time.

Links between Skolem and Markov reachability

Proof sketch

Take instance of Skolem, i.e., a $k \times k$ integer matrix M.

1. Remove negative entries in M.
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    - Then $(M)_{1,2} = \vec{e}^T P_1 \vec{v_1}$, where $\vec{e} = (1, 0, \ldots, 0)^T$ and $\vec{v_1} = (0, 0, 1, -1, 0, \ldots, 0)^T$ are $2k$-dimensional vectors.

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   - By induction, $(M^n)_{1,2} = \vec{e}^T P_1^n \vec{v_1}$.

     - the map sending $\begin{pmatrix} a & b \\ b & a \end{pmatrix}$ to $a - b$ is a homomorphism from the ring of 2×2 symmetric integer matrices to $\mathbb{Z}$

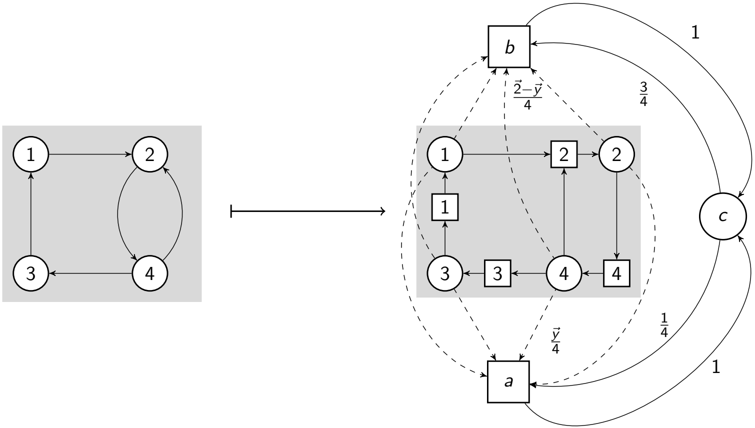
Proof Sketch contd.

Step 2: Re-scale entries to obtain stochastic matrix

- Pick biggest entry in P_1 and divide and then put the remaining mass in a new column. Also add all 1's vector to v_1 to get v_2 pause
- Thus, we have $(M^n)_{1,2} = 0$ iff $\vec{e}^T P_2^n \vec{v_2} = 1$, where P_2 is stochastic $2k+1$-dim matrix and $\vec{v_2}$ has only $0, 1, 2$ entries.

Final Step: Obtaining a co-ordinate vector

- Construct a new Markov chain with double the nodes $(+3)$.



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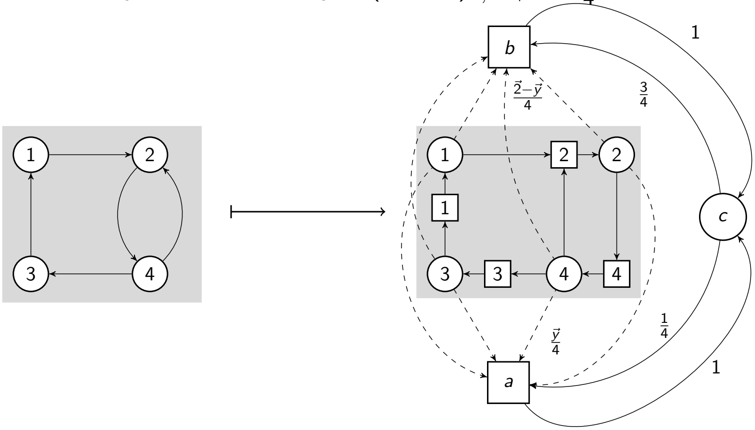
- $(\widetilde{Q}^{2n+1})_{1,2k+1} = \frac{1}{2^{n+2}}(2^n - 1 + \vec{e}^T Q^n \vec{y})$ and we conclude that $\vec{e}^T Q^n \vec{y} = 1$ if and only if $(\widetilde{Q}^{2n+1})_{1,2k+1} = \frac{1}{4}$. □



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- Many probabilistic logics have been defined over trajectories of a Markov chain.
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  - *iLTL* (Kwon, Agha, 2004)
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Corollary

Model checking (i.e., checking whether the system satisfies a property written in the logic) for all these logics is "Skolem-hard".

