Reachability and Regularity problems for Markov chains

S Akshay

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Workshop on Mathematics and Information, IIT Bombay
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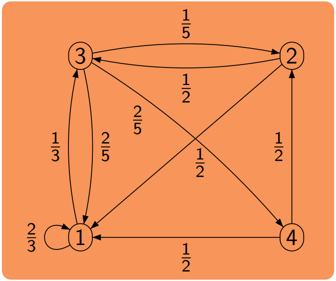
Markov chains: a basic model for probabilistic systems



- Transition system/automaton with probabilities

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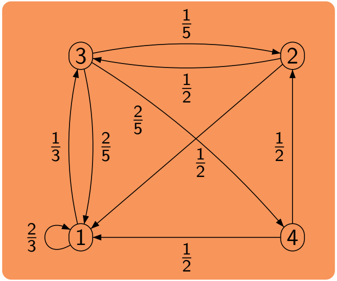

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- Stochastic transition matrix, linear algebraic properties

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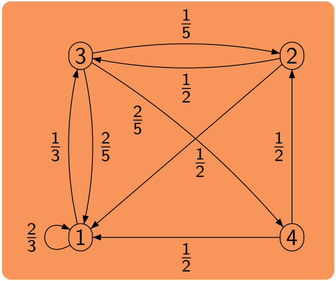

$$\left(\tfrac{1}{2}\ 0\ \tfrac{1}{2}\ 0\right) \times \begin{pmatrix} \frac{2}{3} & 0 & \frac{1}{3} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ \frac{2}{5} & \frac{1}{5} & 0 & \frac{2}{5} \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \end{pmatrix} = \left(\tfrac{8}{15}\ \tfrac{1}{10}\ \tfrac{1}{6}\ \tfrac{1}{5}\right)$$

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- Distribution over states, transformer of distributions

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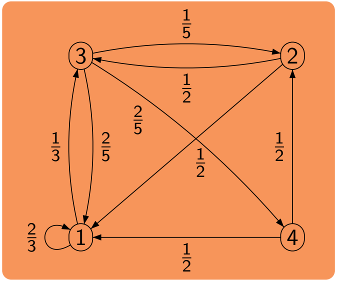

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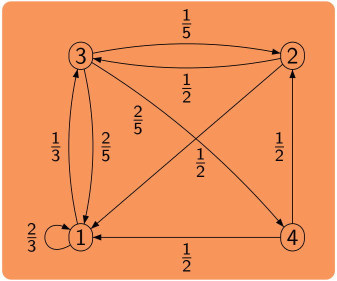

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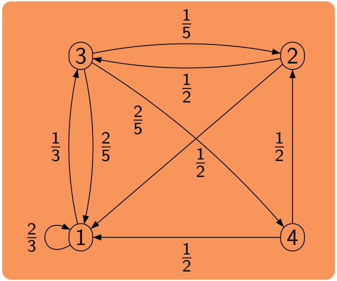

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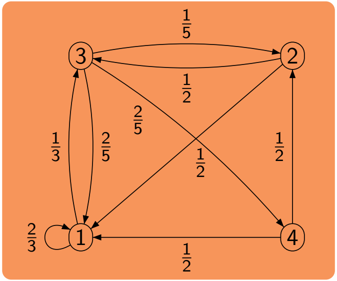

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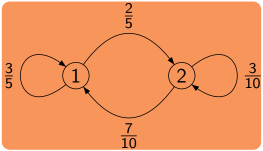

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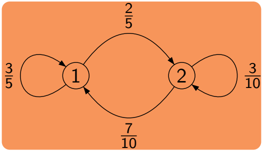

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In general,

We can break into BSCCs (bottom strongly connected components) and analyze probabilities in the limit.

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– Open!

Reachability (is a) problem in Markov chains

In other words,

- given a row-stochastic matrix M, i, j, $r \in \mathbb{Q}$, does there exist $n \in \mathbb{N}$, s.t., $M^n[i,j] = r$?
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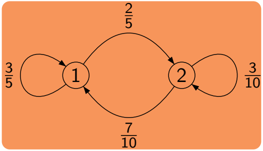

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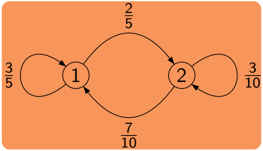

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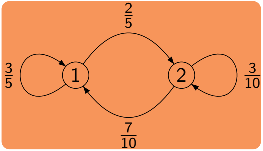

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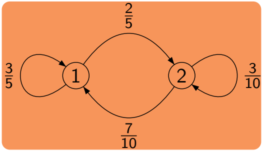

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Hard part: Is the limit point attained in finite time?! What is the behavior around the limit point at all finite times?

