On the Metric-based Approximate Minimization of Markov Chains*

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Aalborg University

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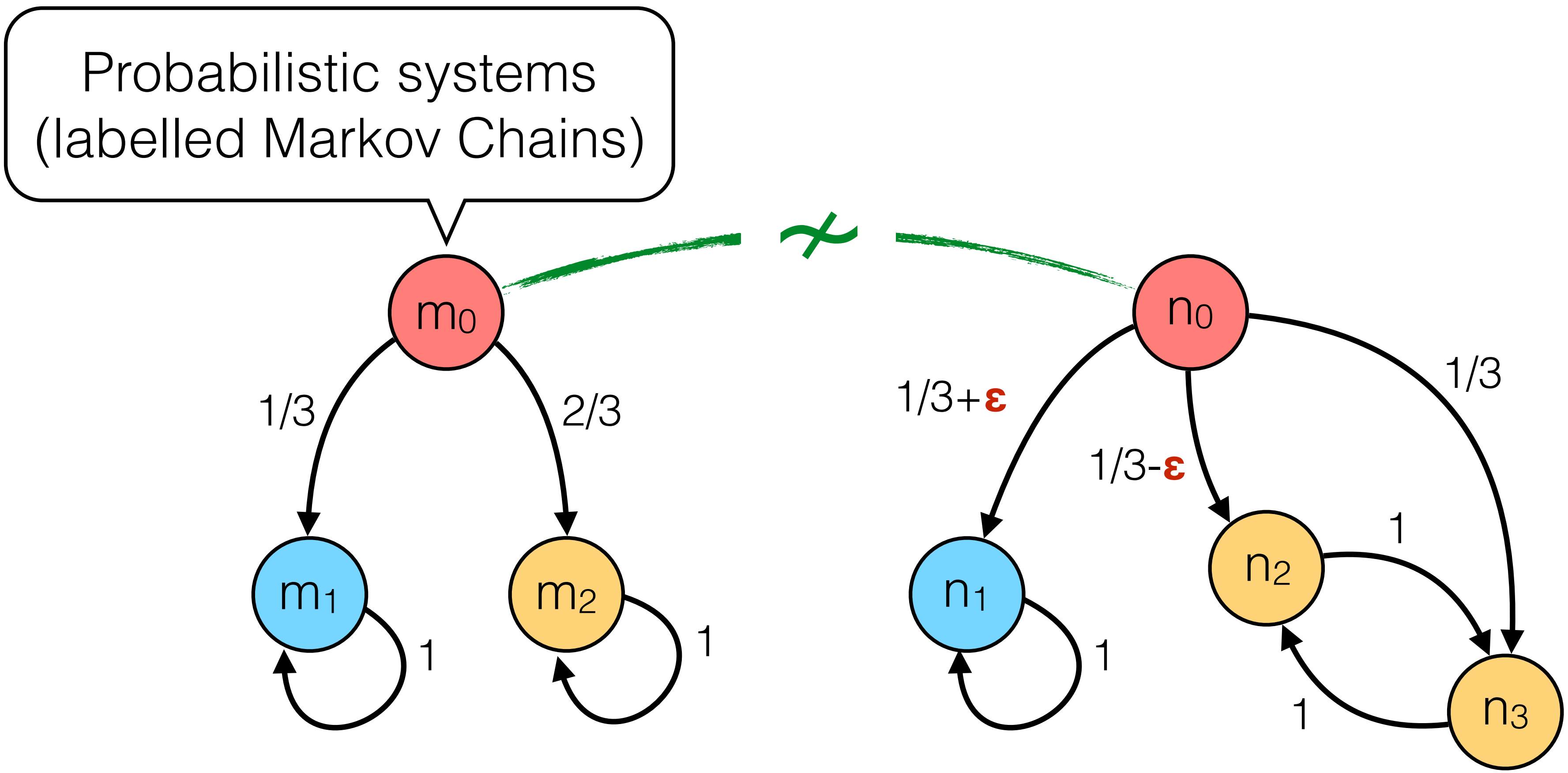
Introduction

- **Moore‘56, Hopcroft‘71:** Minimization algorithm for DFA (*partition refinement wrt Myhill-Nerode equiv.*)
- Minimization via partition refinement:
  - **Kanellakis-Smolka’83:** minimization of LTSs wrt Milner’s strong bisimulation
  - **Baier’96:** minimization of MCs wrt Larsen-Skou probabilistic bisimulation
  - **Alur et al.’92, Yannakakis-Lee’97:** minimization of timed & real-time transition systems.
  - and many more…

A fundamental problem

Jou-Smolka'90 observed that behavioral equivalences are not robust for systems with real-valued data



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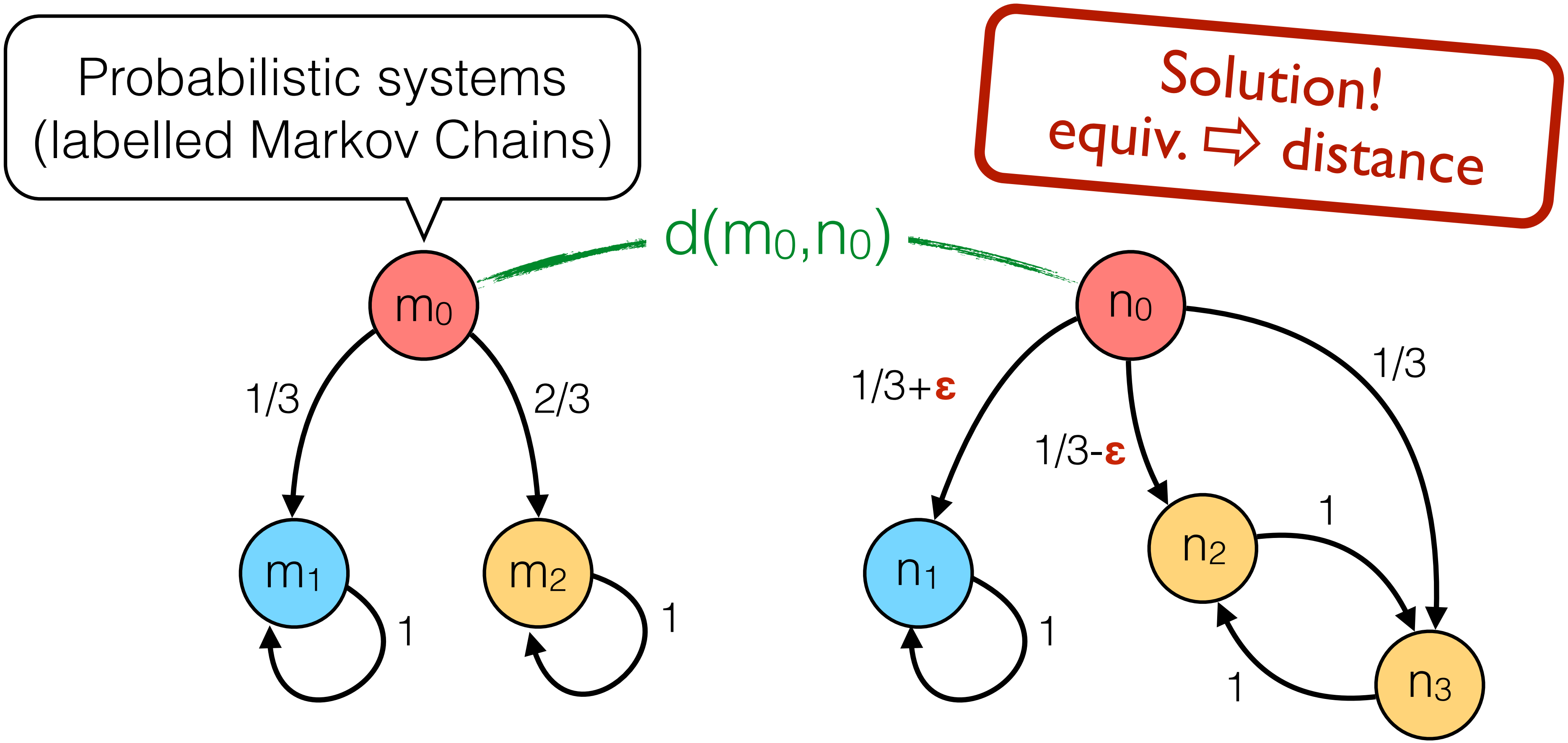

Metric-based Approximate Minimization

Closest Bounded Approximant (CBA)

Minimum Significant Approximant Bound (MSAB)

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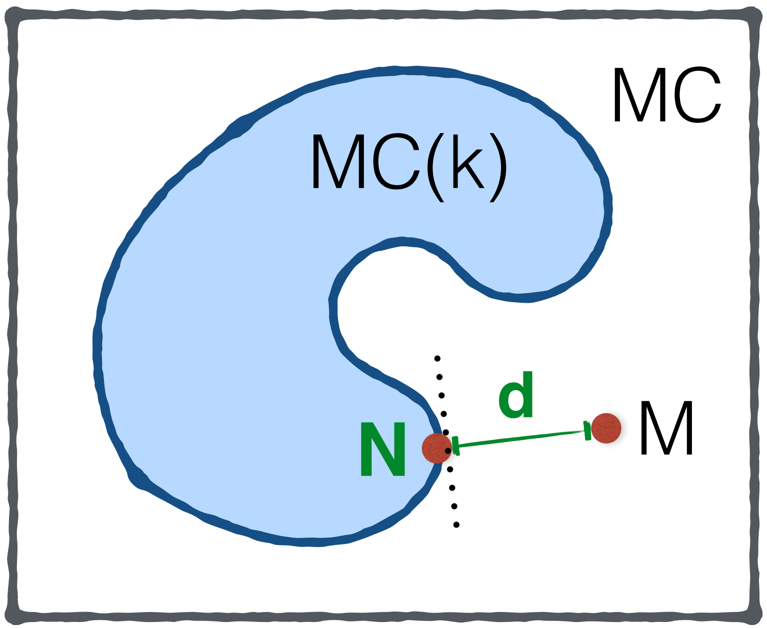

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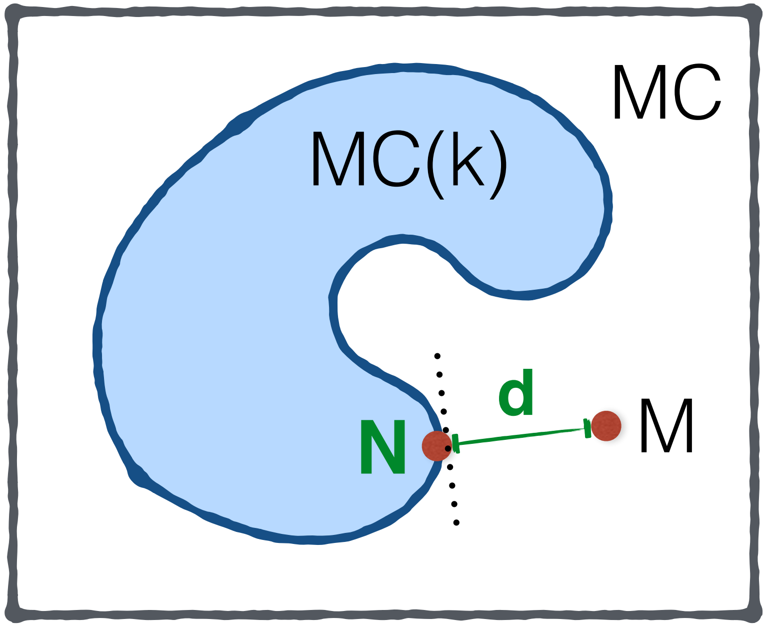

minimize d

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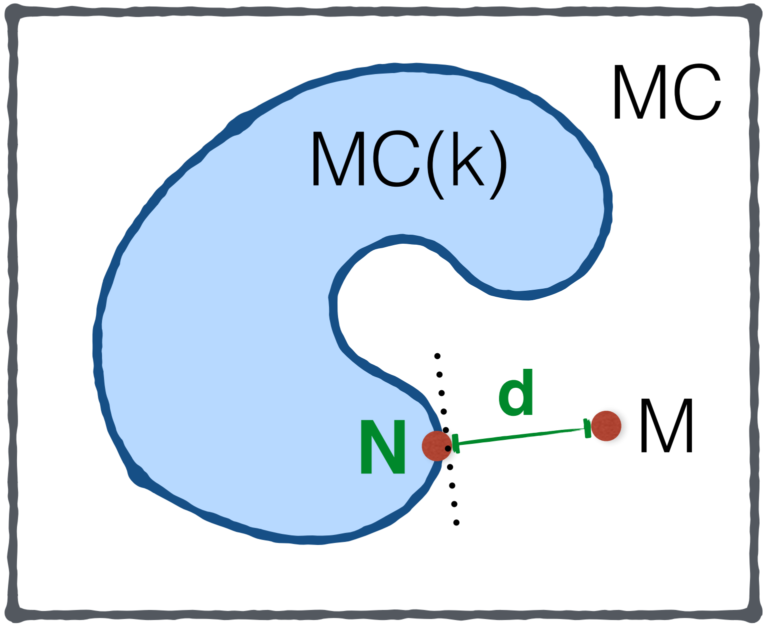

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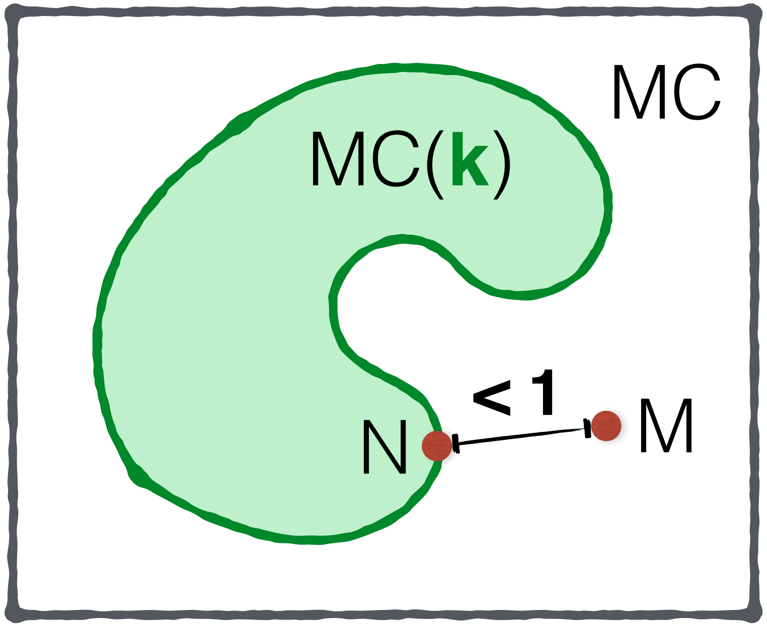

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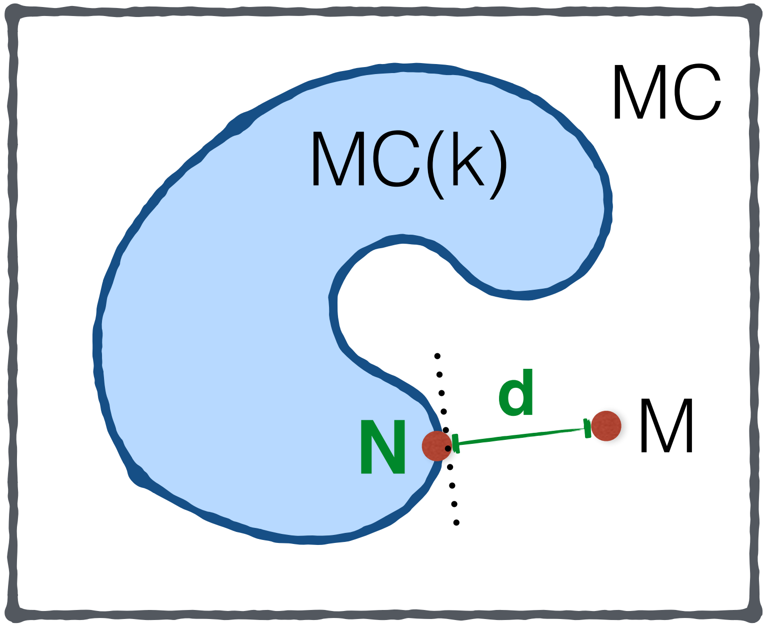

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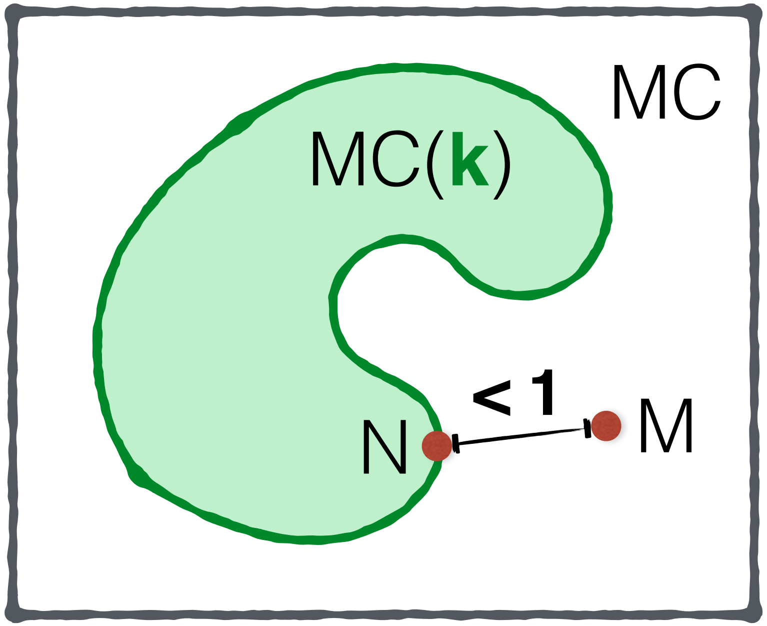

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"To study the complexity of an optimization problem one has to look at its decision variant"

(C. Papadimitriou)

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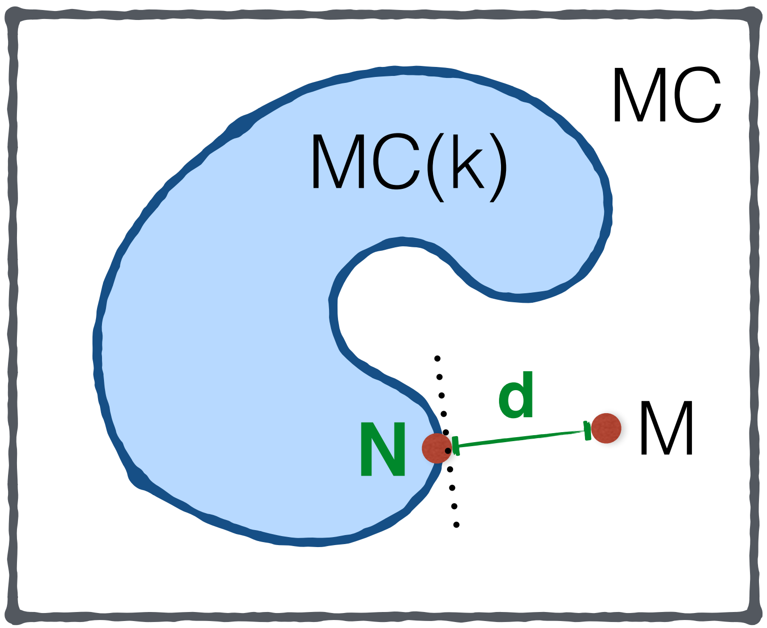

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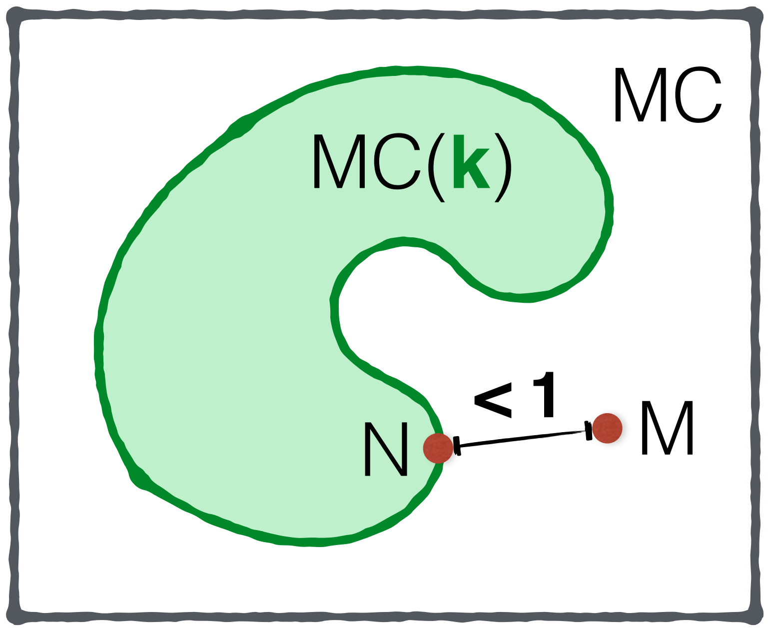

