

Baum-Welch Algorithm for Markov Models Using Algebraic Decision Diagrams

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Abstract—This is a placeholder abstract. The whole template is used in semester projects at Aalborg University (AAU).

1 INTRODUCTION

THE Baum-Welch algorithm is a widely used method for training Markov models in applications such as speech recognition, bioinformatics, and financial modeling [1–3].

Traditionally, the Baum-Welch algorithm relies on matrix-based or recursive approaches to estimate model parameters from observed sequences.

An example of this is the JAJAPY library [4], which implements the Baum-Welch algorithm using a recursive matrix-based approach. This library is designed to learn probabilistic models from partially observable executions, producing observation sequences - also known as traces.

The key strength of JAJAPY lies in its flexibility to accommodate various learning scenarios, along with seamless integration into standard verification workflows using tools like STORM and PRISM. However, the performance of JAJAPY’s Baum-Welch algorithm implementation has been a significant limitation, because of the inherent redundancy in matrix-based representations, which leads to inefficiencies particularly in terms of time and memory consumption, which restricts its scalability to larger models.

To address these challenges, we propose a novel approach that replaces conventional matrices and recursive formulations with Algebraic Decision Diagrams (ADDs). ADDs provide a compact, structured representation of numerical functions over discrete variables, enabling efficient manipulation of large probabilistic models.

By leveraging ADDs, we can exploit the sparsity and structural regularities of Hidden Markov Models (HMMs) and Markov Chains (MCs), significantly reducing memory consumption and accelerating computation.

This paper presents several contributions toward efficient learning of HMMs and MCs models, by leveraging ADDs:

First, we extend the Baum-Welch (BW) algorithm for these models using symbolic computation, reformulating each algorithm step as operations on ADDs, leveraging the CUDD library to carry out these operations symbolically using ADDs.

This reformulation enables efficient calculation of the Markov models in a compact and scalable form.

Secondly, our approach extends previous work on symbolic calculation by accommodating learning from multiple observation sequences for both types of Markov models, broadening the applicability of symbolic learning.

Thirdly, we conduct an experimental evaluation of the scalability of the symbolic Baum-Welch algorithm for a MC from the QComp benchmark set [5], which serves as a standard reference for evaluating the performance of probabilistic model checking algorithms. Our findings suggest that replacing matrices and recursive formulations with ADDs offers a scalable alternative, making Markov model-based learning feasible for larger and more complex datasets.

Additionally, we implement Python bindings for the CUPAAL tool, making it accessible and usable within Python-based machine learning and model-checking workflows, such as JAJAPY.

Finally, using these python bindings we integrate CUPAAL into JAJAPY as JAJAPY 2, enabling users to seamlessly run symbolic probabilistic learning algorithms within JAJAPY.

2 PREVIOUS WORK

In this section, we provide a brief overview of previous work that has influenced our research and has been iterated upon. Specifically, we discuss what these tools are, how they function, who utilizes them, and the motivations behind integrating them into our research. The focus will be on four primary tools: PRISM STORM JAJAPY and CUPAAL.

2.1 Jajapy

JAJAPY provides learning algorithms designed to construct accurate models of a system under learning (SUL) from observed traces. Once learned, these models can be directly exported for formal analysis in tools such as STORM and PRISM.

In this context, we refer to the *training set* as the collection of observation traces used to infer a model of the SUL, and the *test set* as a separate set of traces used to evaluate the quality of the learned model.

JAJAPY supports learning various types of models, depending on the structure of the training data. For clarity, this paper focuses specifically on the new features introduced in JAJAPY 2, which primarily target Markov chains. However, these improvements are equally applicable to other classes of Markov models supported by the tool.

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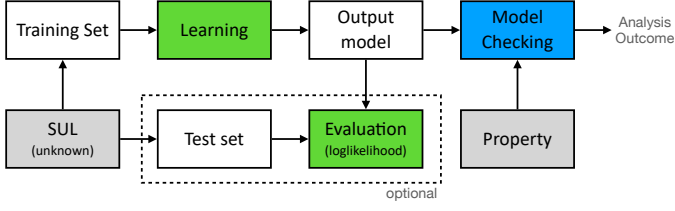


Fig. 1. Modeling and verification workflow using JAJAPY. Phases involving JAJAPY are highlighted in green, while the blue phase represents verification using STORM or PRISM.

At the core of JAJAPY’s learning capabilities are several variants of the Baum-Welch (BW) algorithm [6, 7], adapted for discrete-time Markov chains (MCs), Markov decision processes (MDPs)[8], and continuous-time Markov chains (CTMCs)[9].

Each algorithm requires two inputs: a training set and the desired number of states for the output model. The process begins with the creation of a randomly initialized model (e.g., a Markov chain) and iteratively updates its transition probabilities, increasing the likelihood of transitions that better explain the observed traces.

