Universität Konstanz

Minimization of Weighted Automata

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Introduction

In the last presentation . . .

- two models for stochastic dynamical systems were considered:
  Weighted Automata (WA) and Differential Equations (DE)

- an example for modelling a CRN's dynamics in both models was given:

DE	Solving Chemical Master Equation
WA	Monte Carlo CTMC

Goals specified

1. Implement minimization algorithm for weighted automata [1]. ✓
2. Implement model reduction algorithm for ODEs [2].
3. Develop reproducible benchmarks
4. Write report

What has been done so far

- Software Requirement Specification & Software Design Document
- Random Basis Minimal WA Construction Algorithm by Kiefer/Schützenberger [1]
- Execution of example by Matlab script and hand
- Implementation of minimization & equivalence algorithm, interfaces, TUI, CLI, tests

The Weighted Automaton Minimization Algorithm [1] I

Weighted Automaton $A = (n, \Sigma, \alpha, \mu, \eta)$, where

- n the number of states
- Σ the input alphabet
- α the initial vector with a non-zero value for all starting states
- μ the set of transition matrices, one per input character
- η the final vector with non-zero values for all ending states

The Weighted Automaton Minimization Algorithm [1] II

Reduction to Schwarz-Zippel Lemma (Polynomial Identity Testing) provide bounds on correctness $\frac{n}{K}$

Author claims complexity is in $\mathcal{RNC}$, this is not correct (c.f. later)

In the following slides use forward reduction, the backwards reduction is similar

Basic scheme of the algorithm:
Apply forward reduction to WA, then apply backward reduction on the output of the former

The Weighted Automaton Minimization Algorithm [1] III

- Find a basis F of the prefix space using random vectors r_i
  - Add the vectors of all prefix words up to length n together and multiply this vector by n different factors yielding $\{v_1, \ldots, v_n\}$
  - Factors are derived by random vectors and structure of prefixes
  - Base is then the maximally linear independent subset of $\{\alpha, v_1, \ldots, v_n\}$

- Use basis to do Schützenberger Construction [3]: $\overrightarrow{A} = (\overrightarrow{n}, \Sigma, \overrightarrow{\alpha}, \overrightarrow{\mu}, \overrightarrow{\eta})$ With
  - $\overrightarrow{\mu} = \overrightarrow{F}\mu\overrightarrow{F}^{-1}$ or $\overrightarrow{F}\mu = \overrightarrow{\mu}\,\overrightarrow{F}$
  - $\overrightarrow{\alpha} = e_1$
  - $\overrightarrow{\eta} = \overrightarrow{F}\eta$
  - $\overrightarrow{n} = \text{rank}(\overrightarrow{\mu})$

The Weighted Automaton Minimization Algorithm: Pseudo Code I

```
Algorithm 1: minimize(WeightedAutomaton WA)
Input: A weighted automata WA
Parameters: K setting the maximal random number
Output: A minimal version of WA
begin
    List<Matrix> randVs;
    WeightedAutomaton minWA;

    randVs ← generate_random_vectors(WA, K);
    minWA ← forward_reduction(WA, randVs);

    randVs ← generate_random_vectors(minWA, K);
    minWA ← backward_reduction(minWA, randVs);

    return minWA;
```

Array randVs has size A.n and matrices $r_i \in \{1, \ldots, K \cdot n\}^{\Sigma \times n}$

The Weighted Automaton Minimization Algorithm: Pseudo Code II

Algorithm 2: forward_reduction(WA, randVs)

Input: A weighted automata WA, random vectors randVs
Output: WA transformed by a random minimal forward space base

```
begin
    List<Vector> rhoVectors ← calculate_rho_vectors(WA, randVs);
    Matrix $\overrightarrow{F}$ ← vstack(A.$\alpha$, rhoVectors[0], $\ldots$, rhoVectors[n - 1]);
    int $\overrightarrow{n}$ ← rank($\overrightarrow{F}$);
    $\overrightarrow{F} \leftarrow \overrightarrow{F}[: \overrightarrow{n} - 1, :]$;
    RowVector $\overrightarrow{\alpha}$ ← standard_basis($\overrightarrow{n}$)[0, :];
    Vector $\overrightarrow{\eta} \leftarrow \overrightarrow{F} \cdot \eta$;
    foreach $\mu_i \in WA.\mu$ do
        $\overrightarrow{\mu_i}$ ← Solver($\overrightarrow{F}^T$).solve(($\overrightarrow{F} \cdot \mu_i)^T)^T$;
    return $\left(\overrightarrow{n}, \text{WA}.\Sigma, \overrightarrow{\alpha}, \overrightarrow{\mu}, \overrightarrow{\eta}\right)$;
```

The Weighted Automaton Minimization Algorithm: Pseudo Code III

Algorithm 3: calculate_rho_forward_vectors(WA, randVs)