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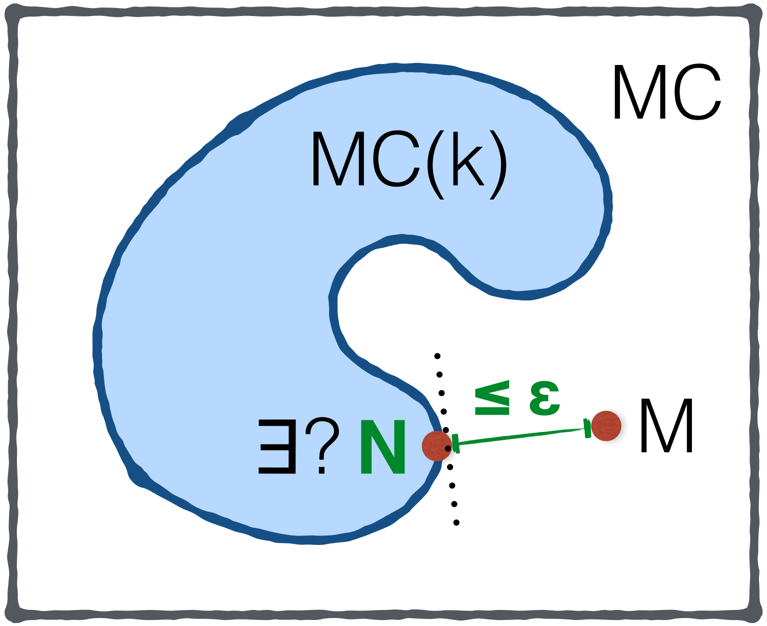

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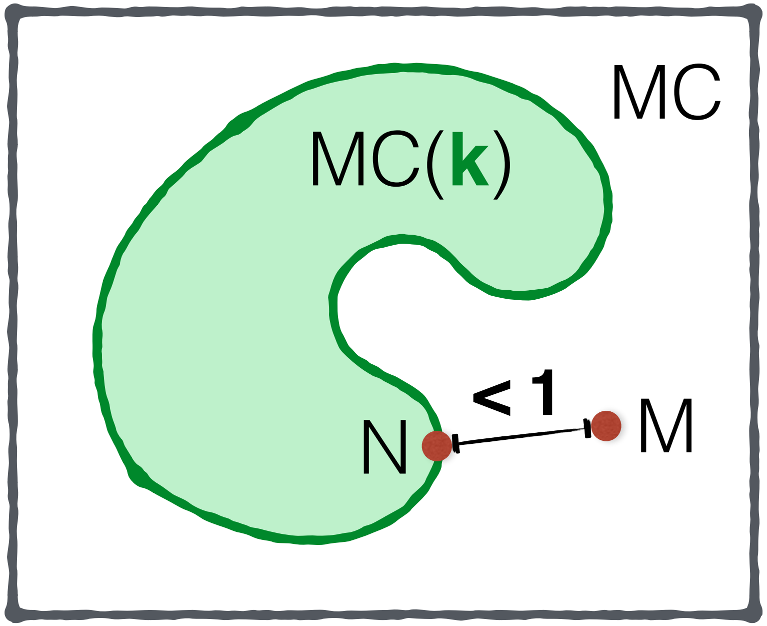

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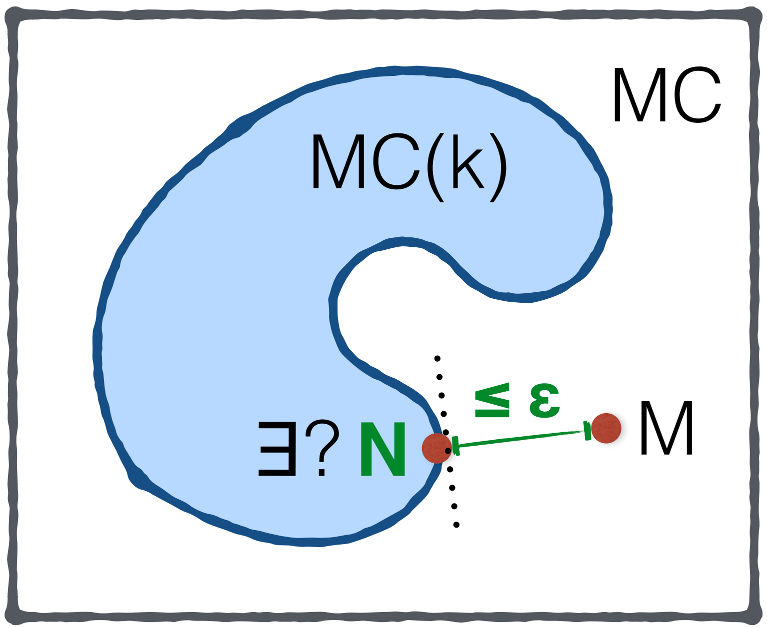

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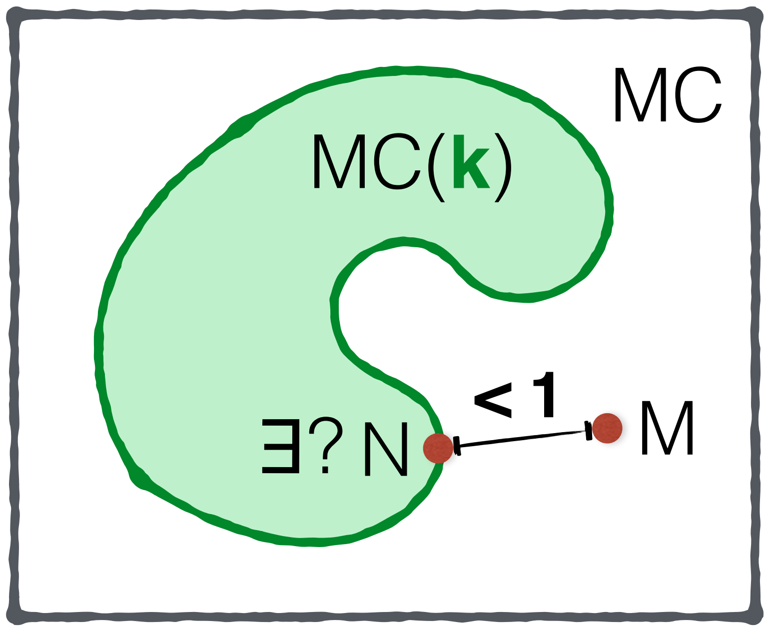
Significant Bounded Approximant (SBA)



given k

What distance on MCs?

a.k.a. Kantorovich distance

(λ-discounted) **Probabilistic Bisimilarity distance** of Desharnais et al. —denoted d_λ

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Theorem (Chen, van Breugel, Worrell 12)

The probabilistic bisimilarity distance
can be computed in polynomial time

Relation with Model Checking

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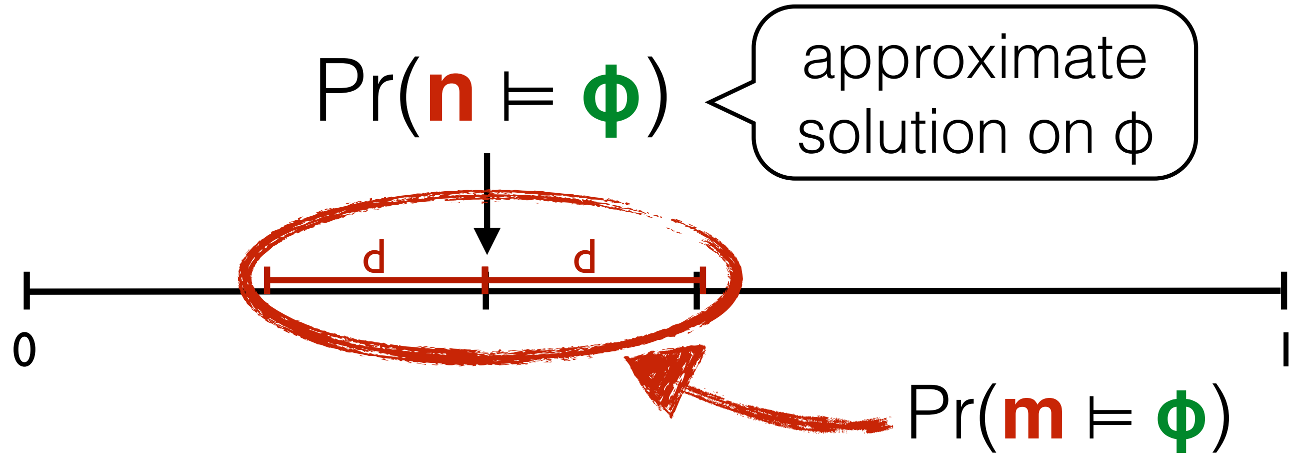
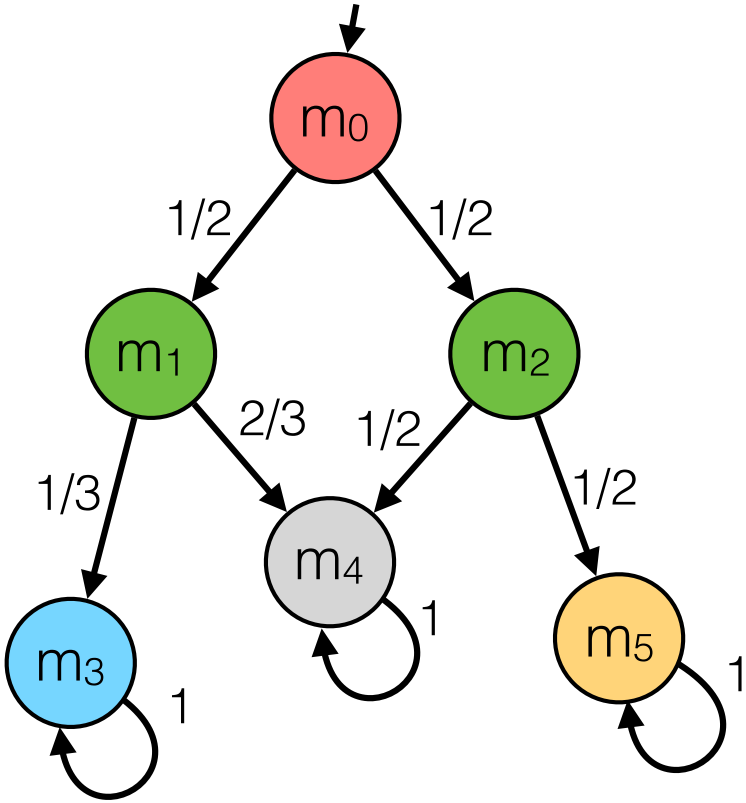
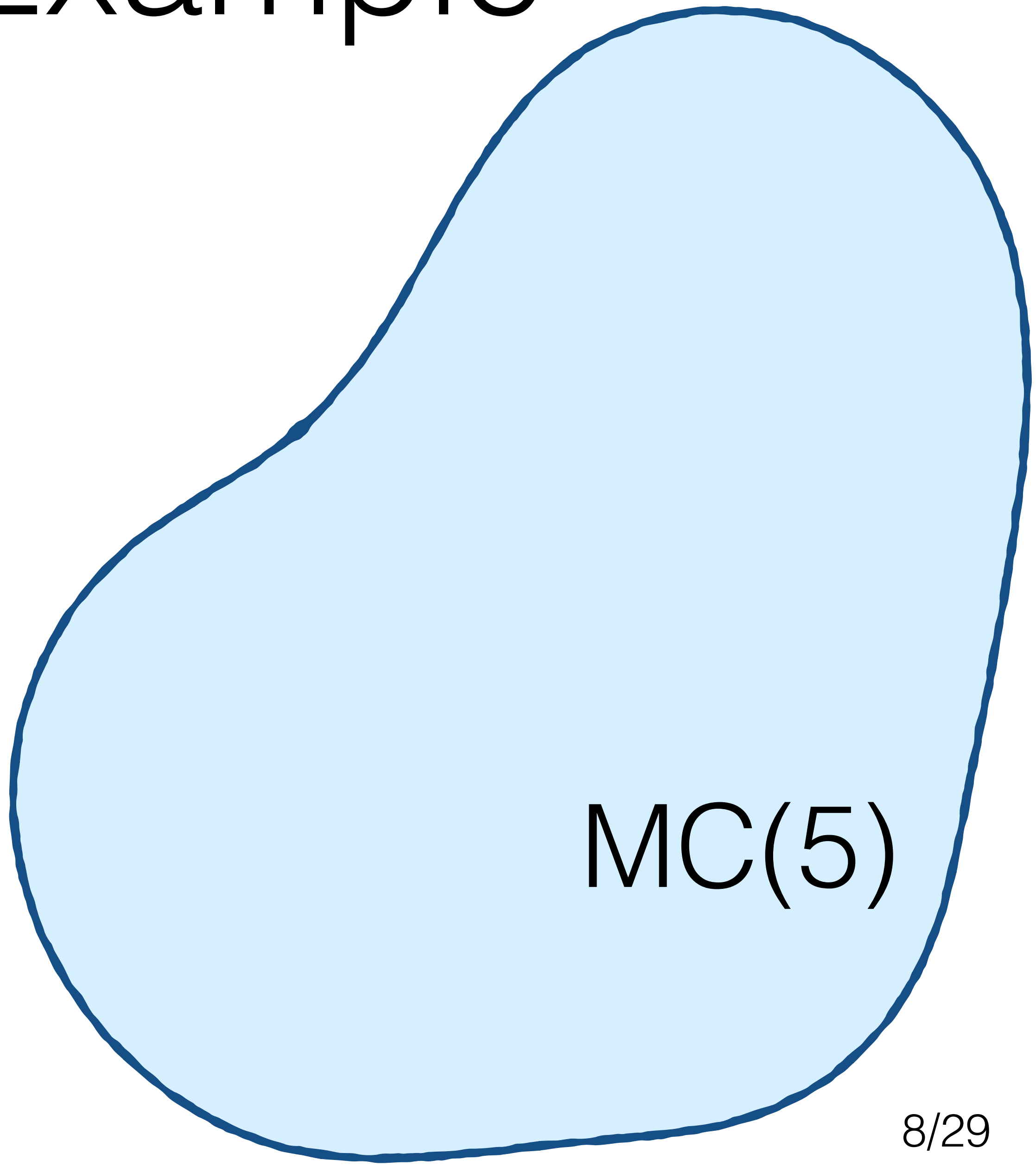
…imagine that $|M| \gg |N|$, we can use N in place of M



CBA: Example*





(*) With respect to the undiscounted probabilistic bisimilarity distance d_1

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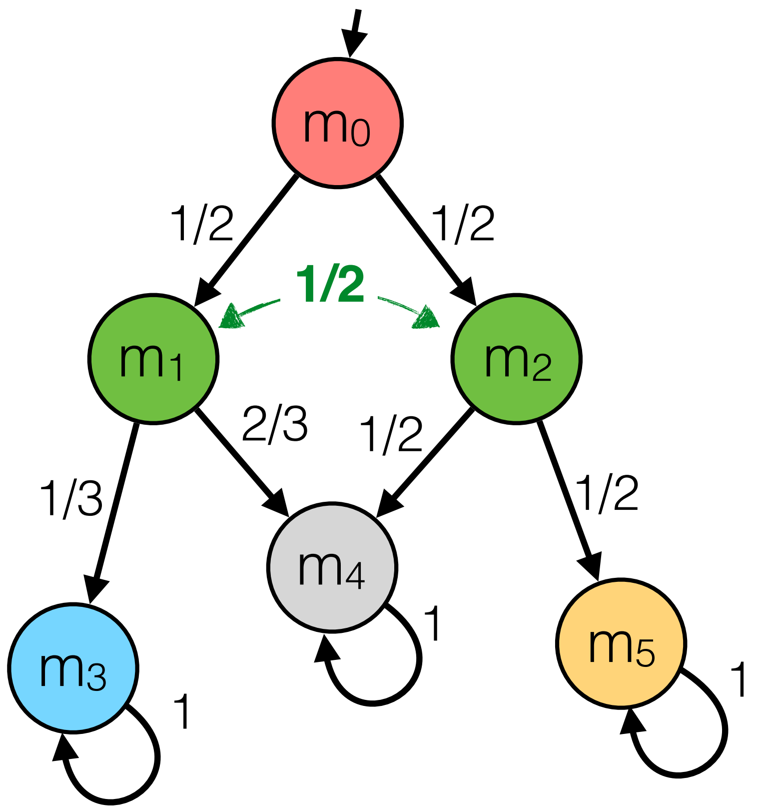

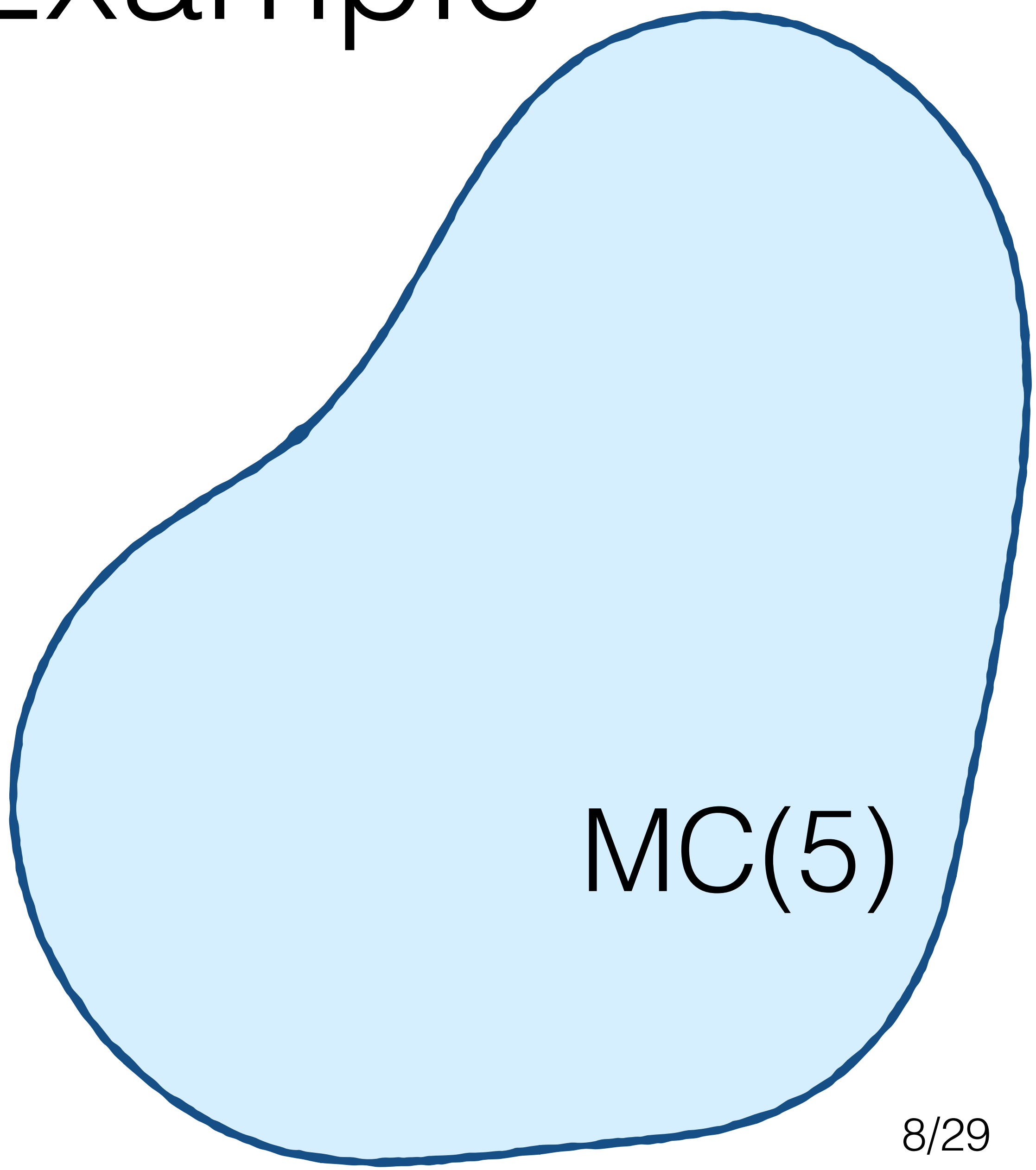

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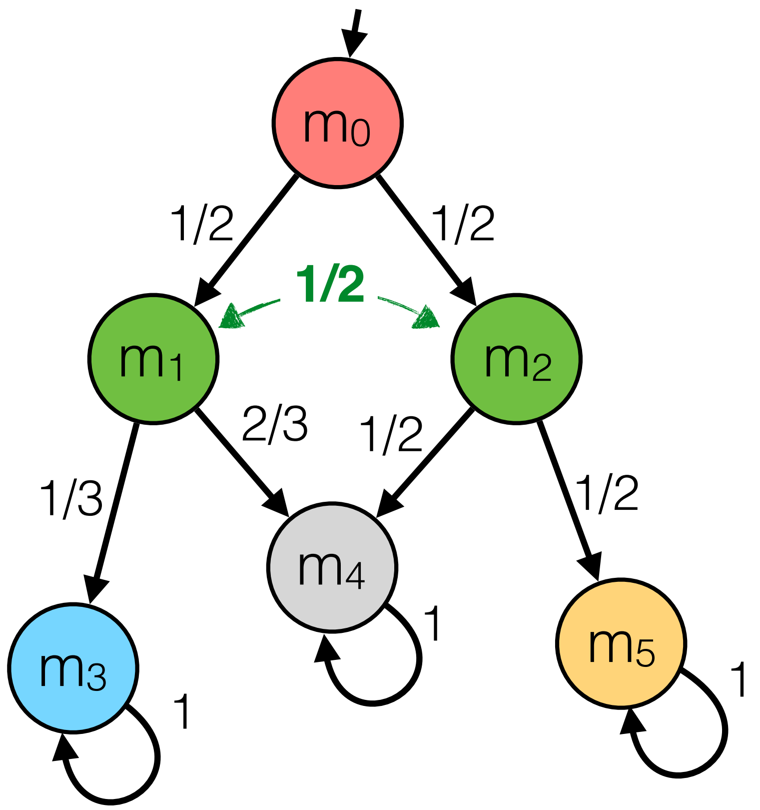