Some related problems

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

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

- Does $\exists n$, such that $M^n(1,1) = 1/3$?
- Also, $\forall n \in \mathbb{N}$, is $\vec{v} \cdot M^n \cdot (1\ 0\ 0) > 1/3$?
- Does $\exists n$ s.t., $\vec{v} \cdot M^n \cdot (1\ 0\ -1) = 0$?

Reasoning about trajectories of Markov chains

- A motivating example (adapted from [Maruthi et al,CMSB'14]): Variation in pop of yeast under stress as shown by a marker.
- A simplistic model as a 3-state Markov chain
  - States: conc of marked yeast in pop – high, med, low
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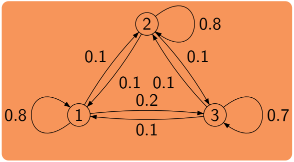

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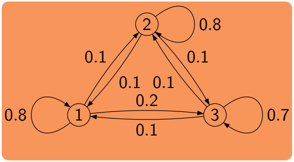

Reasoning about patterns

1. From a given initial distribution, does pop with high conc of marked yeast always stay above 5/12?

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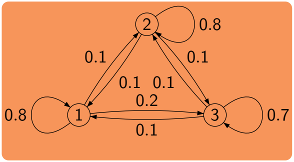

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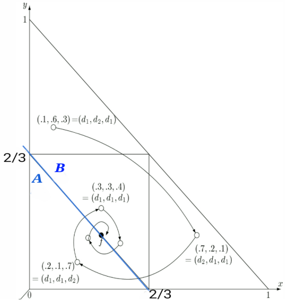
Symbolic dynamics: trajectories



A discretized semantics

- We partition distribution space & label using a finite alphabet.

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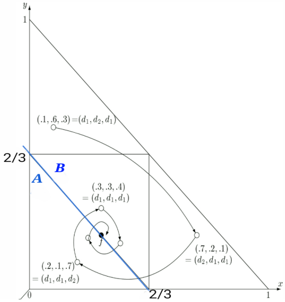

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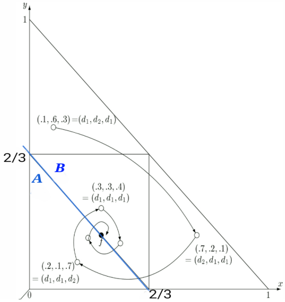

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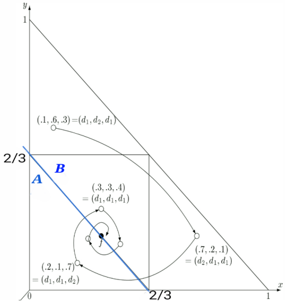

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  - Is the symbolic trajectory BAB^ω?

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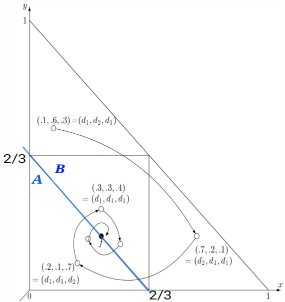

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- We partition distribution space & label using a finite alphabet.
- Thus, symbolic trajectories are words over this finite alphabet of discretized distribution space.

Symbolic dynamics: Trajectories to languages

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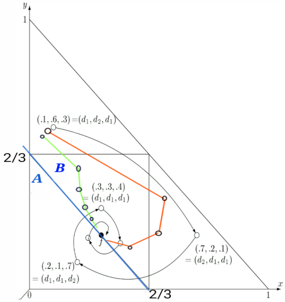

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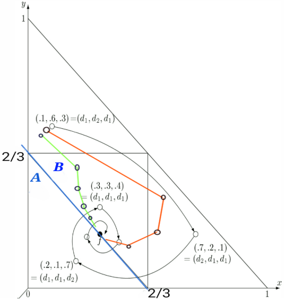

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From words to languages

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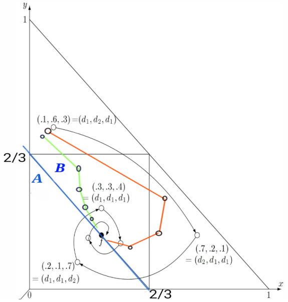

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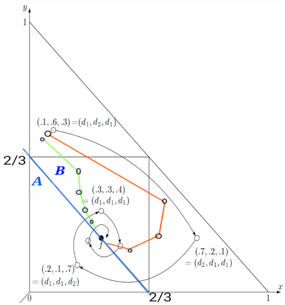

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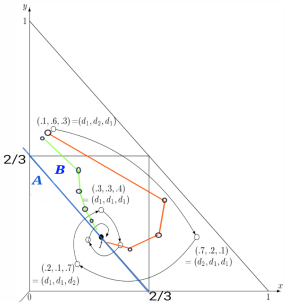

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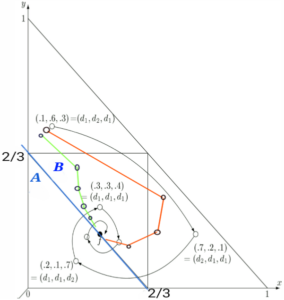

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- Regularity will allow automata-theoretic techniques.
- Can model more complex problems!

