### On the Metric-based Approximate Minimization of Markov Chains\*

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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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### minimize d

Closest Bounded Approximant (CBA)



Minimum Significant Approximant Bound (MSAB)



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Minimum Significant Approximant Bound (MSAB)



minimize k

minimize d

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



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## Talk Outline

### **\*** Probabilistic bisimilarity distance

- fixed point characterization (Kantorovich oper.)
- remarkable properties
- relation with probabilistic model checking

### **\*** Metric-based Optimal Approximate Minimization

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









## Coupling

### **Definition (W. Doeblin 36)**

A coupling of a pair ( $\mu$ , $\nu$ ) of probability distributions on M is a distribution  $\omega$  on M×M such that

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

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

### A quantitative generalization



# A quantitative generalization of probabilistic bisimilarity

The **λ**-discounted *probabilistic bisimilarity pseudometric* is the smallest d<sub>λ</sub>: M×M→[0,1] such that

$$d_{\lambda}(m,n) = \begin{cases} 1 & \text{if } \ell(m) \neq \ell(n) \\ \min_{\boldsymbol{\omega} \in \Omega(\tau(m),\tau(n))} \lambda \sum_{\boldsymbol{u},\boldsymbol{v} \in M} \omega(\boldsymbol{u},\boldsymbol{v}) \ d_{\lambda}(\boldsymbol{u},\boldsymbol{v}) & \text{otherwise} \end{cases}$$

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

### Remarkable properties

**Theorem (Desharnais et. al 99)** 

 $m \sim n$  iff  $d_{\lambda}(m,n) = 0$ 

**Theorem (Chen, van Breugel, Worrell 12)** 

The probabilistic bisimilarity distance can be computed in polynomial time

### Relation with Model Checking

**— Theorem (Chen, van Breugel, Worrell 12)** For all  $\phi \in LTL$  | Pr(m  $\models \phi$ ) - Pr(n  $\models \phi$ ) |  $\leq d_1(m,n)$ 

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



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## The CBA- $\lambda$ problem

 The Closest Bounded Approximant wrt d<sub>λ</sub>
Instance: An MC M, and a positive integer k
Ouput: An MC Ñ, with at most k states minimizing d<sub>λ</sub>(m<sub>0</sub>,ñ<sub>0</sub>)

 $d_{\lambda}(m_0,\tilde{n}_0) = \inf \{ d_{\lambda}(m_0,n_0) \mid N \in MC(k) \}$ we get a solution iff the infimum is a minimum

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

# $$\begin{split} d_{\lambda}(m_0,\tilde{n}_0) &= \inf \left\{ \begin{array}{l} d_{\lambda}(m_0,n_0) \mid \mathbb{N} \in \mathsf{MC}(\mathsf{k}) \right\} \\ &= \inf \left\{ \begin{array}{l} d(m_0,n_0) \mid \Gamma_{\lambda}(\mathsf{d}) \leq \mathsf{d}, \mathbb{N} \in \mathsf{MC}(\mathsf{k}) \right\} \end{split}$$

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### Lemma (Meaningful labels)-

For any N∈MC(k), there exists N'∈MC(k) with labels taken from M, such that  $d_{\lambda}(M,N) \ge d_{\lambda}(M,N')$
#### CBA-λ as a Bilinear Program

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$$d_{m_0,n_0}$$
  
such that  $\lambda \sum_{(u,v) \in M \times N} c_{u,v}^{m,n} \cdot d_{u,v} \leq d_{m,n}$   
 $1 - \alpha_{n,l} \leq d_{m,n} \leq 1$   
 $\alpha_{n,l} \cdot \alpha_{n,l'} = 0$   
 $\sum_{l \in L(\mathcal{M})} \alpha_{n,l} = 1$   
 $\sum_{v \in N} c_{u,v}^{m,n} = \tau(m)(u)$   
 $\sum_{u \in M} c_{u,v}^{m,n} = \theta_{n,v}$   
 $c_{u,v}^{m,n} \geq 0$ 

 $m \in M, n \in N$  $n \in N, l \in L(\mathcal{M}), \ell(m) \neq l$  $n \in N, l, l' \in L(\mathcal{M}), l \neq l'$  $n \in N$  $m, u \in M, n \in N$  $m \in M, n, v \in N$  $m, u \in M, n, v \in N$ 

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| mimimize $d_{m_0,n_0}$   |                 |
|--|-----------------|
| such that $\lambda \sum_{(u,v) \in M \times N} c_{u,v}^{m,n} \cdot d_{u,v} \le d_{m,n}$ $m \in M, n \in N$ |                 |
| $1 - \alpha_{n,l} \le d_{m,n} \le 1 \qquad \qquad n \in N, \ l \in L(\mathcal{M}), \ \ell$                 | $\ell(m)  eq l$ |
| $\alpha_{n,l} \cdot \alpha_{n,l'} = 0 \qquad \qquad n \in N,  l, l' \in L(\mathcal{M})$                    | ), $l \neq l'$  |
| $\sum_{l \in L(\mathcal{M})} \alpha_{n,l} = 1 \qquad \qquad n \in N$                                       |                 |
| $\sum_{v \in N} c_{u,v}^{m,n} = \tau(m)(u) \qquad \qquad m, u \in M, \ n \in N$                            |                 |
| $\sum_{u \in M} c_{u,v}^{m,n} = \theta_{n,v} \qquad \qquad m \in M,  n, v \in N$                           |                 |
| $c_{u,v}^{m,n} \ge 0 \qquad \qquad m, u \in M,  n, v \in N$  | r               |