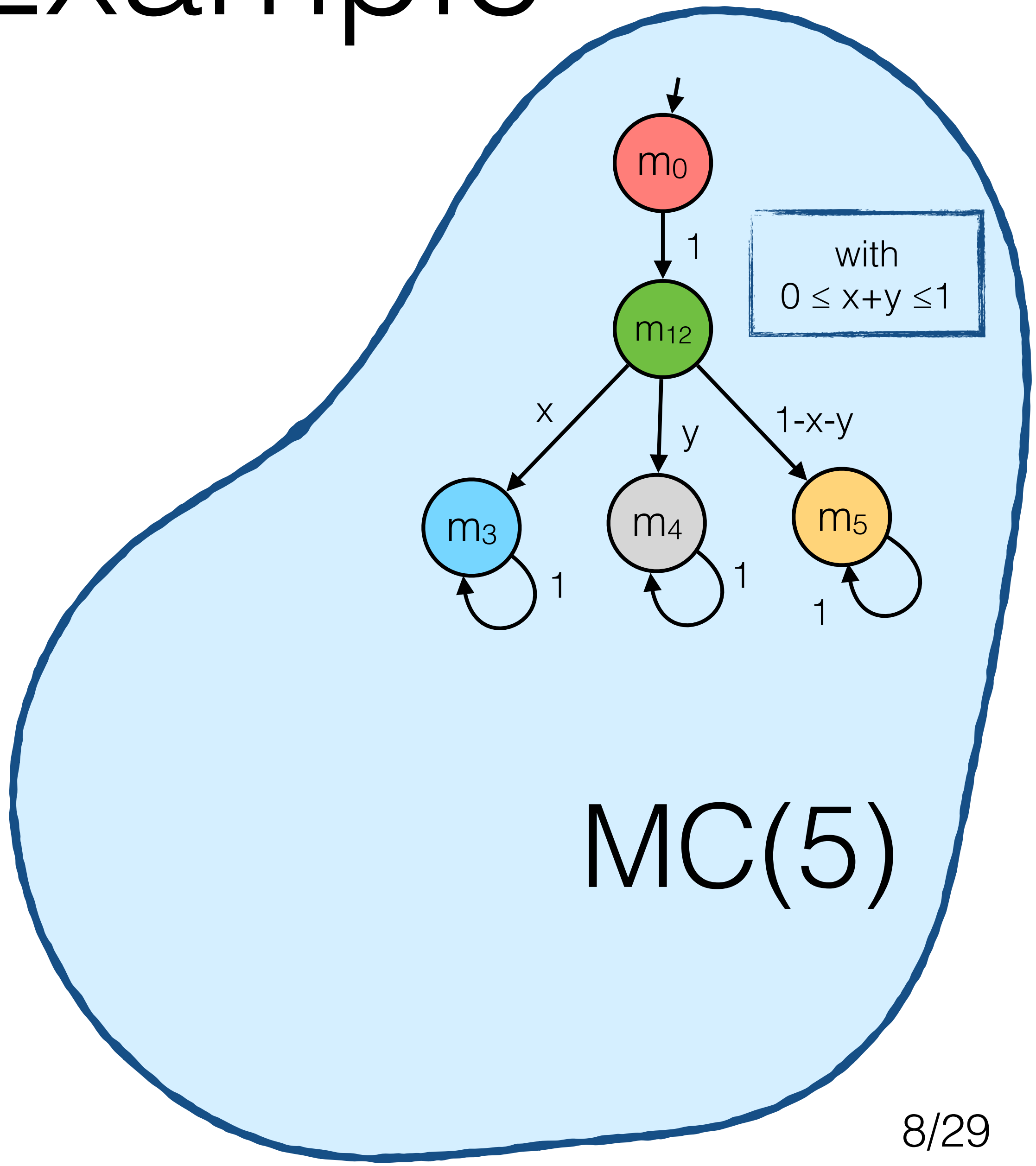

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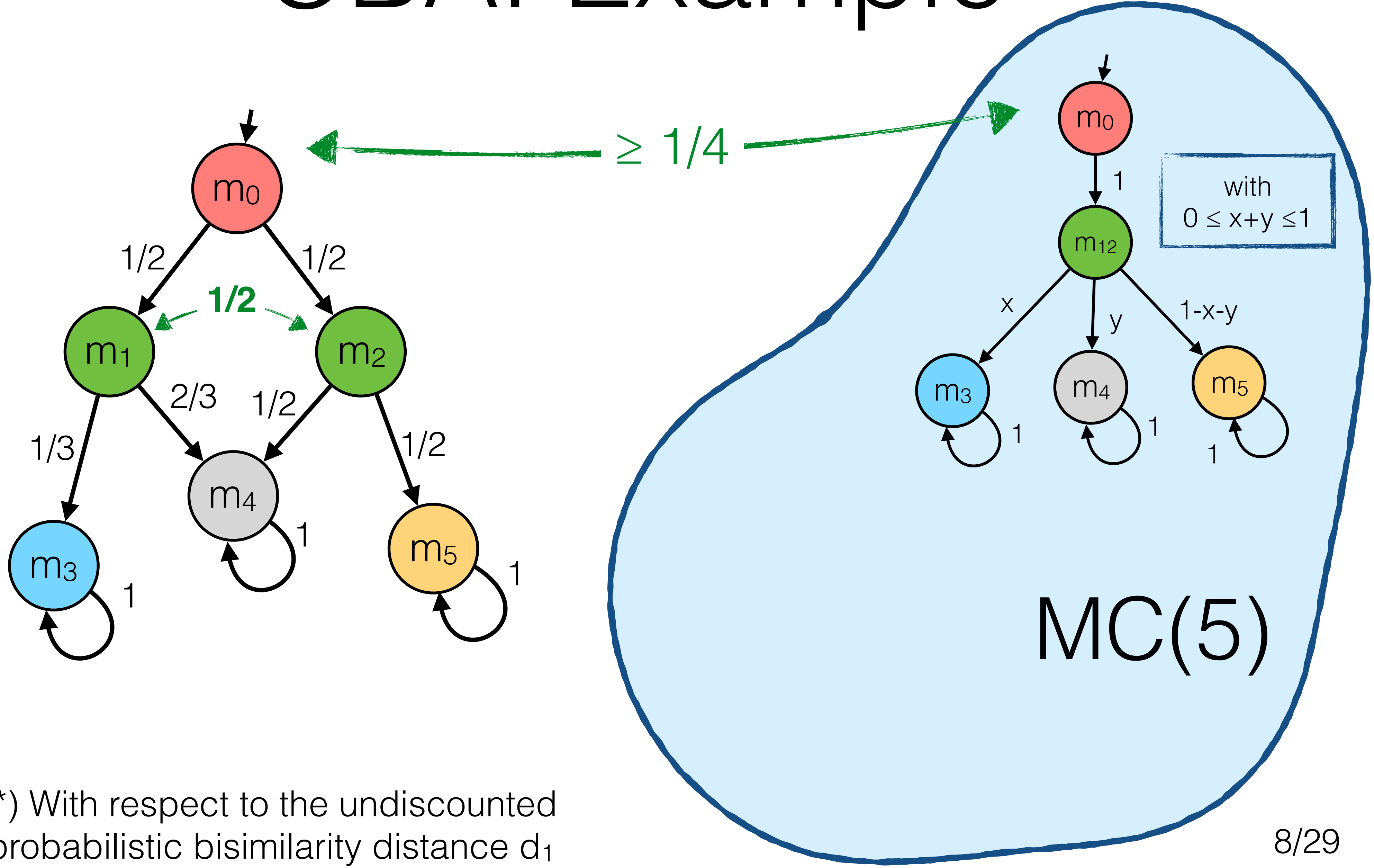

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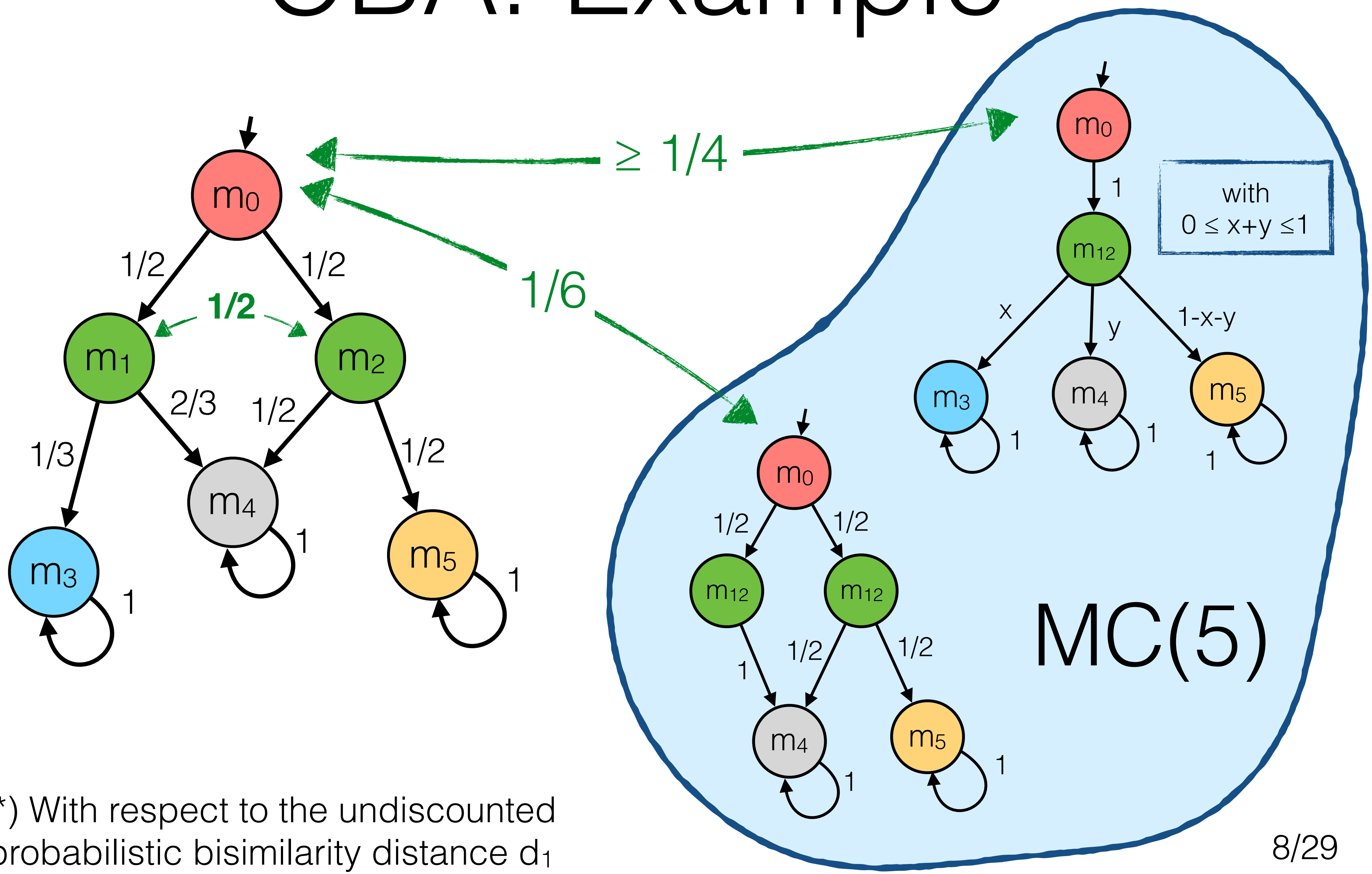

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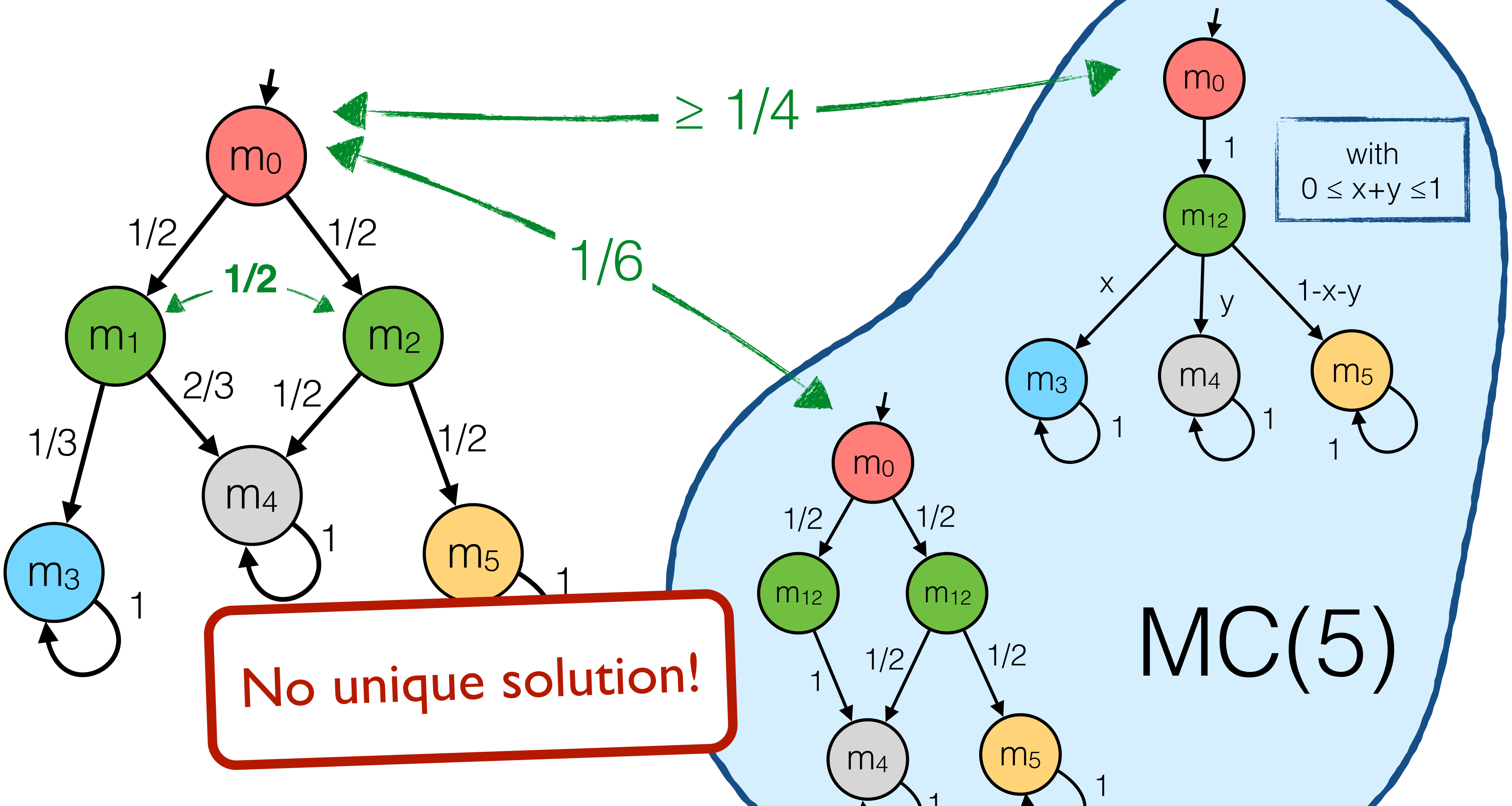

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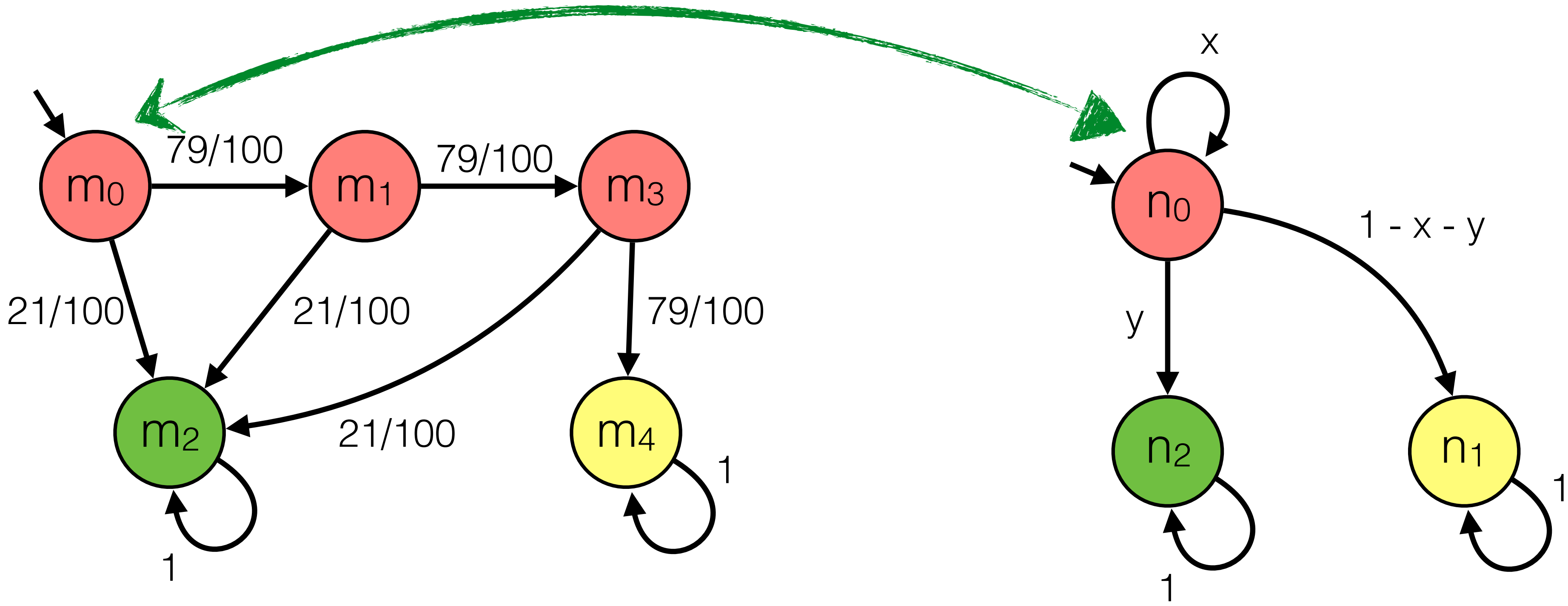

