Languages of Markov Chains

Based on:

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Approximate Verification of the Symbolic Dynamics of Markov Chains JACM'15-LICS'12

Overview of the Talk

- Biological Motivation
- Trajectories of Markov Chains
- Languages of Markov Chains
- Approximations

Population of cells



Setting: Many yeasts. Simplistic model

Each yeast can be in one of 3 states (1 high, 2 med, 3 low concentr. of X)

Experiments: Percentage of yeasts going from state S to state S' => Chance for a yeast to go from state S to state S' (after 5 min).

Image analysis: proportion in state 1 (high concentration of X => marker).

Continuous Abstraction

Non Continuous: Nathalie'sTalk tomorow.

Assume enough yeasts => Proportion in state 1,2,3.

Initial Proportion of cells :

 $P_{init} = \begin{pmatrix} - \\ - \end{pmatrix}$ through image analysis



$$M_{yeast} = \begin{pmatrix} 0.8 & 0.1 & 0.2\\ 0.1 & 0.8 & 0.1\\ 0.1 & 0.1 & 0.7 \end{pmatrix}$$

 $P_{5\min} = M_{yeast} P_{init} \qquad P_{10\min} = M^2_{yeast} P_{init}$

Deterministic concrete trajectory from a given P_{init}

Symbolic Trajectory

Expermiments (image analysis): first less than 5/12 of yeasts in state 1. some time later more than 5/12 of yeasts in state 1. then eventually, less than 5/12 of yeasts in state 1. 5/12 We set up Threshold=5/12 1/3Below threshold: B => finite alphabet {A,B} Above (or equal) threshold: A

So we observed $B^{n1}A^{n2}B^{\omega}$ Symb. Trajectory = infin. word on {A,B} Language of Markov Chain: set of trajectories from Init={ P_{init} | $x \in [0,2/3]$ }

Quantitative Question

Is $B^{n1}A^{n2}B^{\omega}$ in the language of the Markov Chain for some n1,n2?

If yes, for which initial proportion, for which n1,n2?

i.e. for which subset of s in
$$Init = \left\{ \begin{pmatrix} - \\ - \end{pmatrix} \mid x \begin{bmatrix} - \\ - \end{bmatrix} \right\}$$
?

Looks like a verification Question. Use algorithm for solving PCTL* questions on Markov Chains ?

Cannot be modeled with PCTL* [Beauquier Rabinovitch Slissenko CSL'02]

Skolem Problems

Actually, even with a unique initial configuration $P_{init} = \begin{pmatrix} - \\ - \end{pmatrix}$

Trajectory of a Markov chain from P_{init} is B^{ω} ?

as hard as Skolem (question on linear rec. seq. (e.g. Fibonacci)) [Akshay, Antonopoulose, Ouaknine, Worrel, IPL'15]

Decidability? Open for > 40 years. Decidable for <6 states If dec. for 18 states, major breakthrough in diophantines approximations

Simple Markov Chains

Simple: Every Eigen value of Markov Chain has multiplicity 1. -> Markov Chain is diagonalizable.

For simple markov chains,
Trajectory of a Markov chain from some P_{init} is B^ω?
=> decidable for 10 states.
=> for more than 25 states, breakthrough in Diophantines approx

Decidable if Trajectory of a simple Markov chain from some P_{init} is wB^{\u03b2} for some finite word w (ultimate positivity)

[Ouaknine Worrell ICALP'14 (best paper) & ICALP'14]

Eigen Basis

Simple: Markov Chains are diagonalizable.

Express $\mathsf{P}_{\mathsf{init}}$ in the eigen vector basis

$$M_{yeast} = \begin{pmatrix} 0.8 & 0.1 & 0.2\\ 0.1 & 0.8 & 0.1\\ 0.1 & 0.1 & 0.7 \end{pmatrix}$$

$$M \cdot \begin{pmatrix} 5/12 \\ 1/3 \\ 1/4 \end{pmatrix} = \underbrace{1}_{1/4} \begin{pmatrix} 5/12 \\ 1/3 \\ 1/4 \end{pmatrix}; M \cdot \begin{pmatrix} 5/12 \\ -5/12 \\ 0 \end{pmatrix} = \underbrace{0.7}_{0} \begin{pmatrix} 5/12 \\ -5/12 \\ 0 \end{pmatrix}; M \cdot \begin{pmatrix} 5/12 \\ 0 \\ -5/12 \end{pmatrix} = \underbrace{0.6}_{-5/12} \begin{pmatrix} 5/12 \\ 0 \\ -5/12 \end{pmatrix}$$
$$P_{\text{init}} = \begin{pmatrix} 1/3 \\ 1/4 \\ 5/12 \end{pmatrix} = \begin{pmatrix} 5/12 \\ 1/3 \\ 1/4 \end{pmatrix} + \frac{1}{5} \begin{pmatrix} 5/12 \\ -5/12 \\ 0 \end{pmatrix} - \frac{2}{5} \begin{pmatrix} 5/12 \\ 0 \\ -5/12 \end{pmatrix}$$
$$M^{n} P_{\text{init}} = \begin{pmatrix} 5/12 \\ 1/3 \\ 1/4 \end{pmatrix} + \frac{1}{5} \begin{pmatrix} 0.7^{n} \begin{pmatrix} 5/12 \\ -5/12 \\ 0 \end{pmatrix} - \frac{2}{5} \begin{pmatrix} 0.6^{n} \begin{pmatrix} 5/12 \\ 0 \\ -5/12 \end{pmatrix}$$
$$M^{n} P_{\text{init}} \begin{bmatrix} 1 \end{bmatrix} \ge - \qquad \text{iff} \qquad -0.7^{n} \ge -0.6^{n}$$