Other related problems - The Orbit Problem

The Orbit Problem

- Given a $k \times k$ matrix M, k-dim vectors $\vec{x}$ and $\vec{y}$, does $\exists n$ s.t., $\vec{x} \cdot M^n = \vec{y}$?
- Stochastic variant: Given a $k \times k$ stochastic matrix M and k-dim stochastic vectors $\vec{x}$ and $\vec{y}$, does $\exists n$ s.t., $\vec{x} \cdot M^n = \vec{y}$?

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Kannan, Lipton – STOC'80, JACM'86

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- Higher Order Orbit Problem: Given $k \times k$ matrix M, k-dim vector $\vec{x}$, a subspace V of dim $\leq k$, does $\exists n$ s.t., $\vec{x} \cdot M^n \in V$?

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- Skolem problem (does $\exists n$ s.t., $\vec{v} \cdot M^n \cdot \vec{w}^T = 0$?) is special case of the higher order Orbit Problem

Other related problems - The Orbit Problem

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The Orbit problem is decidable in Polynomial time.

Chonev,Ouaknine, Worrell– STOC'12

- High dim Orbit Problem for dim 2 or 3 is in NP^{RP}

Other related problems - Program Termination

Basic undecidability result – Turing 1936

Termination of a generic program with a loop is undecidable:

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But now, let us consider a much simpler case:

An initialized homogeneous linear program

$\vec{x} := \vec{b};\;\; \textbf{while } (\vec{c}^{\,T}\vec{x} > \vec{0}) \;\; \{\vec{x} := A\vec{x}\}$

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Termination problem for simple linear programs

Does an instance of the above program i.e., $\langle \vec{b}; \vec{c}; A \rangle$, terminate?

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Does an instance of the above program i.e., $\langle \vec{b}; \vec{c}; A \rangle$, terminate?

This problem is equivalent to the positivity problem!

Other related problems - Program Termination

Basic undecidability result – Turing 1936

Termination of a generic program with a loop is undecidable:

$$\textbf{while}\ (\mathit{conditions})\ \ \{\mathit{commands}\}$$

But now, let us consider a much simpler case:

An initialized homogeneous linear program

$\vec{x} := \vec{b};\ \ \textbf{while}\ (\vec{c}^T\vec{x} > \vec{0})\ \ \{\vec{x} := A\vec{x}\}$

Termination problem for simple linear programs

Does an instance of the above program i.e., $\langle \vec{b}; \vec{c}; A \rangle$, terminate?

This problem is equivalent to the positivity problem!
– Can rewrite as $\forall n \geq 0$, is $\vec{c}^T \cdot A^n \cdot \vec{b} > 0$?

Termination of Linear Programs

Thus, termination for initialized homogenous linear programs

$\vec{x} := \vec{b};$ **while** $(\vec{c}^T \vec{x} > \vec{0})$ $\{\vec{x} := A\vec{x}\}$ $=$ positivity

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A non-homogenous (initialized) linear program

$$\vec{x} := \vec{b}; \ \textbf{while} \ (B\vec{x} > \vec{e}) \ \{\vec{x} := A\vec{x} + \vec{d}\}$$

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By adding a new scalar variable z,

$\vec{x} := \vec{b}, z = 1;$ **while** $(B\vec{x} - \vec{e}z > 0)$ $\{\vec{x} := A\vec{x} + \vec{d}z; z = z\}$

Termination of Linear Programs

Thus, termination for initialized homogenous linear programs

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while $(B\vec{x} > 0)$ $\{\vec{x} := A\vec{x}\}$

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- Tiwari CAV'04 : termination is decidable (in P) over reals.
- Braverman CAV'06: decidable over rationals.

Conclusion

- Implication for probabilistic verification... several hardness results.
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Simple problems with hard solutions

- Interplay of Markov chain theory, algorithmic complexity theory, number theory...
- And many applications: probabilistic verification, program termination.

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