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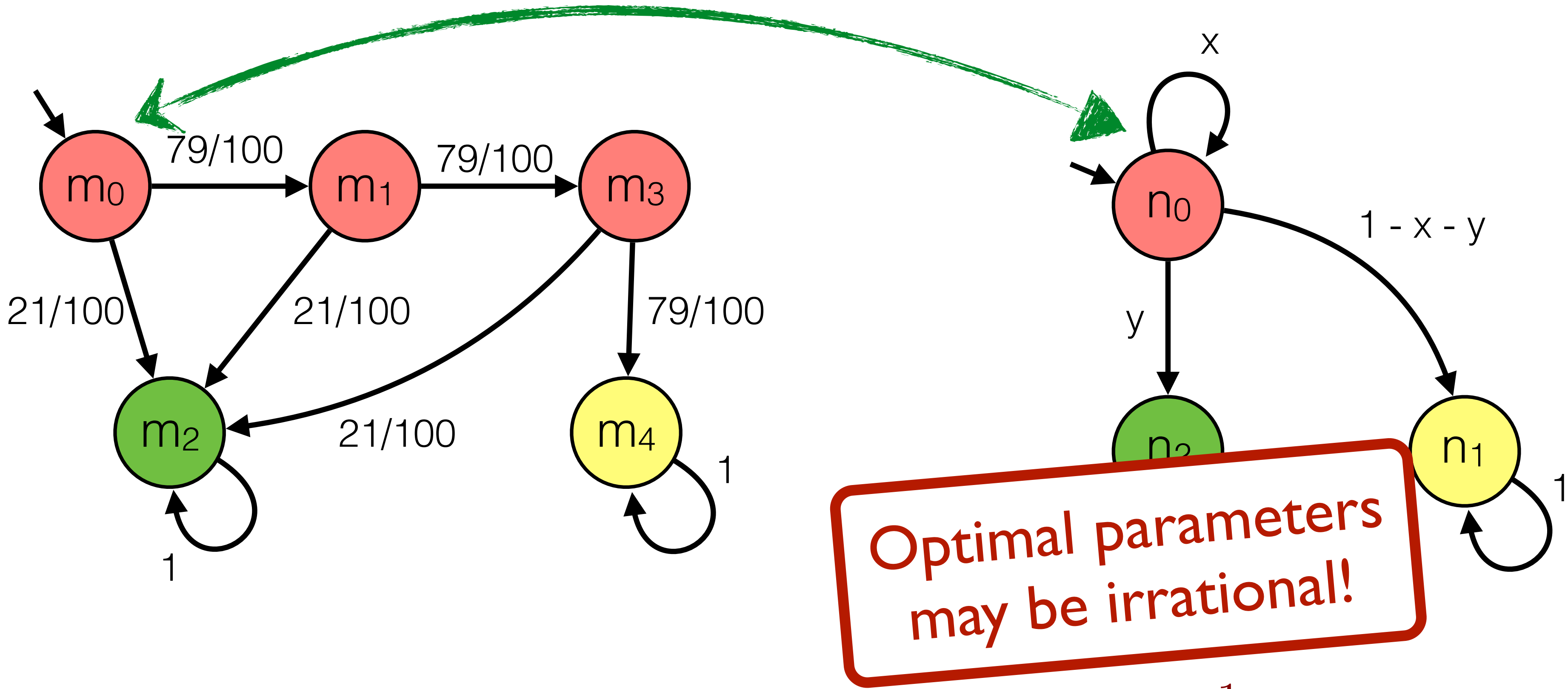

$$x = \frac{1}{30}\left(10 + \sqrt{163}\right)$$

$$y = \frac{21}{200}$$

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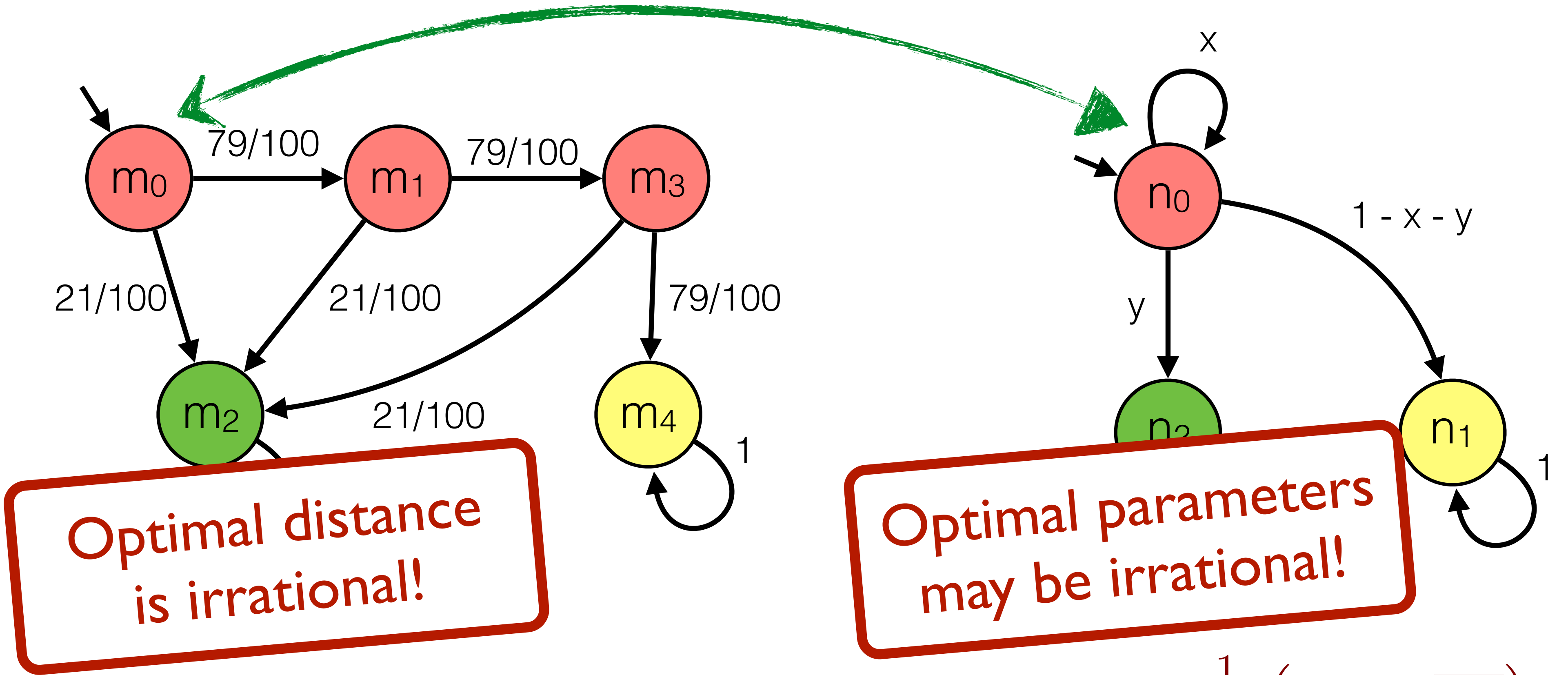

$$\delta(m_0, n_0) = \frac{436}{675} - \frac{163\sqrt{163}}{13500} \approx 0.49$$

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Characterizations + COMPLEXITY results:

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Practical

We proposed an EM-like method to obtain a sub-optimal approximants

Talk Outline

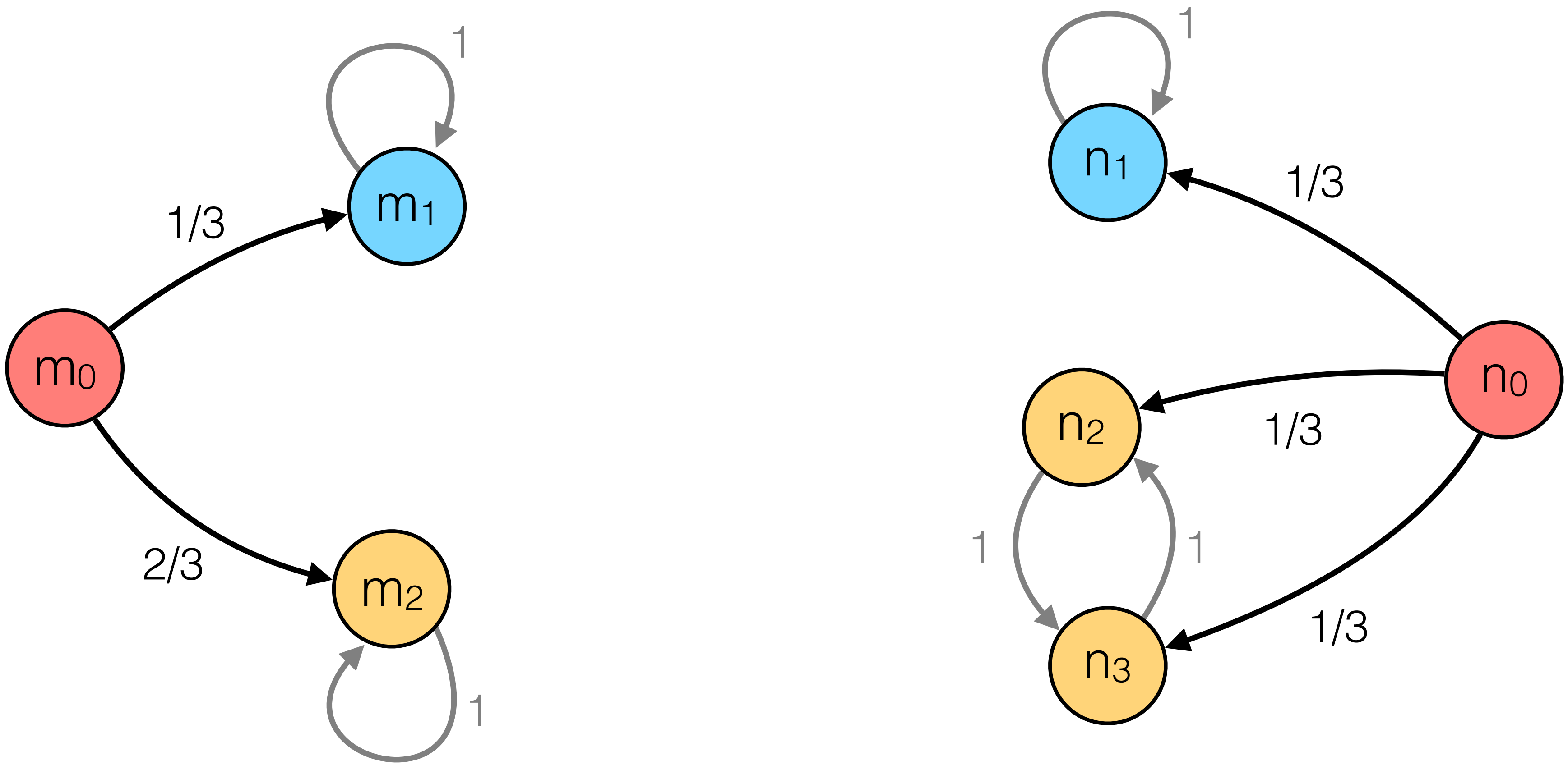
★ **Probabilistic bisimilarity distance**

- fixed point characterization (Kantorovich oper.)

★ **Metric-based Optimal Approximate Minimization**

- *Closest Bounded Approximant* (CBA)
  — bilinear characterization (+ complexity)
- *Minimum Significant Approximant Bound* (MSAB)
  — characterization (+ complexity)
- *Expectation Maximization-like algorithm*
  — 2 heuristics + experimental results

Probabilistic bisimulation



It tries to match the behaviors “quantitatively”

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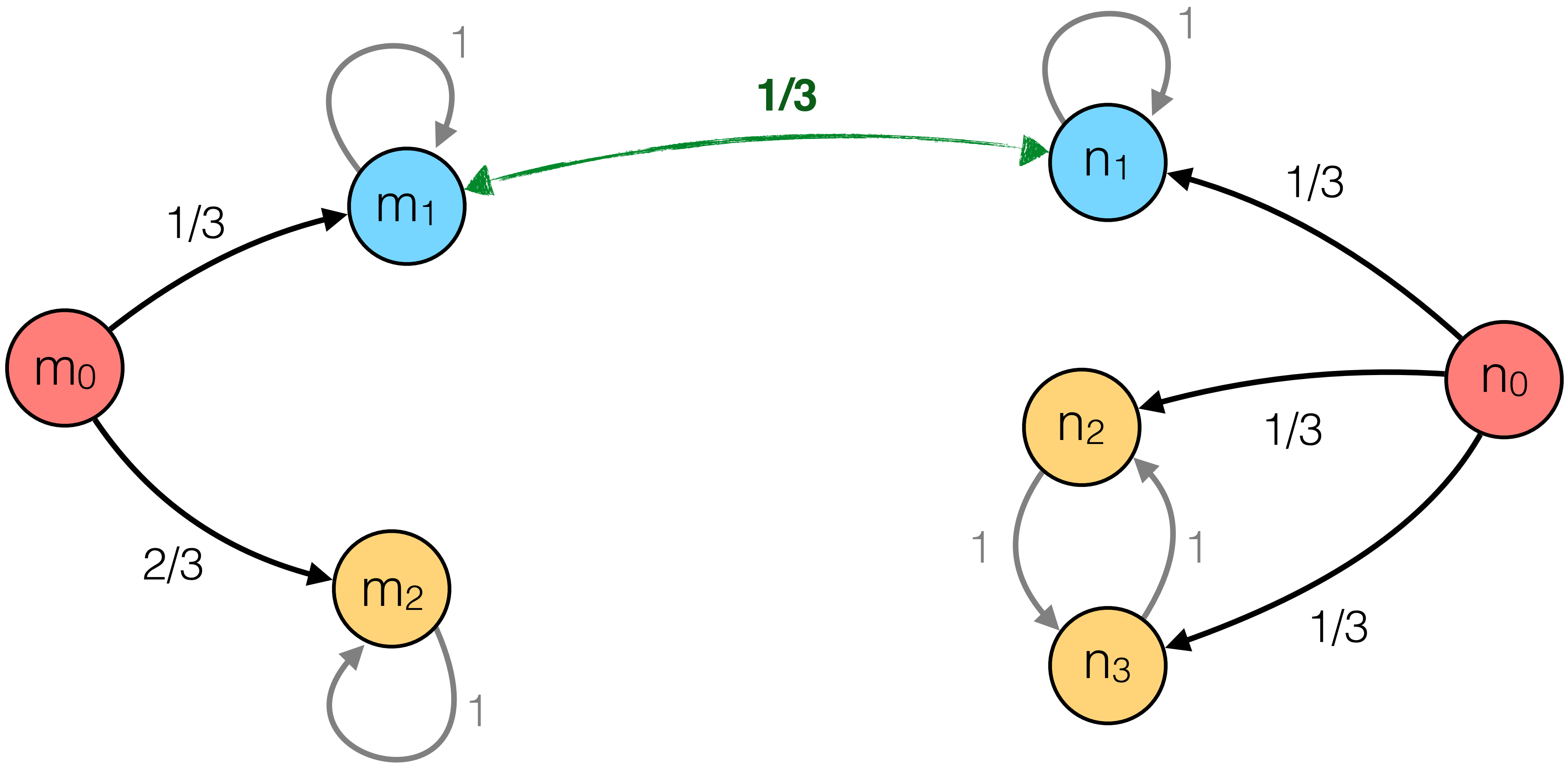

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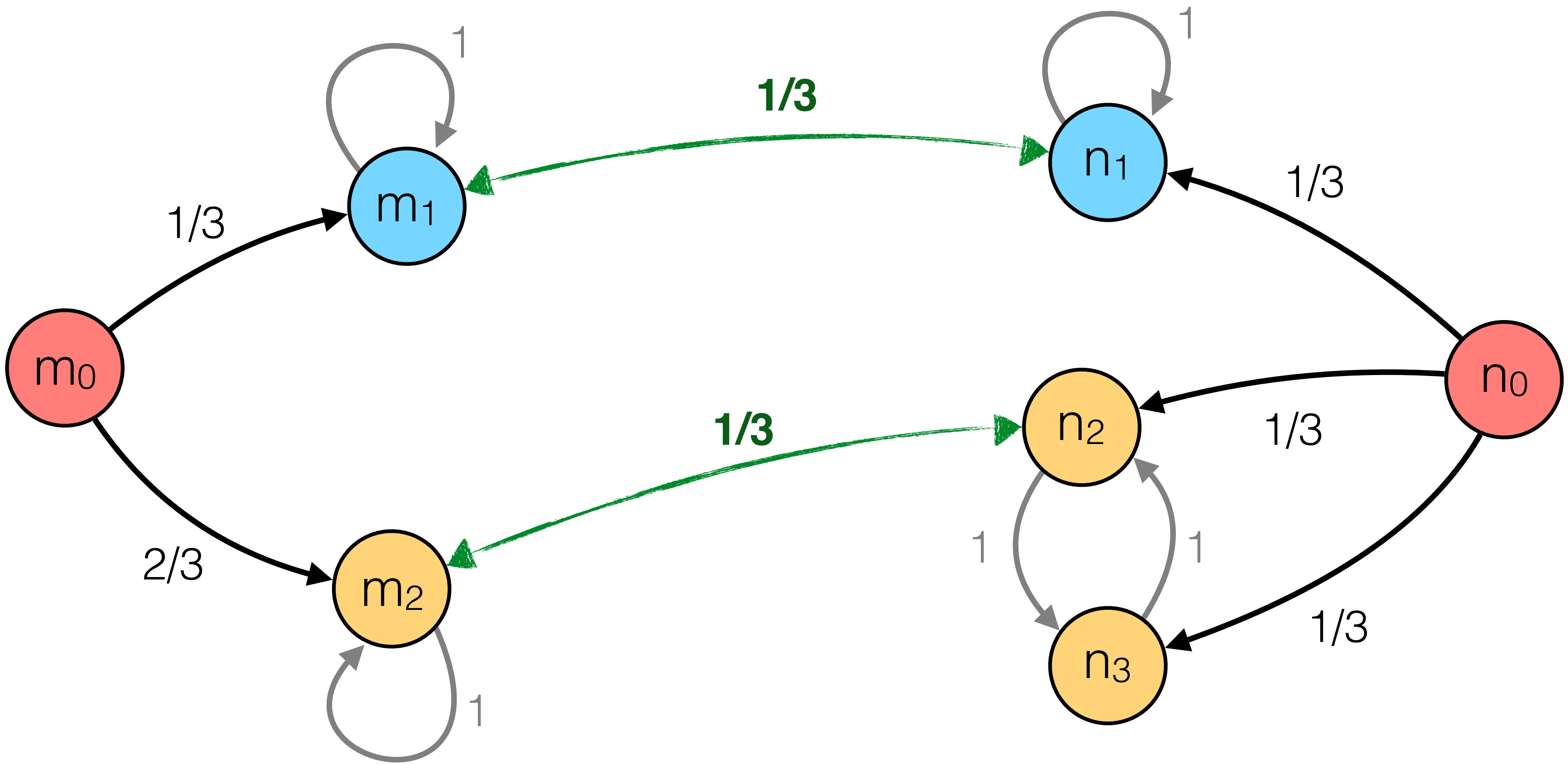