An abstract summary of the problem statements

- M be a Markov chain,
- μ, σ be distributions, *Init* be a set of distributions,
- λ be a threshold value,
- $\mathcal{D}$ be a discretization: for now, consider A, B wrt λ, $w \in \{A, B\}^*$

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2. Why they are interesting/relevant?

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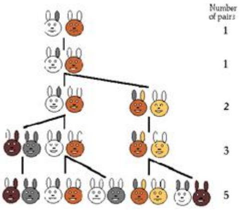
Other links and related problems

Program Termination, Orbit problem, problems for POMDPs

The Fibonacci Sequence



- Fibonacci sequence: $1, 1, 2, 3, 5, 8, 13, 21, \ldots$
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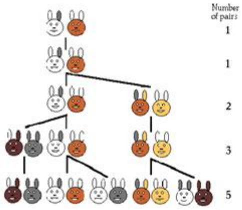

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- But rabbits die! So, $u_n = u_{n-1} + u_{n-2} - u_{n-3}$ where $u_2 = 2, u_1 = u_0 = 1$ Question: Can they ever die out?

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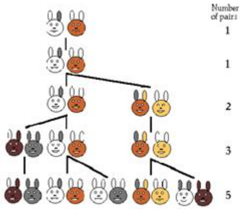

- Fibonacci sequence: $1, 1, 2, 3, 5, 8, 13, 21, \ldots$
- Fibonacci sequence: $u_n = u_{n-1} + u_{n-2}$ where $u_1 = u_0 = 1$
- But rabbits die! So, $u_n = u_{n-1} + u_{n-2} - u_{n-3}$ where $u_2 = 2, u_1 = u_0 = 1$ Question: Can they ever die out?

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

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

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.

Results on Skolem/Positivity problems

- Skolem-Mahler-Lech Theorem (1934, 1935, 1953)
- Decidability of Skolem/Positivity for 2,3,4... in 1981, '85, '05, '06, '09 by various authors.
  - Almost all 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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Bottomline: The general problem is still open!

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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- 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

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Chonev,Ouaknine, Worrell– STOC'12

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

What about lower bounds

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Surprisingly, nothing more is known!

An aside: a new even simpler proof for NP-hardness!

(Part of ongoing work with Nikhil Balaji and Nikhil Vyas...)

Reduction from Subset-Sum problem

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- Gives a (slightly) different NP-complete subclass of Skolem.
- Skolem instances where the eigenvalues are roots of unity (roots of reals?).
- Known to be decidable, but complexity bounds?

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 [IPL'15]

The Markov Reachability Problem is as hard as the Skolem problem

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Theorem [IPL'15]

The Markov Reachability Problem is as hard as the Skolem problem

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 $\mathbb{Z}$

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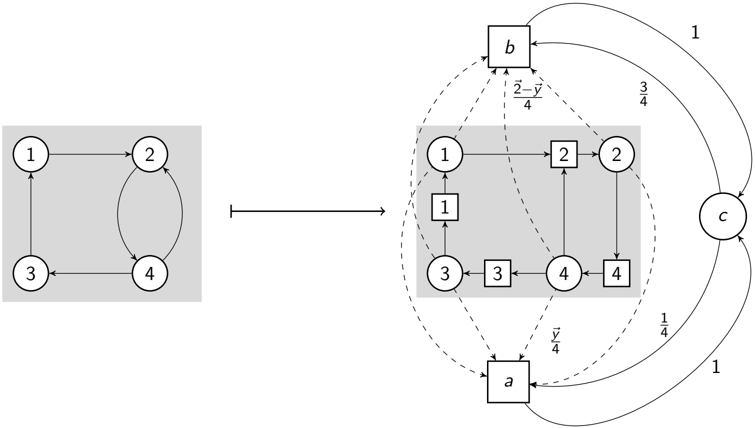
2. Rescale: Pick biggest entry in P_1 and divide;put remaining mass in a new column. Also add all 1's vector to v_1.
   - $(M^n)_{1,2} = 0$ iff $\vec{e}^T P_2^n \vec{v_2} = 1$, where P_2 is stochastic $2k+1$-dim matrix and $\vec{v_2}$ has only $0, 1, 2$ entries.