Symbolic Trajectory from P_{init}: B^k A⁽ⁱ⁾

General Simple Markov Chains

$$M^{n} P_{init} [1] \ge \tau$$
 iff $a_{0} + a_{1} \sigma_{1}^{n} + ... + a_{k} \sigma_{k}^{n} \ge 0$

Trajectories are not always ultimately periodic, even for simple M



Roots of real numbers

If eigen values are roots of real numbers, then trajectories are ultimately periodic

$$M^{n} P_{init} [1] \ge \tau \quad \text{iff} \quad a_{0} + a_{1} \sigma_{1}^{n} + ... + a_{k} \sigma_{k}^{n} \ge 0$$

Let I_k with $\sigma_k^{\ l_k}$ is positive real, Let L=lcm(I_k) and $\rho_k = \sigma_k^{\ L}$

$$M^{Ln} P_{init} [1] \ge \tau$$
 iff $a_0 + a_1 \rho_1^{n} + ... + a_k \rho_k^{n} \ge 0$

 \rightarrow Eventually constant (dominant factor) e.g.: w A^{ω}

→Ultimately periodic of period L ex: L=5, trajectory w' (A B B A B)[®]

Sum up

Property of eigenvalues of Markov chain	Ultimately periodic traj.
Distinct, positive real numbers	🗸 🛛 even ult. constant
Distinct, roots of real numbers	Decidability!
Distinct	× Decidability ?

but positivity/equality approximable [Chadha Kini Viswanathan QEST'14]

What about languages?

set of trajectories from e.g. lnit = {
$$\begin{pmatrix} - \\ - \end{pmatrix}$$
 | x $\begin{bmatrix} - \end{bmatrix}$

Init needs to be a polytope.

Language: not that simple

M_{veast}: eigen values are positive real numbers: 1, 0.7, 0.6

$$\begin{pmatrix} 1/3 \\ 1/4 \\ 5/12 \end{pmatrix} = \begin{pmatrix} 5/12 \\ 1/3 \\ 1/4 \end{pmatrix} + \frac{1}{5} \begin{pmatrix} 5/12 \\ -5/12 \\ 0 \end{pmatrix} - \frac{2}{5} \begin{pmatrix} 5/12 \\ 0 \\ -5/12 \end{pmatrix}$$
 Trajectory: B^k A^{\varphi}

$$\begin{pmatrix} 1/3 \\ 1/3 \\ 1/3 \end{pmatrix} = \begin{pmatrix} 5/12 \\ 1/3 \\ 1/4 \end{pmatrix} - \frac{1}{5} \begin{pmatrix} 5/12 \\ 0 \\ -5/12 \end{pmatrix}$$
 Trajectory: B^{\omega}

When P_{init} converges towards $\begin{pmatrix} 1/3\\ 1/3\\ 1/2 \end{pmatrix}$

Nota finite trajectories trajectory becomes $B^n A^{\omega}$ with n converging to ∞ => Can show that language is B^*A^{ω} U B^{ω}

Language in general

Result: if all eigen values are distincts positive real numbers, Then language is regular for Init a polytope. [AGKV STACS'16]



First, under these conditions, all trajectories are ultimately constant.





In general with Polytope in 1D



max bound e, bound f is a uniform bound for utimately constant.

Polytopes in any Dimension

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Case of e_1...e_z extremities of Polytope with

a_1(e_1) > 0

a_1(e_2)=0, a_2(e_2) < 0

a_1(e_3)=a_2(e_3)=0, a_3(e_3)>0

...

Sign (a_k(e_k))=(-1)^k
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N is the max of the ultimately constant bound for $e_1..e_z$ Result: $L^N_{ult}(H) = (A^*) B^*A^*... B^* A^{o}$

The set of trajectories in $(e_1..e_z)$ **after** N steps: Lemma 1: At most z switch, i.e. Included into $(A^*) B^*A^*... B^* A^{(i)}$ Lemma 2: for all $i_1..i_z$, exists initial distrib with traj: $B^{i_1} A^{i_2} ... B^{i_z} A^{(i)}$

General Dimension: Handle Prefixes



Induction on the highest « z » in the space.