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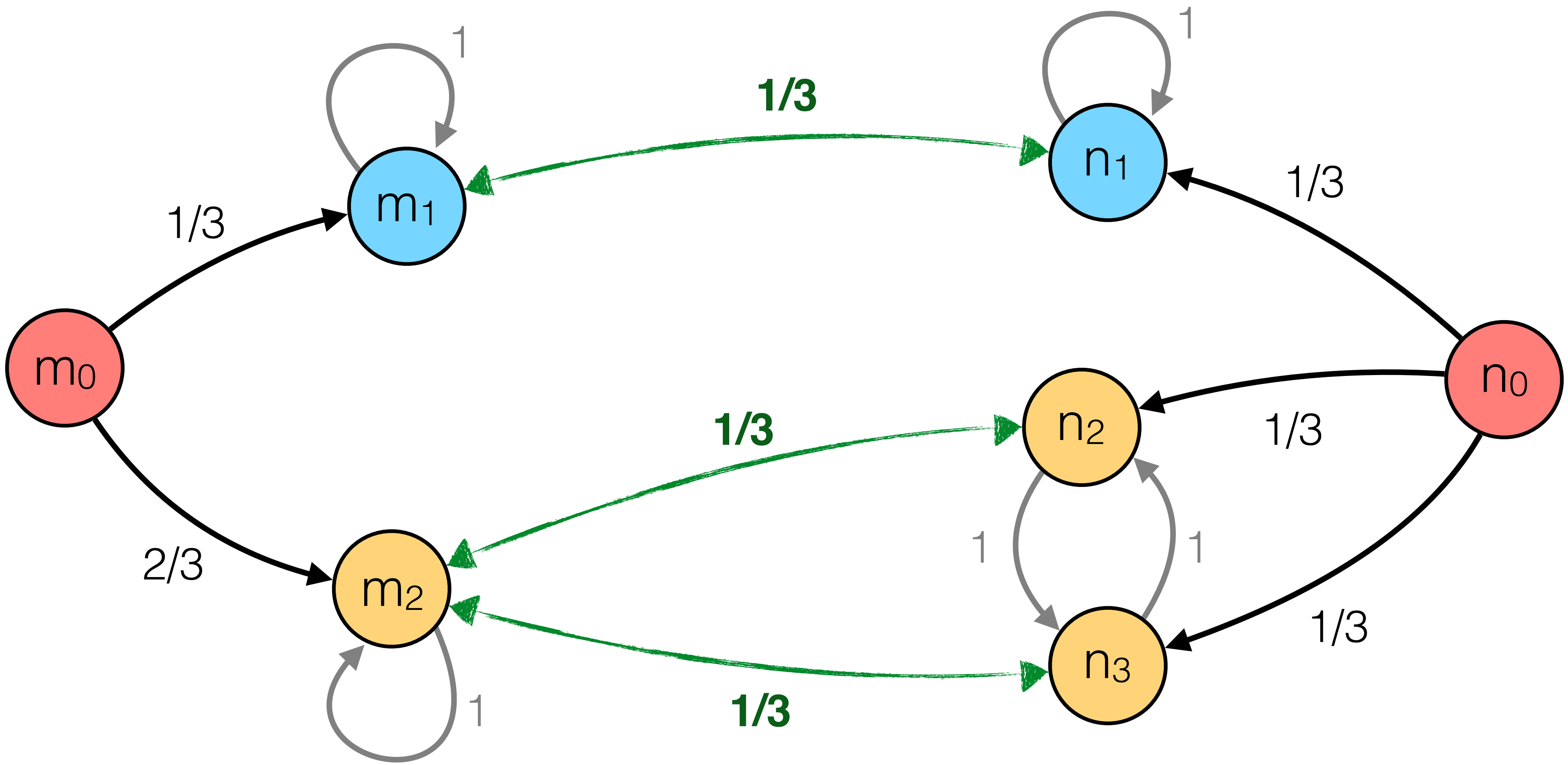

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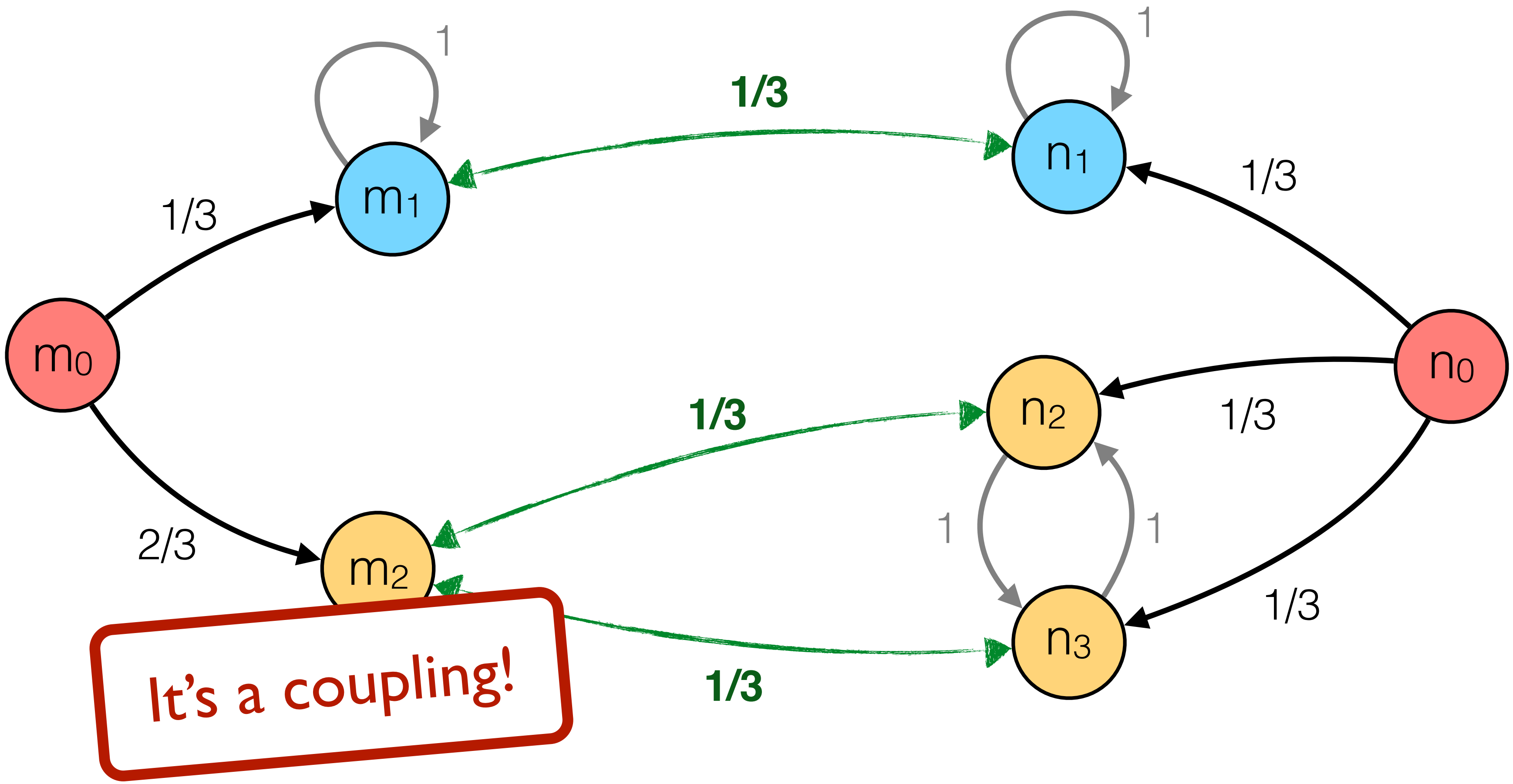

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Coupling

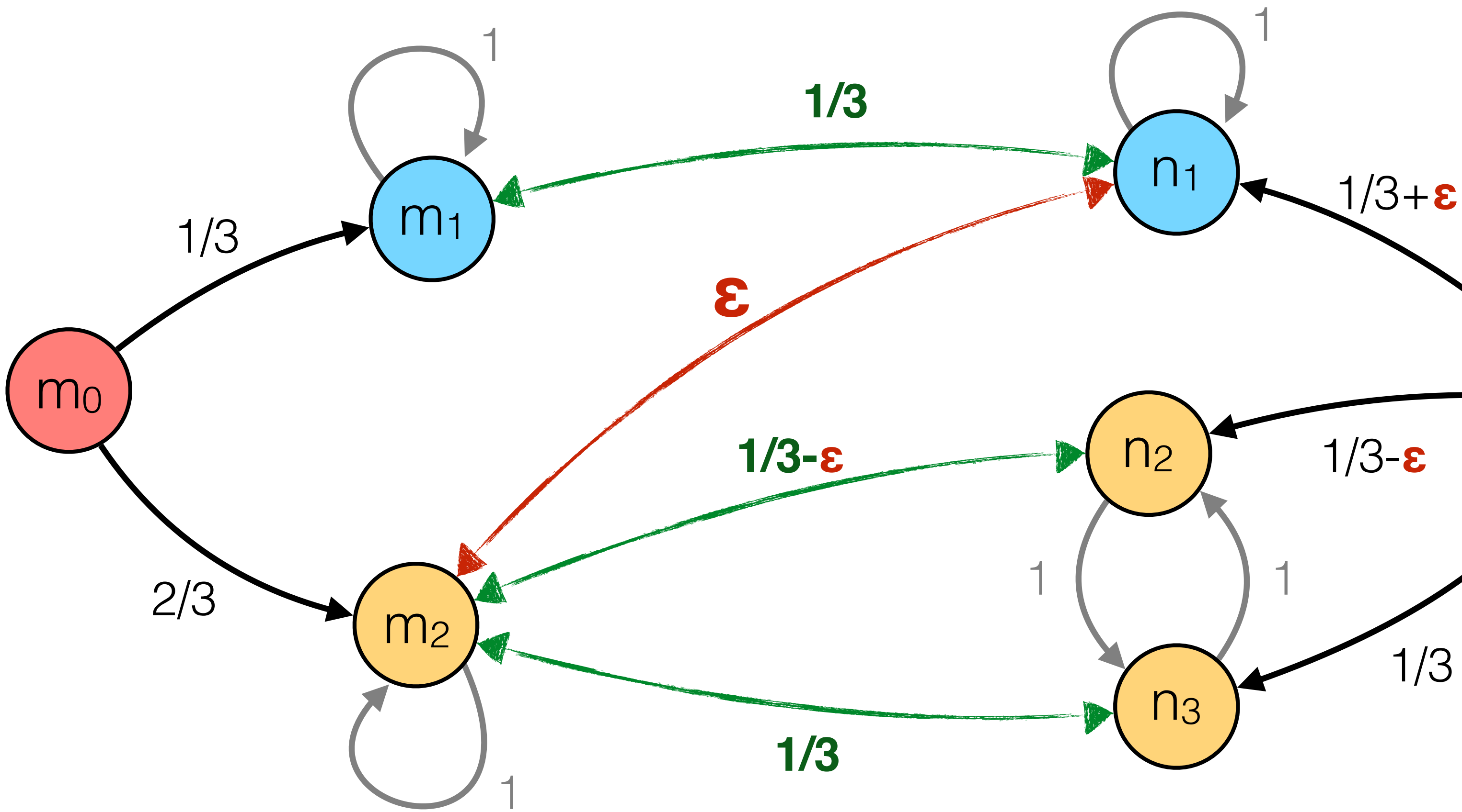
Definition (W. Doeblin 36)

A *coupling* of a pair (μ,ν) of probability distributions on M is a distribution ω on M×M such that

- $\sum_{n \in M} \omega(m,n) = \mu(m)$ *(left marginal)*
- $\sum_{m \in M} \omega(m,n) = \nu(n)$ *(right marginal)*.

One can think of a coupling as a measure-theoretic relation between probability distribution

A quantitative generalization



$$\text{minimize} \sum_{u,v \in M} \omega(u,v)\, d(u,v)$$

A quantitative generalization of probabilistic bisimilarity

(Desharnais et al.'99 & Worrell-van Breugel'00)

The **λ**-discounted **probabilistic bisimilarity pseudometric** is the smallest $d_\lambda : M \times M \to [0,1]$ such that

$$d_\lambda(m,n) = \Gamma_\lambda(d_\lambda) = \begin{cases} 1 & \text{if } \ell(m) \neq \ell(n) \\ \lambda\, K(d_\lambda)(\tau(m),\tau(n)) & \text{otherwise} \end{cases}$$

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transition probabilities

Kantorovich distance

$$K(d)(\mu,\nu) = \min_{\omega \in \Omega(\mu,\nu)} \sum_{u,v \in M} \omega(u,v)\, d(u,v)$$

Talk Outline

- ★ **Probabilistic bisimilarity distance**
  - fixed point characterization (Kantorovich oper.)

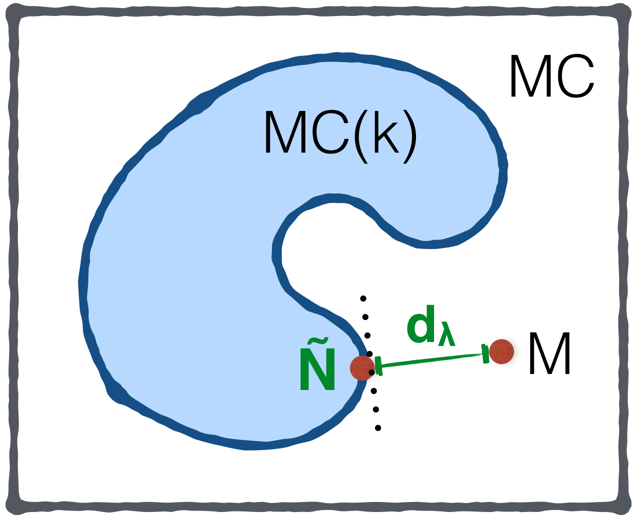
- ★ **Metric-based Optimal Approximate Minimization**
  - *Closest Bounded Approximant* (CBA)
    — bilinear characterization + complexity
  - *Minimum Significant Approximant Bound* (MSAB)
    — complexity (+ characterization)
  - *Expectation Maximization-like algorithm*
    — 2 heuristics + experimental results

The CBA-λ problem

CBA wrt d_λ

Instance: An MC M, and $k \in \mathbb{N}$

Output: An MC Ñ, with at most k states minimizing $d_\lambda(m_0, \tilde{n}_0)$



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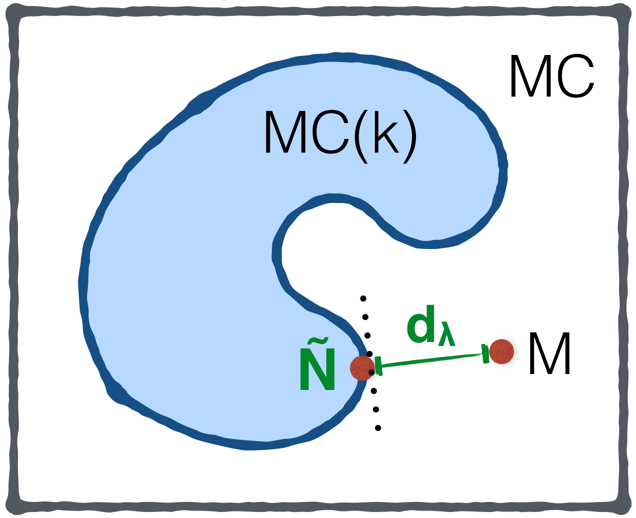

$$d_\lambda(m_0, \tilde{n}_0) = \inf \{ d_\lambda(m_0, n_0) \mid N \in MC(k) \}$$

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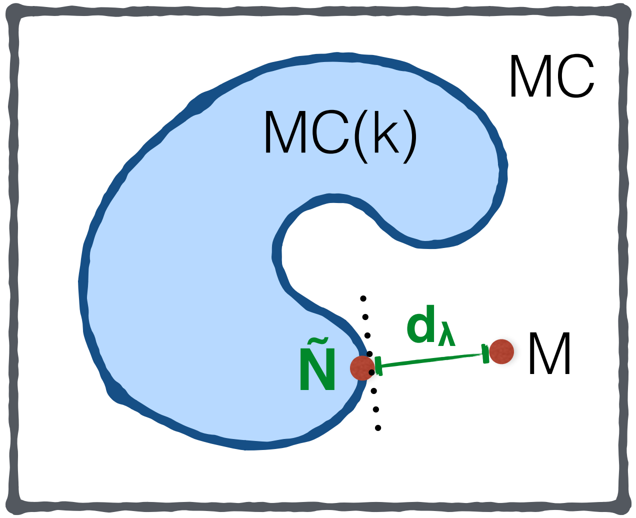

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we get a solution iff the infimum is a minimum

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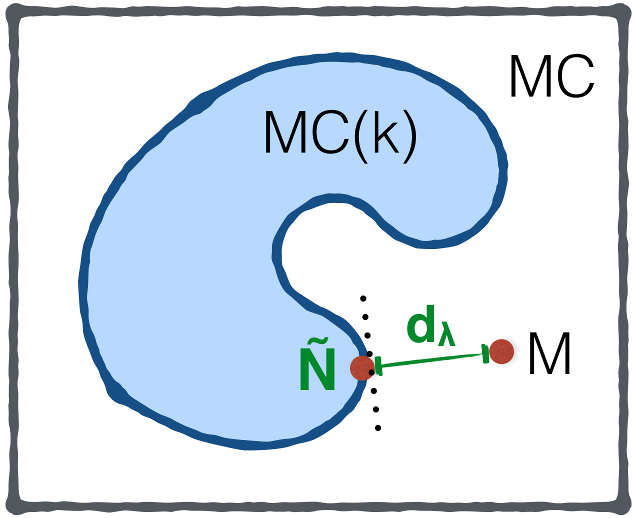

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generalization of bisimilarity quotient

CBA-λ as a Bilinear Program

$d_\lambda(m_0, \tilde{n}_0) = \inf \{ d_\lambda(m_0, n_0) \mid N \in MC(k) \}$

CBA-λ as a Bilinear Program

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$$= \inf \{ d(m_0,n_0) \mid \Gamma_\lambda(d) \leq d,\ N \in MC(k) \}$$

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$d_\lambda(m_0,\tilde{n}_0) = \inf \{ d_\lambda(m_0,n_0) \mid N \in MC(k) \}$
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$$
\begin{array}{lll}
\text{mimimize} & d_{m_0,n_0} & \\
\text{such that} & d_{m,n} = 1 & \ell(m) \neq \alpha(n) \\
& \lambda \sum_{(u,v)\in M\times N} c^{m,n}_{u,v} \cdot d_{u,v} \leq d_{m,n} & \ell(m) = \alpha(n) \\
& \sum_{v\in N} c^{m,n}_{u,v} = \tau(m)(u) & m,u \in M,\ n \in N \\
& \sum_{u\in M} c^{m,n}_{u,v} = \theta_{n,v} & m \in M,\ n,v \in N \\
& c^{m,n}_{u,v} \geq 0 & m,u \in M,\ n,v \in N
\end{array}
$$

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$= \inf \{ d(m_0, n_0) \mid \Gamma_\lambda(d) \leq d, N \in MC(k) \}$

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	$\sum_{v \in N} c^{m,n}_{u,v} = \tau(m)(u)$	$m, u \in M,\ n \in N$
	$\sum_{u \in M} c^{m,n}_{u,v} = \theta_{n,v}$	$m \in M,\ n, v \in N$
	$c^{m,n}_{u,v} \geq 0$	$m, u \in M,\ n, v \in N$

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such that	$d_{m,n} = 1$	$\ell(m) \neq \alpha(n)$
	$\lambda \sum_{(u,v) \in M \times N} c^{m,n}_{u,v} \cdot d_{u,v} \leq d_{m,n}$	$\ell(m) = \alpha(n)$
	$\sum_{v \in N} c^{m,n}_{u,v} = \tau(m)(u)$	$m, u \in M,\ n \in N$
	$\sum_{u \in M} c^{m,n}_{u,v} = \theta_{n,v}$	$m \in M,\ n, v \in N$
	$c^{m,n}_{u,v} \geq 0$	$m,$

variable!

N = {1…k}

CBA-λ as a Bilinear Program

$$d_\lambda(m_0,\tilde{n}_0) = \inf \{\, d_\lambda(m_0,n_0) \mid N \in MC(k) \,\}$$
$$= \inf \{\, d(m_0,n_0) \mid \Gamma_\lambda(d) \leq d,\ N \in MC(k) \,\}$$

$$\begin{array}{lll}
\text{mimimize} & d_{m_0,n_0} & \\
\text{such that} & d_{m,n} = 1 & \\
 & \lambda \sum_{(u,v)\in M\times N} c^{m,n}_{u,v} \cdot d_{u,v} \leq d_{m,n} & \ell(m) = \alpha(n) \\
 & \sum_{v\in N} c^{m,n}_{u,v} = \tau(m)(u) & m,u \in M,\ n \in N \\
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 & c^{m,n}_{u,v} \geq 0 & m,
\end{array}$$

what labels should the MC N have?

variable!

N = {1…k}

CBA-λ as a Bilinear Program

Lemma (Meaningful labels)

For any $N \in MC(k)$, there exists $N' \in MC(k)$ with labels taken from M, such that $d_\lambda(M,N) \geq d_\lambda(M,N')$

CBA-λ as a Bilinear Program

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& 1 - \alpha_{n,l} \leq d_{m,n} \leq 1 & n \in N,\, l \in L(\mathcal{M}),\, \ell(m) \neq l \\
& \alpha_{n,l} \cdot \alpha_{n,l'} = 0 & n \in N,\, l, l' \in L(\mathcal{M}),\, l \neq l' \\
& \sum_{l \in L(\mathcal{M})} \alpha_{n,l} = 1 & n \in N \\
& \sum_{v\in N} c^{m,n}_{u,v} = \tau(m)(u) & m, u \in M,\, n \in N \\
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\end{array}
$$

CBA-λ as a Bilinear Program

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\end{array}
$$

CBA-λ as a Bilinear Program

this characterization has two main consequences…

1. CBA-λ admits always a solution (finite intersection of closed subsets)
2. CBA-λ can be approximated up to any precision

Complexity of CBA-λ

actually, its decision variant!