Final Step: Obtaining a co-ordinate vector - fixing v_2

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



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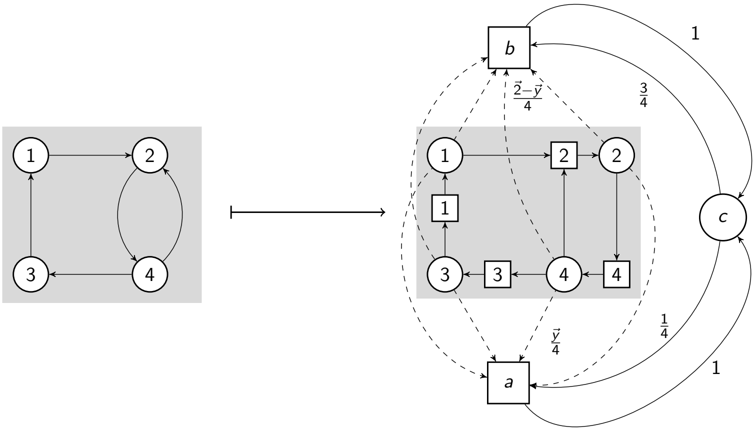

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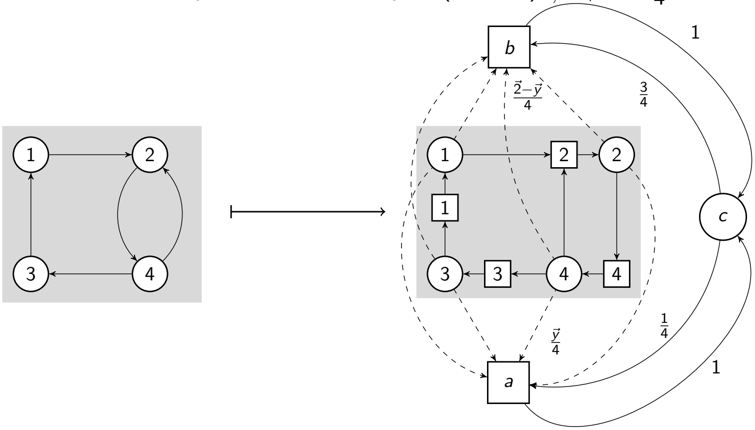
- Thus $\vec{e}^T Q^n \vec{y} = 1$ if and only if $(\widetilde{Q}^{2n+1})_{1,2k+1} = \frac{1}{4}$. □



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Corollary

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

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1. The problem statements
2. Why they are interesting/relevant?

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Other links and related problems

Program Termination, Orbit problem, problems for POMDPs

Properties of trajectories

Recall: Given a Markov chain M and a distribution μ, we define

- (symbolic) trajectory $w \in \{A, B\}$, where $w_i = A$ iff $\mu \cdot M^i \geq \lambda$

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Qn: How hard is it to describe them? Are they periodic?

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$$M_0 = \begin{pmatrix} 0.6 & 0.1 & 0.3 \\ 0.3 & 0.6 & 0.1 \\ 0.1 & 0.3 & 0.6 \end{pmatrix} \text{ and } \delta_0 = \begin{pmatrix} \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{2} \end{pmatrix}$$

- Threshold $\lambda = 1/3$, initial distribution δ_0.
- Trajectory projected on first component is not regular.
- Reason is that eigenvalues are $1, re^{i\theta}, re^{-i\theta}$ with $r = \sqrt{19}/10, \theta = \cos^{-1}(4/\sqrt{19})$.

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What about the language/regularity of symbolic dynamics?

Results on the symbolic dynamics: Approximate

Recall:

- Let *Init*, the set of initial distributions *Init*, be a convex polytope (or product of intervals).
- The language $L(M, Init)$ of a Markov chain M is the set of words over the set of all initial distributions.

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Approximation results

- "For all $\epsilon > 0$, does there exist n_ϵ s.t., prob to be in Goal after n_ϵ steps is at least $1/2 - \epsilon$?" is decidable.
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  –[Chadha et al., '14] tackle such problems in unary PFA.
- Decidability for more general approximations of symbolic dynamics, valid for LTL-style queries
  – [Agarwal et. al, '12,'15]

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Theorem [A., Genest, Karelovic, Vyas,'16]

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- Under above conditions, all trajectories are ult. constant.
- For each trajectory σ, there exists $n_\sigma \in \mathbb{N}$, after which it is constant A^ω or B^ω.

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Idea: Break into ultimate and finite prefixes and analyze the points where sign changes (switches from A to B or vice versa).

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The Markov reachability problem

1. The problem statements
2. Why they are interesting/relevant?

Links to the Skolem problem

- Another seemingly easy but hard problem!

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- For a single trajectory.
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Other links and related problems

Program Termination, Orbit problem, problems for POMDPs

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Basic undecidability result – Turing 1936

Termination of a generic program with a loop is undecidable:

while (*conditions*) {*commands*}

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An initialized homogeneous linear program

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

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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

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

Conclusion

Simple problems with hard solutions

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A yawning gap in complexity/decidability

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