In the picture, z=3, n(dimension)=4 Take w touching (h,g) and touching (h,g,f) with a point not touching h or g And touching (h,g,f,e) with a point not touching (hfg). We can prove that for some i, w Aⁱ B A^{\omega} is a trajectory continuity argument w Aⁱ B^{\omega} is a trajectory => wAⁱA*B*A^{\omega} included into trajectory w A^{\omega} is a trajectory

In general



Induction on the highest « z » in the space.

Remove points with trajectory wAⁱA*B*A^{ω} and w'AⁱA*B*A^{ω} It remains a finite union of convex polyhedra with lower « z »

Hence the language is a finite union of regular set, hence it is regular.

Sum up

Property of eigenvalues of Markov chain	Regular language	Ultimately periodic traj.		
Distinct, positive real numbers	✓ decidable	\checkmark		
Distinct, roots of real numbers	× Decidability	✓		
Distinct	× ?	×		

but approximable [AAGT LICS'12]

Distinct roots of real numbers: not regular.

	0	1	0	0	0	0	0]
	0	0	1	0	0	0	0
	0	0	0	1	0	0	0
$M_1 =$	0	0	0	0	1	0	0
	0	0	0	0	0	1	0
	0	0	0	0	0	0	1
	$\frac{1}{512}$	$\frac{8r+3}{512}$	$\frac{3+3r}{64}$	$\frac{13+16r}{128}$	$\frac{9+2r}{32}$	$\frac{1+4r}{16}$	$\frac{1-r}{2}$

Approximation for Markov Chains.

Irreducible aperiodic chains

$$M = \begin{pmatrix} 0.3 & 0.7 & 0\\ 0.5 & 0 & 0.5\\ 0.8 & 0 & 0.2 \end{pmatrix}$$



M is irreducible aperiodic because:

$$M^{2} = \begin{pmatrix} .44 & .21 & .35 \\ .55 & .35 & 0.1 \\ .4 & .56 & .04 \end{pmatrix}$$

Approximations for irreducible aperiodic chains:

Irreducible aperiodic: unique stationary distribution **f**. Fix $\varepsilon => \text{ exists K}$ such that $|M^{K}u - f| < \varepsilon$ for all initial distribution **u**.

 $\begin{array}{l} \mathsf{A}_1..\mathsf{A}_n \text{ is an } (\epsilon,\mathsf{K})\text{-approximate symbolic trajectory of} \\ & a \text{ concrete } \text{trajectory } \mathsf{d}_1..\mathsf{d}_n \text{ if} \\ \mathsf{d}_i \in \mathsf{A}_i \text{ for all } i{<}\mathsf{K} \text{ and } \mathsf{d}_i \text{ is } \epsilon\text{-close to } \mathsf{A}_i \text{ for } i{>}\mathsf{K}. \end{array}$

Exact symbolic trajectory from init: ABBABBBABBBBA... Epsilon => K=4, Approx symbolic trajectories: ABBABBAA..., ABBABBAB..., ABBABBBA..., ABBABBBB....

We get ABBABB (A or B)* is regular.

Approximations for irreducible aperiodic chains:

Th: Given MC + Init (set), it is decidable [AAGT, LICS'12] whether:

For some concrete trajectory w, there does not exists a approx trajectory satisfying ϕ ,

 \Rightarrow w does not satisfies ϕ .

=> system does not satisfy ϕ .

For all concrete trajectory w, all approx traj satisfy φ => all w satisfies φ.

 \Rightarrow system satisfies ϕ .

Undetermined: for all concrete trajectory, there exists approximate trajectroty satisfying ϕ , but not for all.

=> Refine ε to reduce number of approx trajectories.

Irreducible Periodic chains



M is periodic of period 3.

M³ is irreducible aperiodic on disconnected partition of nodes.

Consider M³ from Init, Consider M³ from M Init, Consider M³ from M² Init

Not irreducible chains



- Stationary distributions have weight 0 for non bottom SCC (1; 2-3, 4). \Rightarrow Analyse the bottom SCC with earlier algorithm.
- Tough part: Analyse non bottom SCC to get weights for bottom SCC, depending on Initial distribution (algorithm close to PCTL Mod. Check.)
- + uniform K over all initial distrib => allow to lift results to Languages

Polytope of initial Distributions

uniform K over all initial distrib => allow to lift results to Languages

Consider each extremities e1..en of the initial polytope. Use linearity!

Compute the way they weight in the different BSCC e = $\Sigma \lambda i$ ei => weight(e,BSCCk) = $\Sigma \lambda i$ weight(ei,BSCCk)

 \Rightarrow Easy to compute the possible ultimately ϵ -reccuring set of letters

Then compute set of bounded prefixes with some ultimate set of letters, easy to compute as well.

Conclusion

Markov Chain (Unary PFA): Simplistic formalism but still many open problems.

Even taking restrictive hypothesis, not easy to describe their behavior.

But quantitative analysis of population is possible under strong hypothesis or with approximations.