Complexity of CBA-λ

actually, its decision variant!

Complexity Upper-bound

BA-λ is in **PSPACE**

Proof sketch: *we can encode the question ⟨M,k,ε⟩∈BA-λ to that of checking the feasibility of a set of bilinear inequalities. This can be encoded as a decision problem for the existential theory of the reals, thus it can be solved in PSPACE [Canny—STOC88].*

Complexity of CBA-λ

actually, its decision variant!

Complexity Upper-bound

BA-λ is in **PSPACE**

Complexity lower-bound

BA-λ is **NP-hard**

Proof idea: *we provide a reduction from VERTEX COVER.*
(see the appendix for a sketch of the reduction)

Complexity of CBA-λ

actually, its decision variant!

Complexity Upper-bound

BA-λ is in **PSPACE**

Complexity lower-bound

BA-λ is **NP-hard**

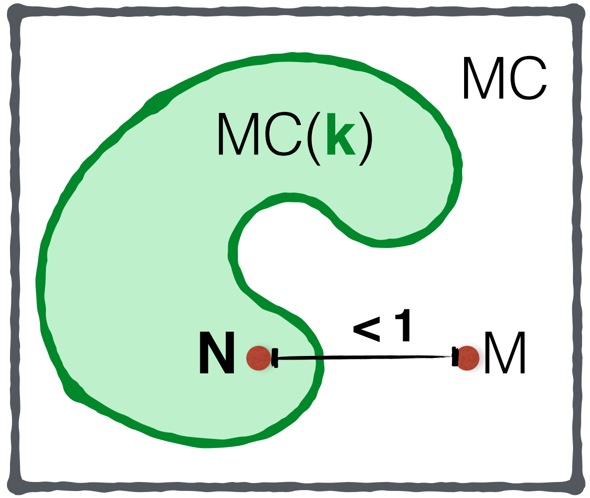
unlikely to solve CBA as simple linear program

The MSAB-λ problem

The MSAB wrt d_λ

Instance: An MC M

Output: The smallest k such that $d_\lambda(m_0,n_0)<1$, for some $N \in MC(k)$



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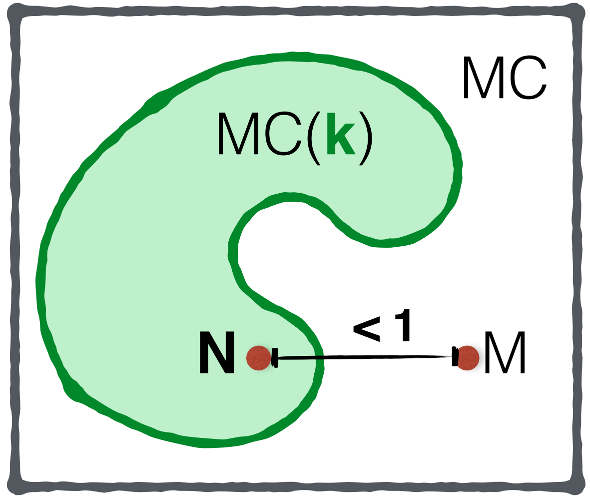

For **λ<1**, the MSAB-λ problem is trivial, because the solution is always k=1

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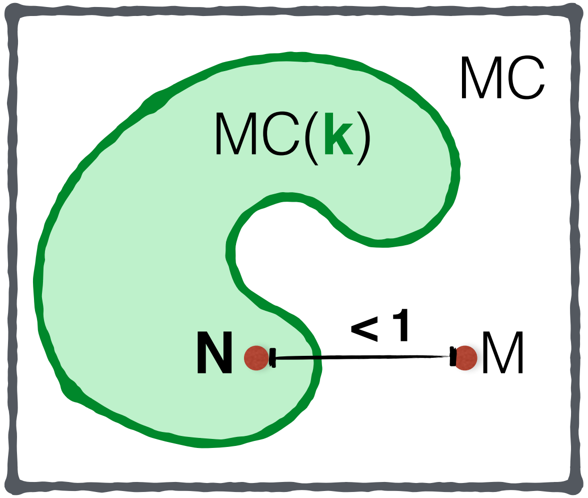

For **λ<1**, the MSAB-λ problem is trivial, because the solution is always k=1

For **λ=1**, the same problem is surprisingly difficult…

Complexity of MSAB-1

actually, its decision variant!

Theorem

SBA-1 is **NP-complete**

Proof idea: *we provide a reduction from VERTEX COVER.*
(see the appendix for a sketch of the reduction)

Towards an Algorithm…

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- The CBA can be solved as a bilinear program. Theoretically nice, but practically unfeasible!

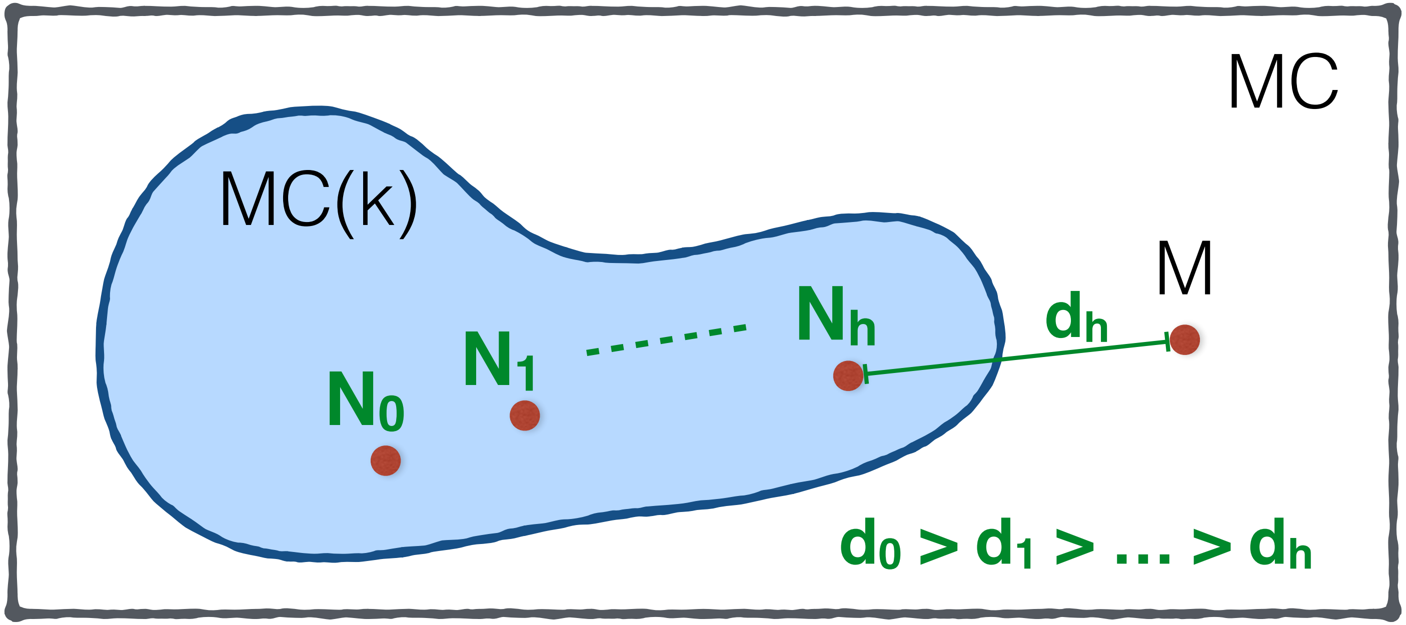
  (our implementation in PENBMI can handle MCs with at most 5 states…)

Towards an Algorithm…

- The CBA can be solved as a bilinear program. Theoretically nice, but practically unfeasible!
  (our implementation in PENBMI can handle MCs with at most 5 states…)

- We are happy with **sub-optimal solutions** if they can be obtained by a practical algorithm.

EM-like Algorithm



- Given the MC M and an initial approximant N_0
- it produces a sequence $N_0, \ldots, N_h$ of approximants having strictly decreasing distance from M
- N_h may be a sub-optimal solution of CBA-λ

EM-like Algorithm

Algorithm 1

Input: $\mathcal{M} = (M, \tau, \ell)$, $\mathcal{N}_0 = (N, \theta_0, \alpha)$, and $h \in \mathbb{N}$.

1. $i \leftarrow 0$
2. **repeat**
3. $\quad i \leftarrow i + 1$
4. $\quad$ compute $\mathcal{C} \in \Omega(\mathcal{M}, \mathcal{N}_{i-1})$ such that $\delta_\lambda(\mathcal{M}, \mathcal{N}_{i-1}) = \gamma_\lambda^{\mathcal{C}}(\mathcal{M}, \mathcal{N}_{i-1})$
5. $\quad \theta_i \leftarrow \textsc{UpdateTransition}(\theta_{i-1}, \mathcal{C})$
6. $\quad \mathcal{N}_i \leftarrow (N, \theta_i, \alpha)$
7. **until** $\delta_\lambda(\mathcal{M}, \mathcal{N}_i) > \delta_\lambda(\mathcal{M}, \mathcal{N}_{i-1})$ or $i \geq h$
8. **return** $\mathcal{N}_{i-1}$

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Intuitive Idea

UpdateTransition assigns greater probability to transitions that are most representative of the behavior of M

Two update heuristics

- **Averaged Marginal (AM)**: given N_k we construct N_{k+1} by averaging the marginal of certain "coupling variables" obtained by optimizing the number of occurrences of the edges that are most likely to be seen in M.

- **Averaged Expectations (AE)**: similar to the above, but now the N_{k+1} looks only the expectation of the number of occurrences of the edges likely to be found in M.

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UpdateTransition in polynomial time for both heuristics!

Case	$\|M\|$	k	$\lambda = 1$				$\lambda = 0.8$			
			δ_λ-init	δ_λ-final	#	time	δ_λ-init	δ_λ-final	#	time
IPv4 (AM)	23	5	0.775	0.054	3	4.8	0.576	0.025	3	4.8
	53	5	0.856	0.062	3	25.7	0.667	0.029	3	25.9
	103	5	0.923	0.067	3	116.3	0.734	0.035	3	116.5
	53	6	0.757	0.030	3	39.4	0.544	0.011	3	39.4
	103	6	0.837	0.032	3	183.7	0.624	0.017	3	182.7
	203	6	–	–	–	TO	–	–	–	TO
IPv4 (AE)	23	5	0.775	0.109	2	2.7	0.576	0.049	3	4.2
	53	5	0.856	0.110	2	14.2	0.667	0.049	3	21.8
	103	5	0.923	0.110	2	67.1	0.734	0.049	3	100.4
	53	6	0.757	0.072	2	21.8	0.544	0.019	3	33.0
	103	6	0.837	0.072	2	105.9	0.624	0.019	3	159.5
	203	6	–	–	–	TO	–	–	–	TO
DrkW (AM)	39	7	0.565	0.466	14	259.3	0.432	0.323	14	252.8
	49	7	0.568	0.460	14	453.7	0.433	0.322	14	420.5
	59	8	0.646	–	–	TO	0.423	–	–	TO
DrkW (AE)	39	7	0.565	0.435	11	156.6	0.432	0.321	2	28.6
	49	7	0.568	0.434	10	247.7	0.433	0.316	2	46.2
	59	8	0.646	0.435	10	588.9	0.423	0.309	2	115.7

Table 1. Comparison of the performance of EM algorithm on the IPv4 zeroconf protocol and the classic Drunkard's Walk w.r.t. the heuristics AM and AE.

Future Work

- **Conjecture 1:** (with Nathanaël Fijalkow)
  Is BA-1 is SUM-OF-SQUARE-ROOTS-hard

- **Conjecture 2:** (by Borja Balle)
  for $\lambda<1$, BA-λ is in NP (hence NP-complete!)

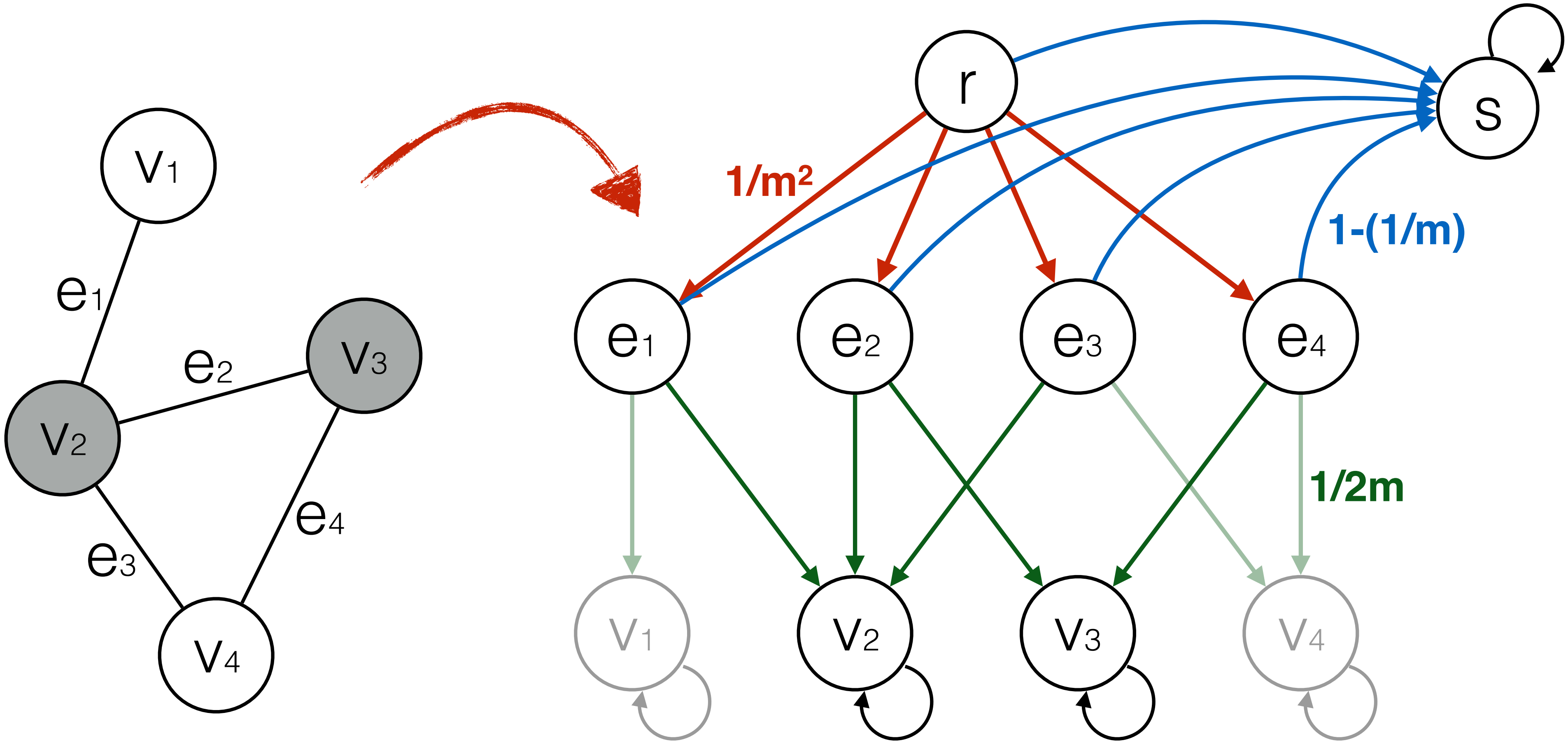
- Real/better EM-heuristics?

- What about different models/distances?

Thank you
for your attention

Appendix

BA-λ is NP-hard

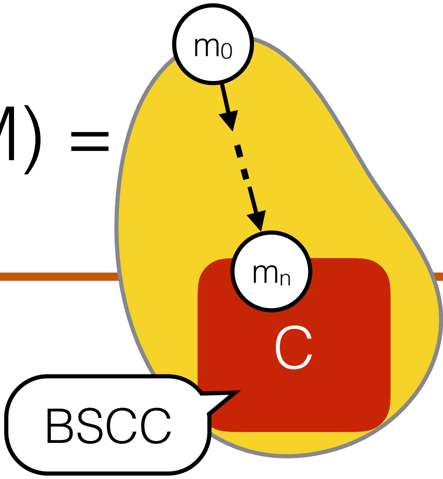


⟨G,h⟩∈VERTEX COVER iff ⟨M_G, m+h+2, $\lambda^2/2m^2$⟩∈BA-λ

Characterization of SBA-1

Lemma

Assume M be maximally collapsed. Then,

$\langle M,k \rangle \in$SBA-1 iff $\mathcal{G}(M)$ =  and $h+|C| \leq k$

number of labels in $m_0 \ldots m_{n-1}$

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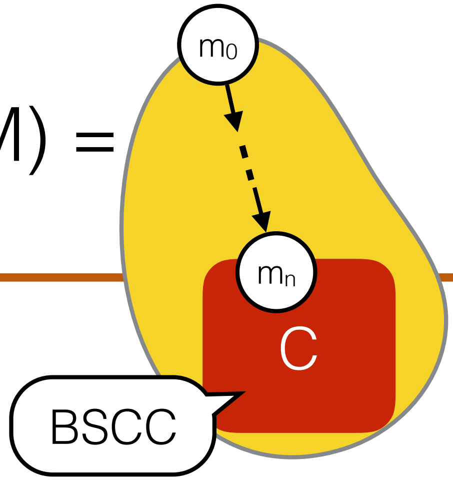
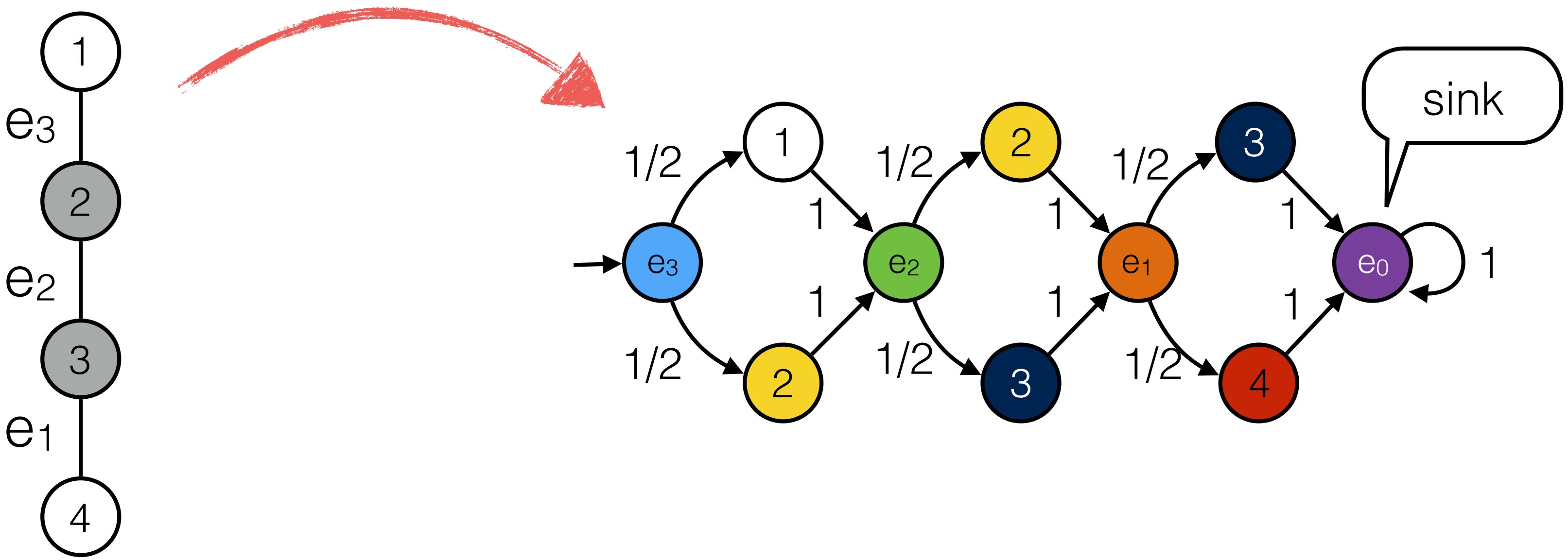


and $h+|C| \leq k$

number of labels in $m_0 \ldots m_{n-1}$

Proof sketch: *compute with Tarjan's algorithm all the SCCs of $\mathcal{G}(M)$. Then non deterministically choose a BSCC and a path to it. In poly-time we can count the number of labels in the path and the size of the BSCC.*