#### 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- $\lambda$

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# Bounded Approximant threshold wrt d<sub>λ</sub> Instance: An MC M, a positive integer k, and a rational ε>0 Output: yes iff there exists N with at most k

states such that  $d_{\lambda}(m_0, n_0) \leq \epsilon$ 

### Complexity upper bound



**Proof sketch:** we can encode the question  $\langle M,k,\varepsilon \rangle \in BA-\lambda$  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].

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

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**Instance:** An MC M **Ouput:** The smallest k such that  $d_{\lambda}(m_0,n_0) < 1$ , for some N  $\in$  MC(k)

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For  $\lambda=1$ , the same problem is surprisingly difficult...

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– Significant Bounded Approximant wrt d<sub>1</sub> – Instance: An MC M and a positive k Ouput: yes iff there exists N with at most k states such that d<sub>1</sub>(m<sub>0</sub>,n<sub>0</sub>)<1.</p>

# Complexity of MSAB-1

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#### Theorem

SBA-1 is NP-complete

#### SBA-1 ⊆ **NP**



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**Proof sketch:** compute with Tarjan's algorithm all the SCCs of G(M). Then non deterministically choose a BSCC and a path to it. In polytime 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:

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

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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...)
- 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<sub>0</sub>
- it produces a sequence N<sub>0</sub>, ..., N<sub>h</sub> of approximants having strictly decreasing distance from M
- $N_h$  may be a sub-optimal solution of CBA- $\lambda$



# EM-like Algorithm

#### Algorithm 1

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

- 1.  $i \leftarrow 0$
- 2. repeat

3. 
$$i \leftarrow i+1$$

- 4. 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.  $\theta_i \leftarrow \text{UPDATETRANSITION}(\theta_{i-1}, \mathcal{C})$

6. 
$$\mathcal{N}_i \leftarrow (N, \theta_i, \alpha)$$

- 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<sub>k</sub> we construct N<sub>k+1</sub> 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<sub>k+1</sub> looks only the expectation of the number of occurrences of the edges likely to be found in M.

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| Case         | M   | $I \mid k$ | $\lambda = 1$            |                           |    | $\lambda = 0.8$ |                          |                           |    |       |
|--------------|-----|------------|--------------------------|---------------------------|----|-----------------|--------------------------|---------------------------|----|-------|
|              |     |            | $\delta_{\lambda}$ -init | $\delta_{\lambda}$ -final | #  | time            | $\delta_{\lambda}$ -init | $\delta_{\lambda}$ -final | #  | time  |
| IPv4<br>(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          | _                        | _                         | —  | ТО              | _                        | —                         | _  | ТО    |
| IPv4<br>(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          | _                        | _                         |    | ТО              | _                        | _                         | _  | ТО    |
| DrkW<br>(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                    | _                         | _  | ТО              | 0.423                    | —                         | _  | ТО    |
| DrkW<br>(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.

#### What we have seen

#### **Theoretical**

Metric-based state space reduction for MCs

- 1. Closest Bounded Approximant (CBA) encoded as a bilinear program
- 2. Bounded Approximant (BA) PSPACE & NP-hard for all  $\lambda \in (0,1]$
- 3. Significant Bounded Approximant (SBA) NP-complete for  $\lambda = 1$

#### **Practical**

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

#### Future Work

- Is BA-λ SUM-OF-SQUARE-ROOTS-hard?
   (conjecture: for λ<1, BA-λ is in NP)</li>
- Can we obtain a real/better EM-heuristics?
- What about different models/distances?
- What about different constraints? —beyond minimization!

# Thank you for your attention

Appendix

#### BA- $\lambda$ is NP-hard



 $\langle G,h \rangle \in VERTEX \ COVER \ iff \ \langle M_G, m+h+2, \lambda^2/2m^2 \rangle \in BA-\lambda$ 

# EM-like algorithm (experimental results)

#### IPv4 Zero Conf Protocol Averaged Marginal (AM)

#### Input model



#### IPv4 Zero Conf Protocol Averaged Marginal (AM)



#### IPv4 Zero Conf Protocol Averaged Marginal (AM)


## IPv4 Zero Conf Protocol Averaged Marginal (AM) $d_{0.9}(M,N_0) \approx 0.67$ Input model $d_{0.9}(M,N_1) \approx 0.043$ 0.2 0.5 0\5 0.473684 0.526316 0.5 0.5 05 2 d<sub>0.9</sub>(M,N<sub>2</sub>) ≈ 0.041 0.0909091

## IPv4 Zero Conf Protocol Averaged Expectations (AE)



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## IPv4 Zero Conf Protocol Averaged Expectations (AE)

