Input: A weighted automata WA, random vectors randVs
Output: Candidate vectors as base of the Forward space

```
begin
    List<(Word, Vector)> words ← generate_words_forward(WA, WA.n);
    for $i = 0$ to $randVs.length - 1$ do
        for $j = 0$ to $words.length - 1$ do
            $v_i$ += words[j].vector * get_word_factor(words[j].word, randVs[i]);
    return $\{v_0, \ldots, v_{\text{randVs.length}-1}\}$;
```

Algorithm 4: get_word_factor(WA, randVs)

Input: Word w, randVs random vector
Output: WA transformed by a random minimal forward space base

```
begin
    result ← 1;
    for $i = 0$ to do
        result *= randVs(word[i], i);
```

The Weighted Automaton Minimization Algorithm: Pseudo Code IV

Algorithm 5: generate_words_forward(WA, randVs)

Input: A weighted automata WA, length of words k
Output: List of Tuples of word and corresponding vector

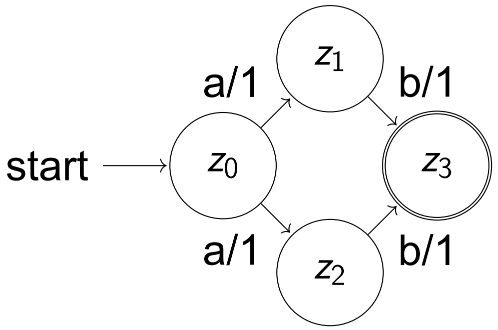
```
begin
    List<Word, Vector> result;
    if $k == 1$ then
        result = ;
        foreach $\mu_i \in WA.\mu$ do
            vect $\leftarrow$ WA.$\alpha \cdot \mu_i$;
            if !vect.isZero() then
                result.add(i, vect);
    else
        result = generate_words_forward(WA, $k-1$);
        for (word, wVector) $\in$ result do
            if word.length $==$ k - 1 then
                foreach $\mu_i \in WA.\mu$ do
                    vect $\leftarrow$ wVector$\cdot\mu_i$;
                    if !vect.isZero() then
                        newWord $\leftarrow$ word;
                        newWord.append(i);
                        result.add(newWord, vect);
    return result;
```

The Weighted Automaton Minimization Algorithm: Example I

Weighted automaton $\mathcal{A} = (n, \Sigma, \mu, \alpha, \eta)$ with

- $n = 3$,
- $\Sigma = \{a, b\}$,
- $\alpha = (1, 0, 0, 0)$,
- $\eta = (0, 0, 0, 1)$,

- $\mu(a) = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$,
- $\mu(b) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}$.



The Weighted Automaton Minimization Algorithm: Example II

$$r^{(1)} = \begin{pmatrix} 9 & 5 & 5 & 7 \\ 6 & 11 & 2 & 1 \end{pmatrix}; \quad r^{(2)} = \begin{pmatrix} 2 & 3 & 1 & 2 \\ 12 & 3 & 9 & 4 \end{pmatrix} r^{(3)} = \begin{pmatrix} 2 & 7 & 9 & 10 \\ 1 & 11 & 2 & 6 \end{pmatrix} r^{(4)} = \begin{pmatrix} 4 & 5 & 2 & 10 \\ 5 & 9 & 5 & 5 \end{pmatrix}$$

$$\alpha\mu(a)r_i + \alpha\mu(a)\mu(b)r_i = (0,1,1,0)r_i + (0,0,0,2)r_i$$

$$v_1 = 9 \cdot (0,1,1,0) + 9 \cdot 11 \cdot (0,0,0,2) = (0,9,9,198)$$

$$v_2 = 2 \cdot (0,1,1,0) + 2 \cdot 3 \cdot (0,0,0,2) = (0,2,2,12)$$

$$v_3 = 2 \cdot (0,1,1,0) + 2 \cdot 11 \cdot (0,0,0,2) = (0,2,2,44)$$

$$v_4 = 4 \cdot (0,1,1,0) + 4 \cdot 9 \cdot (0,0,0,2) = (0,4,4,72)$$

$$\overrightarrow{F} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 9 & 9 & 198 \\ 0 & 2 & 2 & 12 \end{pmatrix}$$

The Weighted Automaton Minimization Algorithm: Example III

$$\overrightarrow{F}\mu(\sigma) = \overrightarrow{\mu}(\sigma)\overrightarrow{F} \equiv \overrightarrow{\mu}(\sigma) = \overrightarrow{F}\mu(\sigma)\overrightarrow{F}_R^{-1}$$

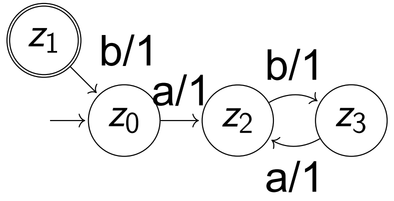
$$\overrightarrow{\mu}(a) = \begin{pmatrix} 0 & \frac{-1}{24} & \frac{11}{16} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \overrightarrow{\mu}(b) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{8} & \frac{-9}{16} \\ 0 & \frac{1}{36} & \frac{-1}{8} \end{pmatrix}$$

$$\overrightarrow{\eta} = \overrightarrow{F}\eta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 9 & 9 & 198 \\ 0 & 2 & 2 & 12 \end{pmatrix} \cdot (0,0,0,1)^T = (0,198,12)^T$$

$$\Rightarrow \overrightarrow{\mathcal{A}} = (3, \{a, b\}, \overrightarrow{\mu}, (1,0,0), (0,198,12)^T)$$