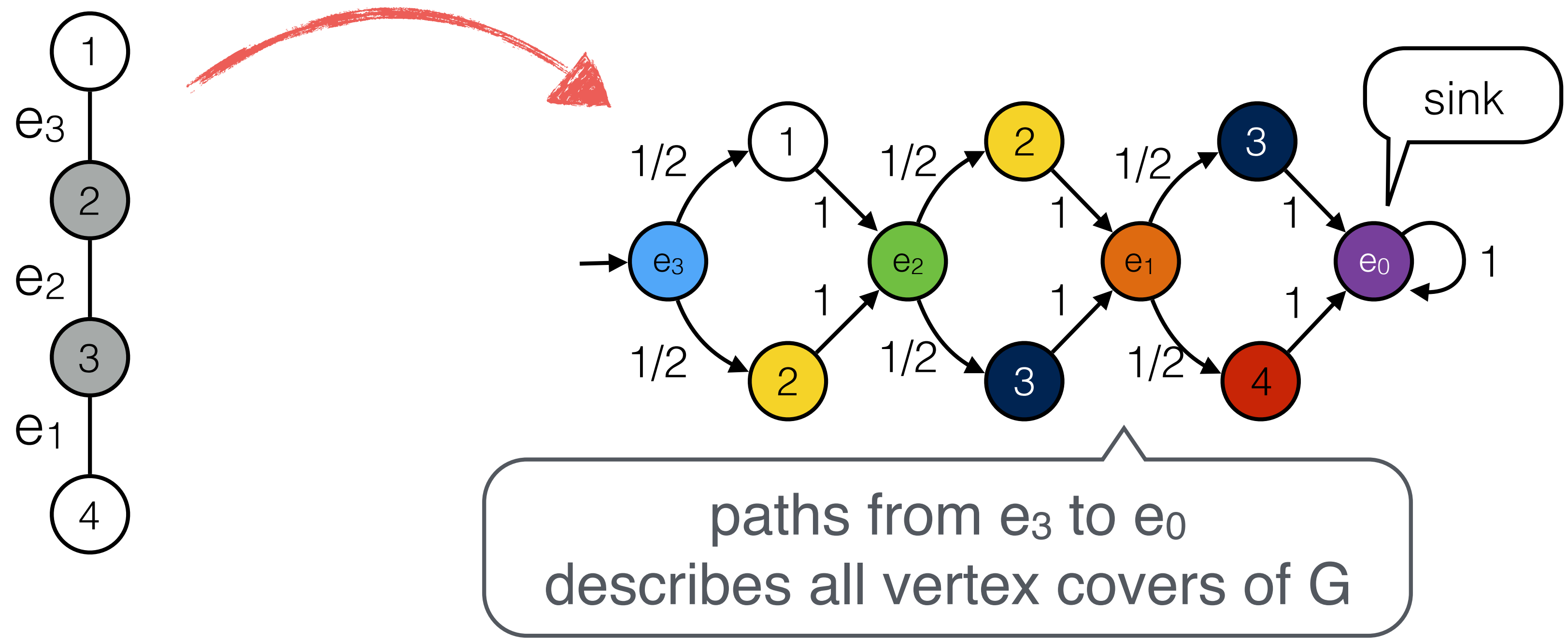
SBA-1 is **NP-hard**



Proof sketch: *by reduction to VERTEX COVER:*

$\langle G,h \rangle \in VERTEX\ COVER$ *iff* $\langle M_G, h+m+1 \rangle \in SBA\text{-}1$

SBA-1 is **NP-hard**



Proof sketch: *by reduction to VERTEX COVER:*

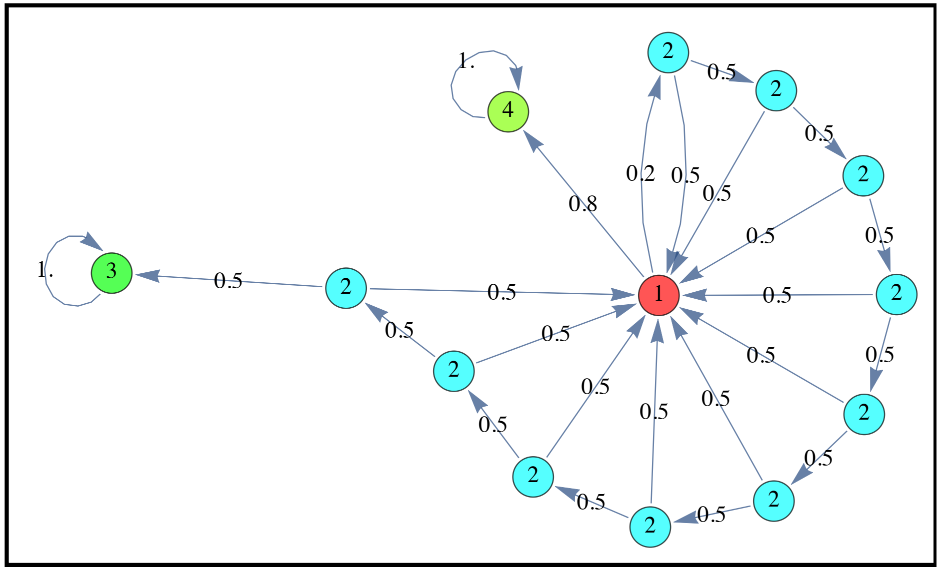
$\langle G,h\rangle \in$ *VERTEX COVER* *iff* $\langle M_G, h+m+1\rangle \in$ *SBA-1*

EM-like algorithm
(experimental results)

IPv4 Zero Conf Protocol

Averaged Marginal (AM)

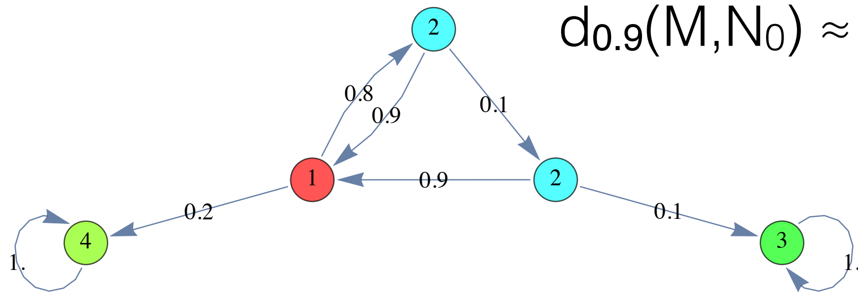
Input model



IPv4 Zero Conf Protocol

Averaged Marginal (AM)

$d_{0.9}(M,N_0) \approx 0.67$



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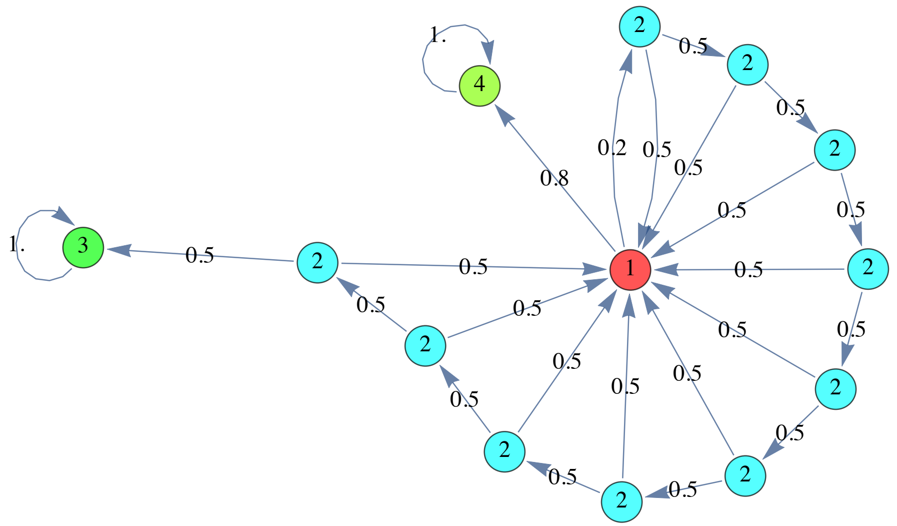

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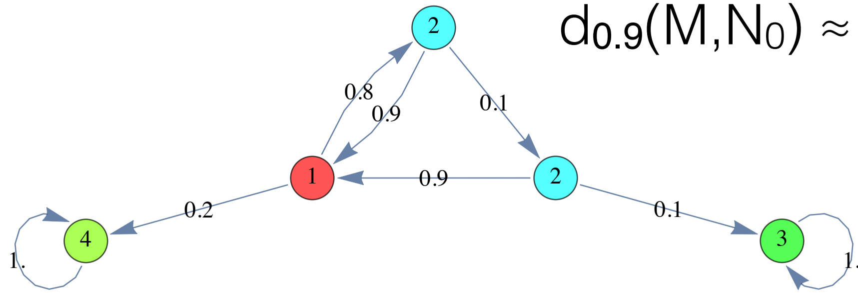
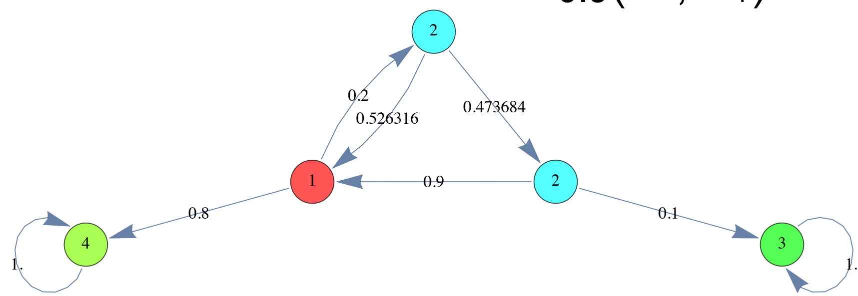
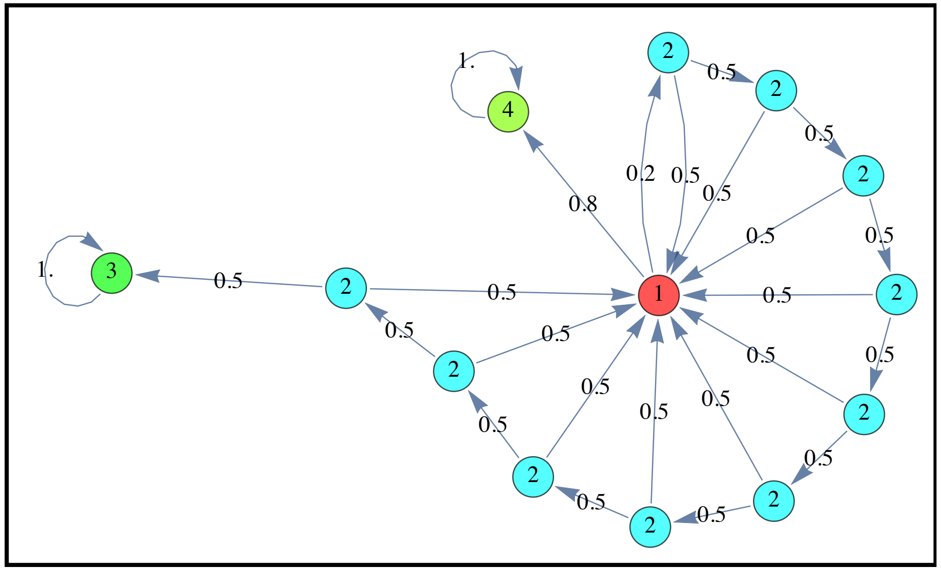


$d_{0.9}(M,N_1) \approx 0.043$



Input model



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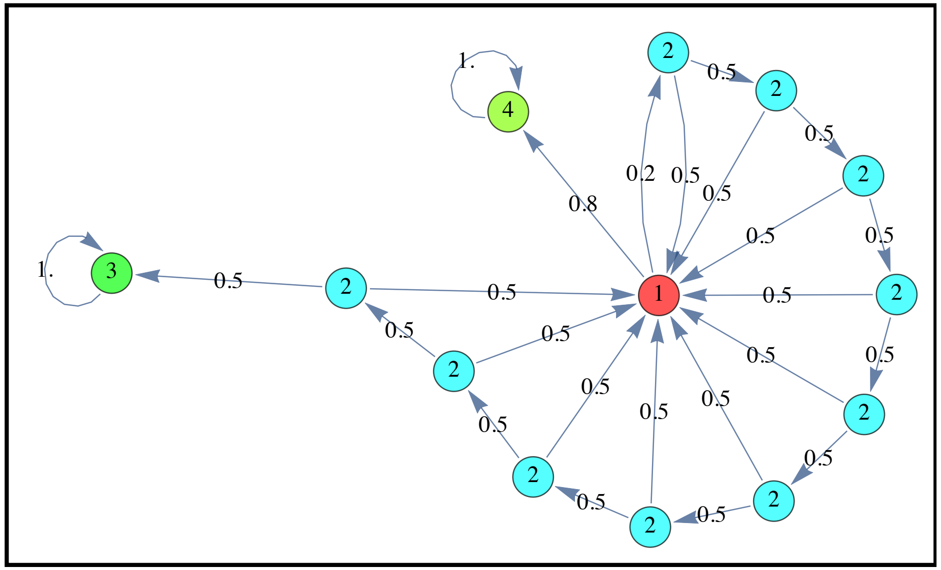

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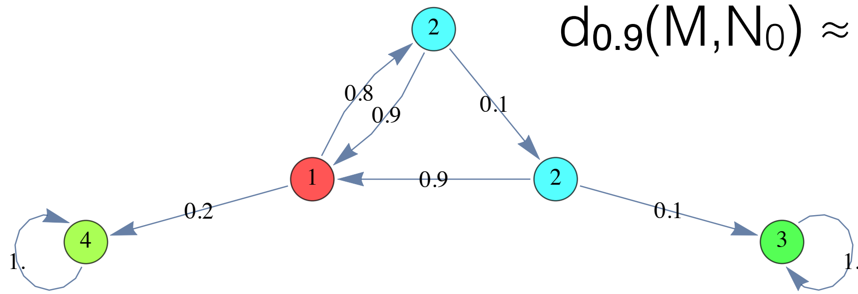

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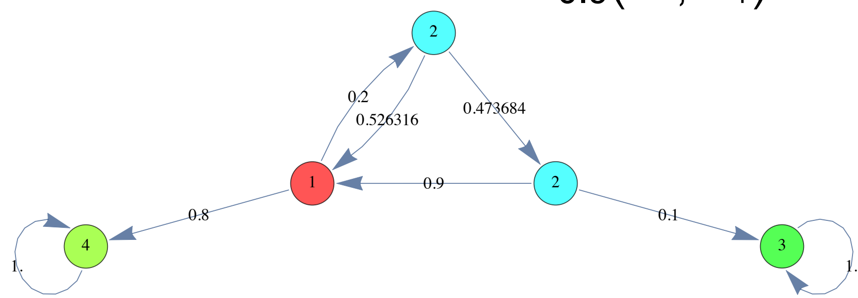
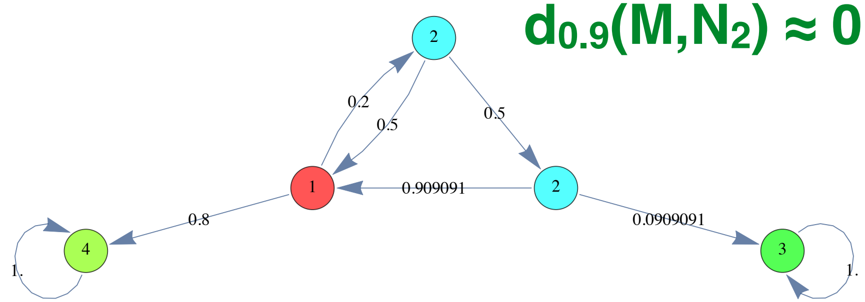


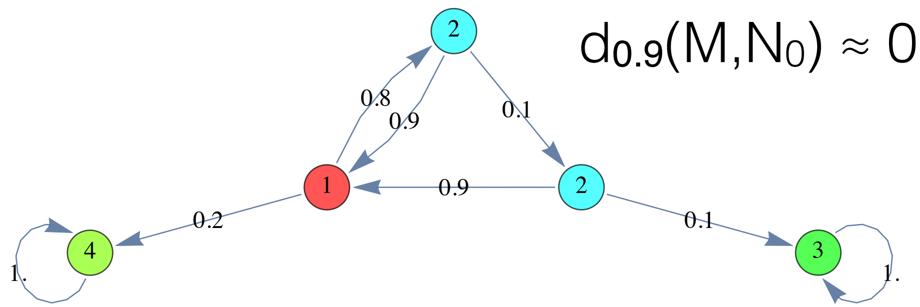
$d_{0.9}(M,N_2) \approx 0.041$



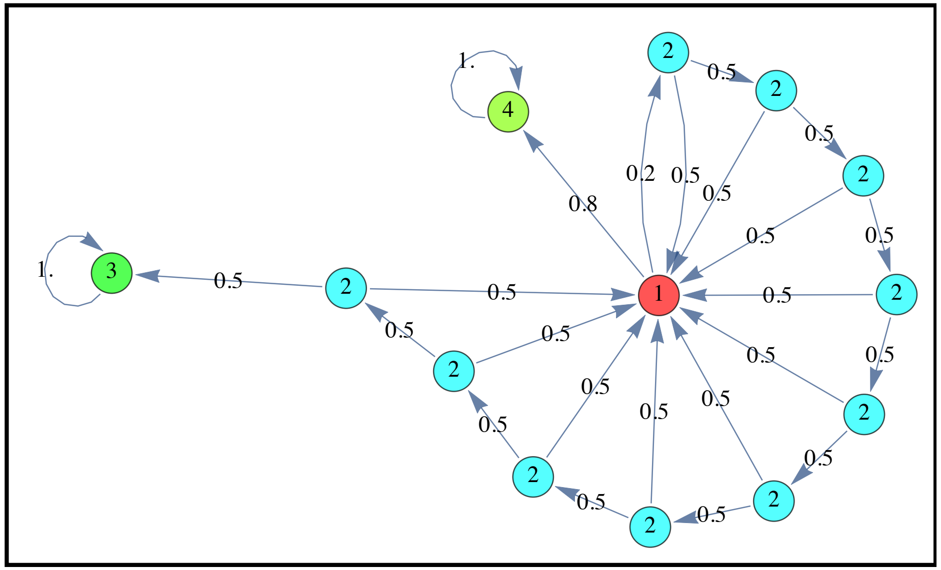
IPv4 Zero Conf Protocol

Averaged Expectations (AE)

$d_{0.9}(M,N_0) \approx 0.67$



Input model



IPv4 Zero Conf Protocol

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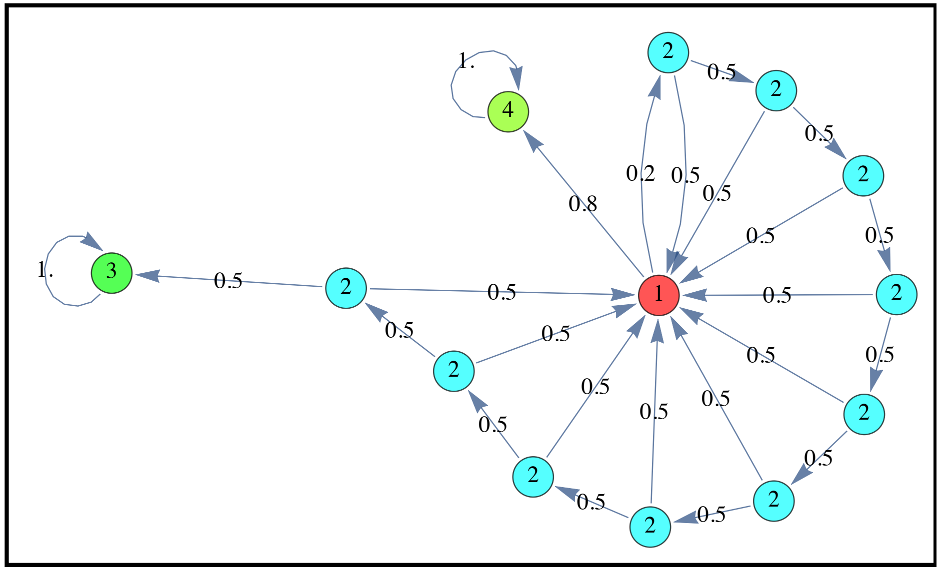

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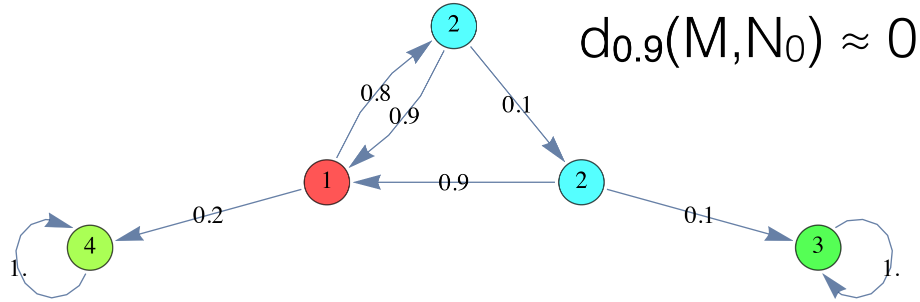
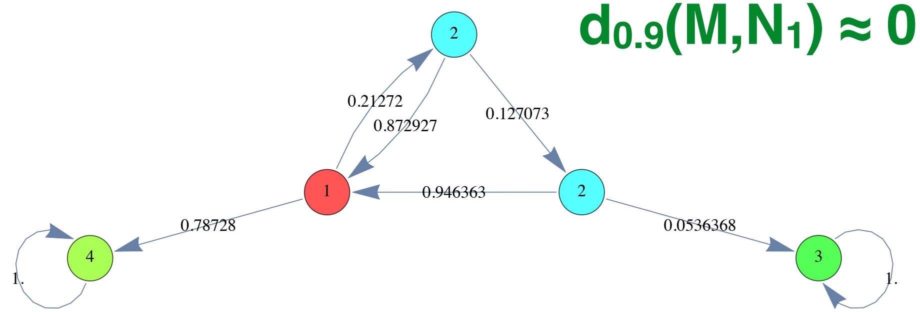


$d_{0.9}(M,N_1) \approx 0.08$



IPv4 Zero Conf Protocol

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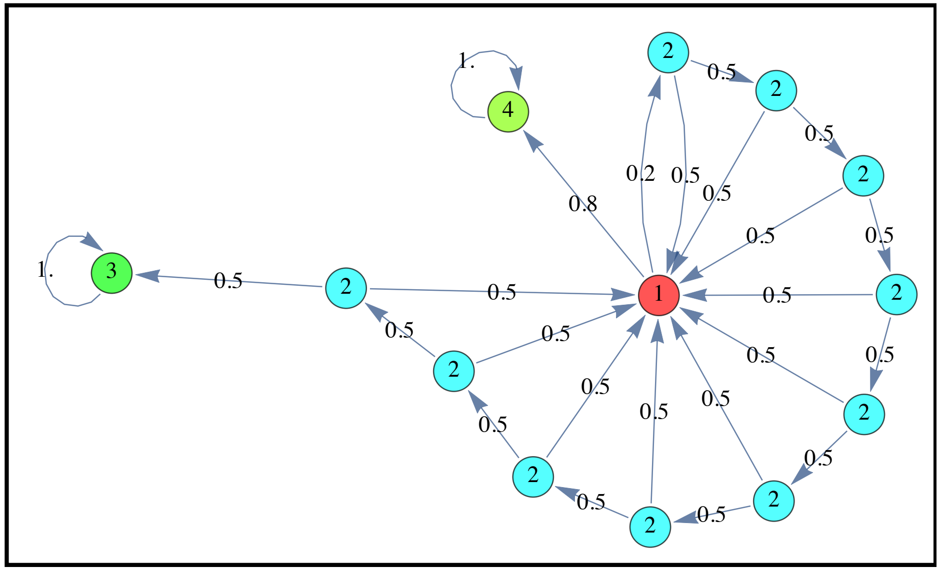

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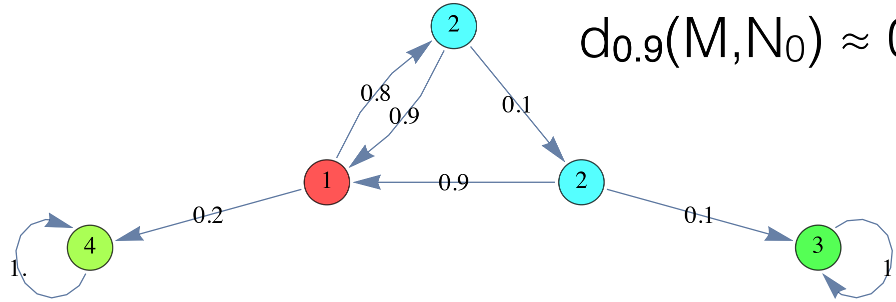
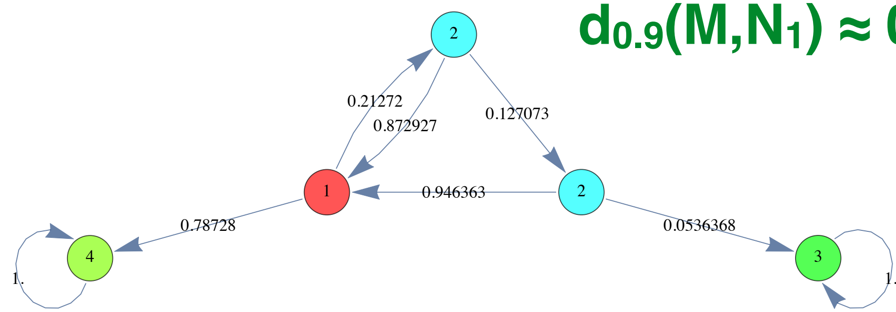
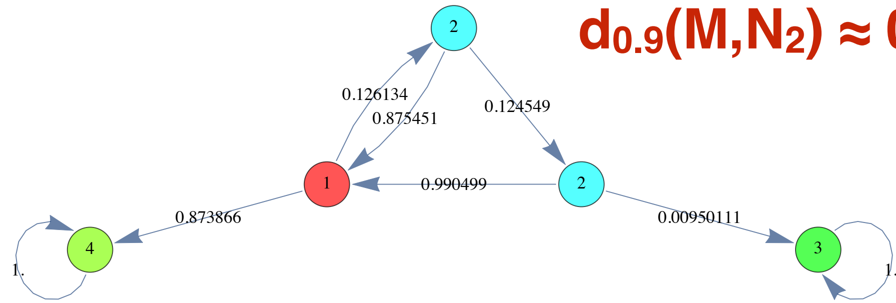


$d_{0.9}(M,N_1) \approx 0.08$



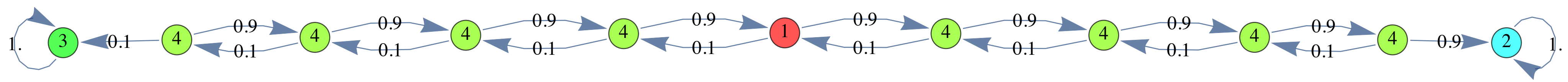
$d_{0.9}(M,N_2) \approx 0.11$



Drunkard's Walk

Averaged Marginal (AM)

Input model



Drunkard's Walk

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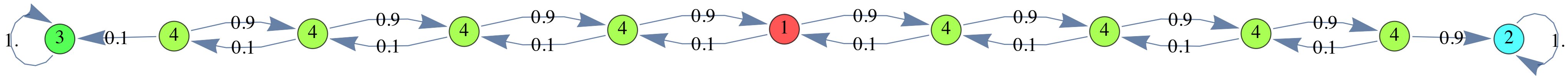
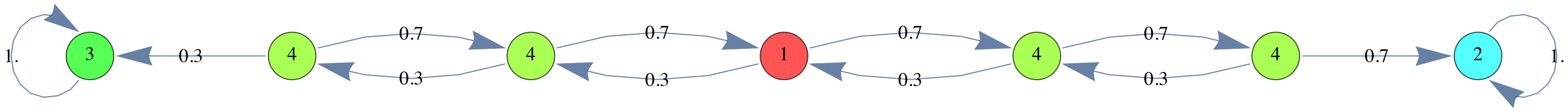


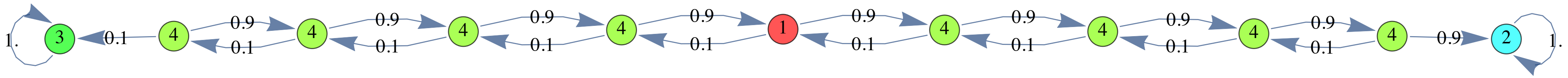


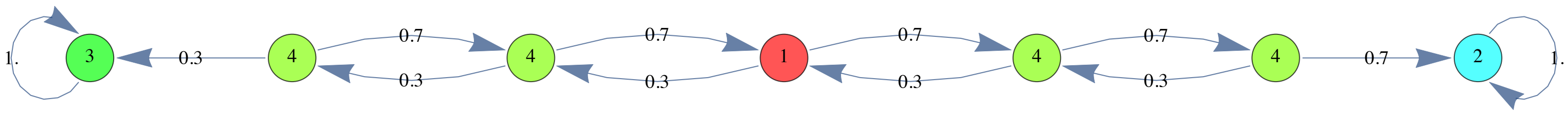
$d_{0.9}(M,N_0) \approx 0.64$

Drunkard's Walk

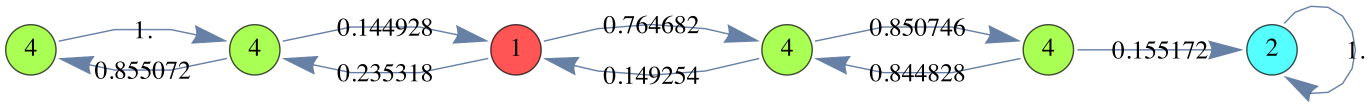
Averaged Marginal (AM)

Input model





$d_{0.9}(M,N_0) \approx 0.64$

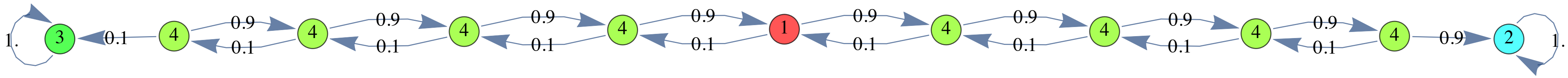


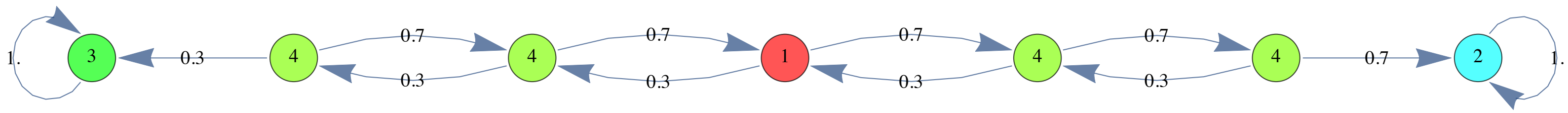
$d_{0.9}(M,N_1) \approx 0.56$

Drunkard's Walk

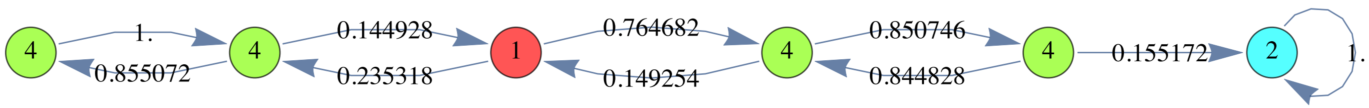
Averaged Marginal (AM)

Input model

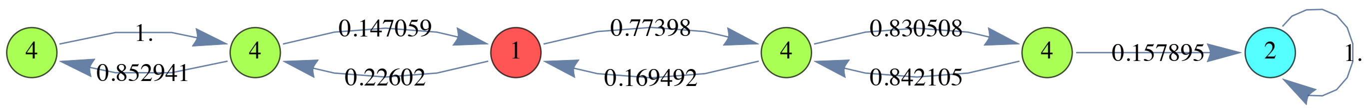




$d_{0.9}(M,N_0) \approx 0.64$



$\mathbf{d_{0.9}(M,N_1) \approx 0.56}$

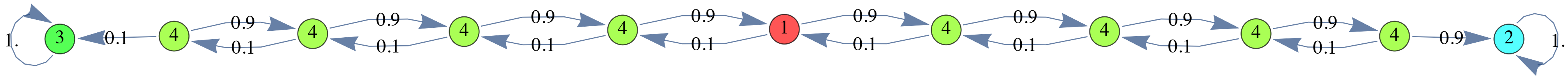


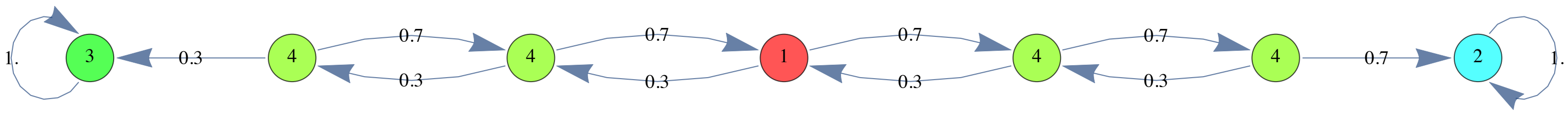
$\mathbf{d_{0.9}(M,N_2) \approx 0.567}$

Drunkard's Walk

Averaged Expectations (AE)

Input model



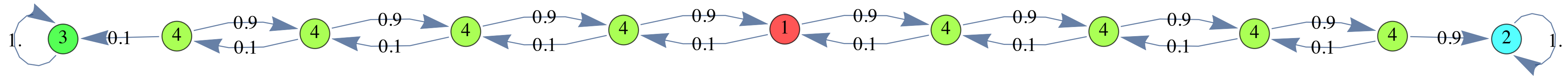


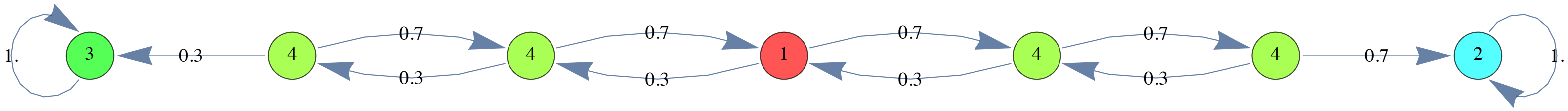
$\delta_{0.9}(M, N_0) \approx 0.64$

Drunkard's Walk

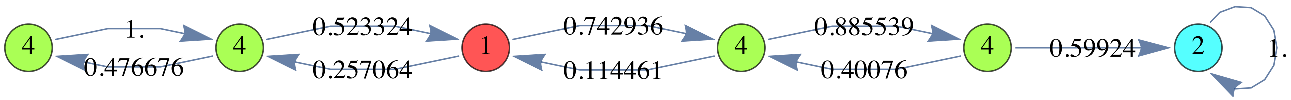
Averaged Expectations (AE)

Input model





$\delta_{0.9}(M,N_0) \approx 0.64$

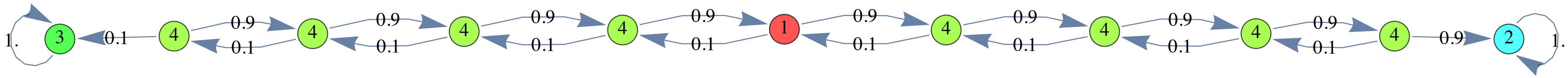


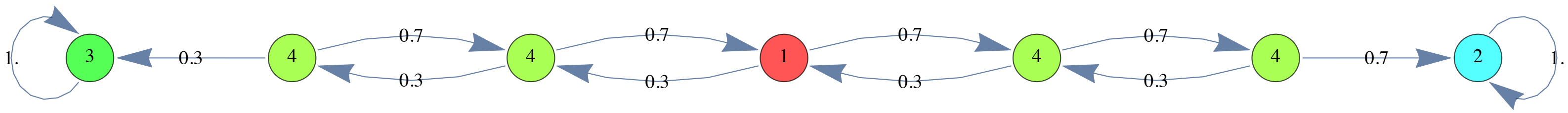
$\delta_{0.9}(M,N_1) \approx 0.56$

Drunkard's Walk

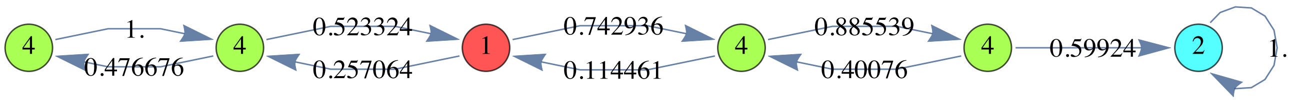
Averaged Expectations (AE)

Input model

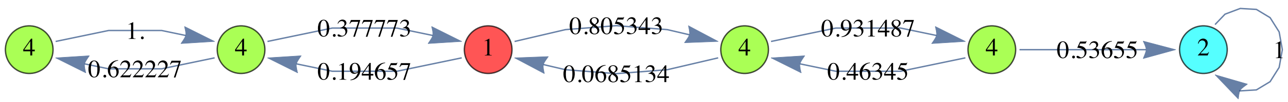




$\delta_{0.9}(M,N_0) \approx 0.64$



$\delta_{0.9}(M,N_1) \approx 0.56$

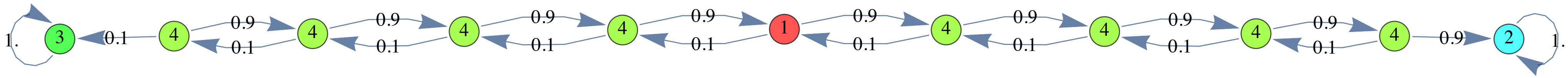


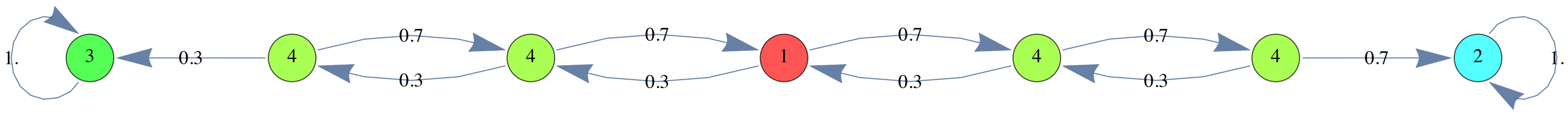
$\delta_{0.9}(M,N_2) \approx 0.543$

Drunkard's Walk

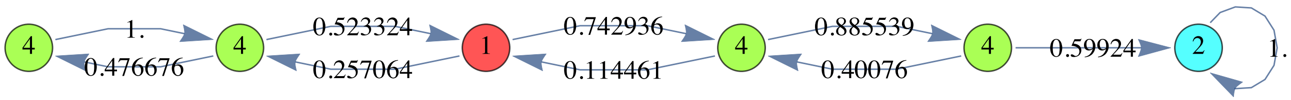
Averaged Expectations (AE)

Input model

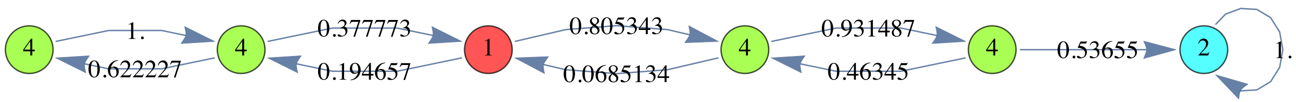




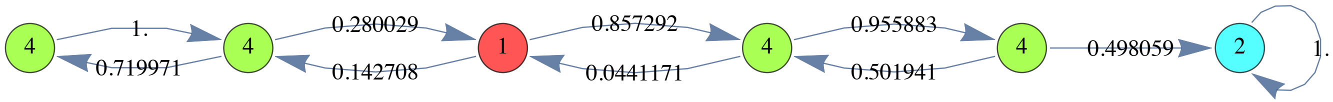
$\delta_{0.9}(M,N_0) \approx 0.64$



$\delta_{0.9}(M,N_1) \approx 0.56$



$\delta_{0.9}(M,N_2) \approx 0.543$



$\boldsymbol{\delta_{0.9}(M,N_3) \approx 0.540}$