Weighted Automata Equivalence Algorithm [1]

Zeroness Problem:
$\forall w \in \Sigma^* : A(w) = 0$ $\longrightarrow$

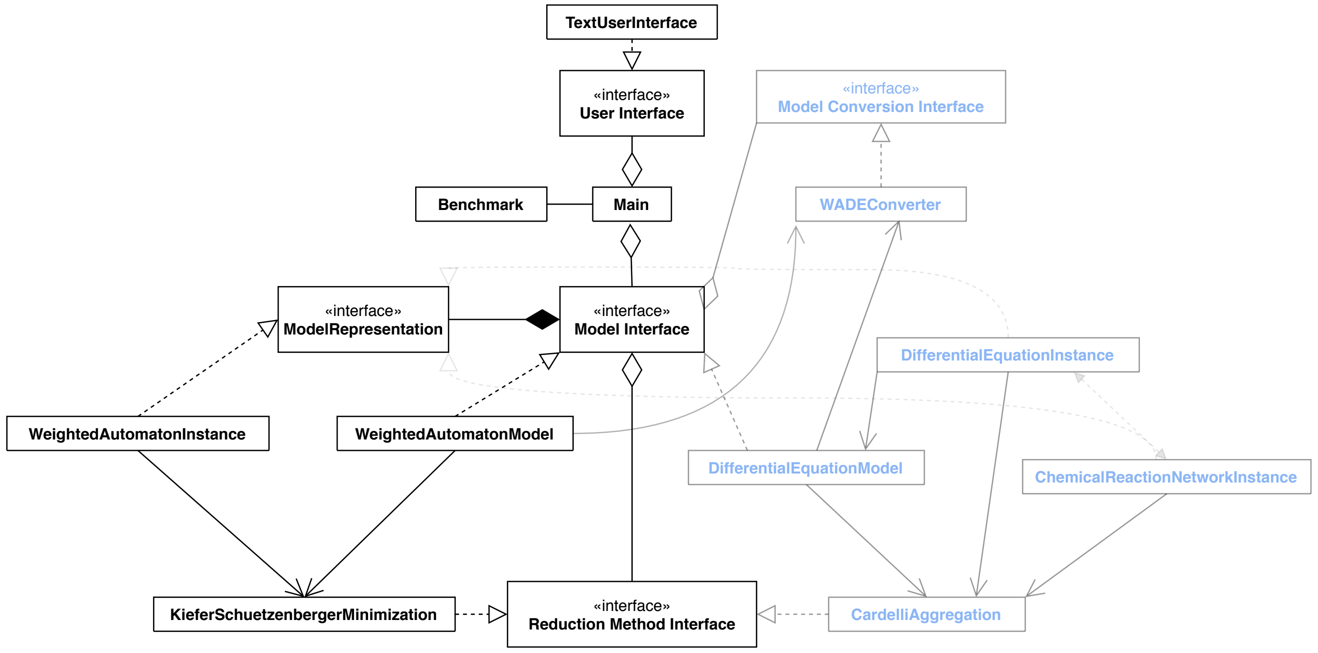

$$\begin{tikzcd} z_1 \arrow[dr, "b/1"] & & & \\ \arrow[r] & z_0 \arrow[r, "a/1"] & z_2 \arrow[r, bend left, "b/1"] & z_3 \arrow[l, bend left, "a/1"] \end{tikzcd}$$

$\Rightarrow \forall w \in \Sigma^* : A(w) = 0$

x

e

Implementation Details I


TextUserInterface
«interface»
User Interface
«interface»
Model Conversion Interface
Benchmark
Main
WADEConverter
«interface»
ModelRepresentation
«interface»
Model Interface
DifferentialEquationInstance
WeightedAutomatonInstance
WeightedAutomatonModel
DifferentialEquationModel
ChemicalReactionNetworkInstance
KieferSchuetzenbergerMinimization
«interface»
Reduction Method Interface
CardelliAggregation

Implementation Details II

Sparse vs. Dense Matrices

Templates,Concepts and Eigen Wrapper

OpenMP multi-threadding pragmas

further optimization possibilities

Code & Demo

Up Next

Previously greyed out part: Ordinary Differential Equations & Cardelli et al. [2]

What's the connection now? extremely sloppy notation ahead:

$$\text{LTS} \leftrightarrow \text{WA} \leftrightarrow \text{PA} \leftrightarrow \text{MC} \leftrightarrow \text{Rule-based Modeling} \leftrightarrow \text{ODE} \leftrightarrow \text{DE}$$

Bibliography

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