The efficiency and accuracy of the learning process depends heavily on the choice of the initial hypothesis. To improve convergence and model quality, JAJAPY allows users to supply a custom initial hypotheses in several formats, including STORMPY sparse models, PRISM-files, or native JAJAPY model definitions.

An example of using JAJAPY to learn a 10-state Markov chain from a training set, starting from a random initial hypothesis, is shown in Listing 1.

```

1 import jajapy
2 training_set = jajapy.loadSet("Path/to/data")
3 type(training_set) # list
4
5 learned_model = jajapy.BW().fit(training_set,
6     nb_states=10)
7 type(learned_model) # stormpy.SparseDtmc

```

Listing 1. Example of using JAJAPY’s BW implementation to learn a 10-state Markov chain from a training set.

JAJAPY supports reading PRISM files, using STORM (through STORMPY), as well as direct verification of learned model, through properties, provided the properties are supported. Alternatively, the model can be exported to PRISM’s format for verification using the PRISM model checker.

2.2 CuPAAL

CuPAAL is a tool developed in C++ that extends the work done in JAJAPY by implementing the Baum-Welch algorithm with an ADD-based approach instead of a recursive method. The goal of CuPAAL is to leverage ADDs to improve the efficiency of learning Markov models, particularly in large-scale applications where traditional recursive methods may become computationally expensive.

CuPAAL has undergone multiple iterations. Initially, it implemented a partial ADD-based approach, where only the calculation of the alpha and beta values of the Baum-Welch algorithm were implemented using ADDs. This partial implementation served as an initial proof-of-concept to determine

whether incorporating ADDs could yield performance benefits compared to the recursive approach employed by JAJAPY.

Following promising results from the partial implementation, further development led to a fully ADD-based version of CuPAAL for HMMs. This iteration replaced all recursive computations with ADDs, enabling more efficient execution, particularly for large models. The transition to a fully ADD-based approach demonstrated the potential for significant computational savings and scalability improvements, reinforcing the viability of this method for broader applications beyond our initial research scope.

Because there is no notion of HMM in the PRISM formalism, we’ve implemented the BW algorithm for use with MCs. Given the similarities between these model types, we’ve reused a lot of the previous work in the implementation.

By building upon JAJAPY and developing CuPAAL, we have been able to evaluate the impact of using ADDs in probabilistic model learning.

3 PRELIMINARIES

This section provides an overview of the theoretical background necessary to understand the rest of the article. For ease of reference Appendix B contains a table of symbols used in the paper.

We begin by defining the key concepts of a HMM and a MC, which are the two main models used in this report, then go on to introduce the BW, which is a widely used algorithm for training HMMs, and showing how it can be adapted to handle multiple observation sequences using matrix operations.

3.1 Hidden Markov Model

Hidden Markov Models (HMMs) were introduced by Baum and Petrie in 1966 [10] and have since been widely used in various fields, such as speech recognition [1], bioinformatics [2], and finance [3].

A HMM is a statistical model that describes a system that evolves over time. The system is assumed to hold the Markov property, meaning that the future state of the system only depends on the current state and not on the past states. The system is also assumed to be unobservable, meaning that the states are hidden and cannot be directly observed. Instead, the system emits observations, which are used to infer the hidden states.

Definition 1 (Hidden Markov Model). *A Hidden Markov Model (HMM) is a tuple $\mathcal{M} = (S, L, \omega, \tau, \pi)$, where:*

- S is a finite set of states.
- L is a finite set of labels.
- $\omega : S \rightarrow D(L)$ is the emission function.
- $\tau : S \rightarrow D(S)$ is the transition function.
- $\pi \in D(S)$ is the initial distribution.

$D(X)$ denotes the set of probability distributions over a finite set X . The emission function ω describes the probability of emitting a label given a state. The transition function τ describes the probability of transitioning from one state to another. The initial distribution π describes the probability of starting in a given state.

An example of a HMM is a weather model where the hidden state represents the actual weather (sunny, rainy, or cloudy), but we only observe indirect signals, such as whether someone is carrying an umbrella or wearing sunglasses.

3.2 Markov Chain

A Markov Chain (MC), named after Andrei Markov, is a stochastic model widely used in different fields of study [7].

Definition 2 (Markov Chain). *A Markov Chain (MC) is a tuple $\mathcal{M} = (S, L, \omega, \tau, \pi)$ identical to the HMM structure above except that the emission function is deterministic: for every $s \in S$ there is a single label $l = \omega(s)$ emitted with probability 1.*

In other words, the emission function ω is a function that maps each state to a single label $l \in L$, meaning that each state emits exactly and only one label. Two distinct states may emit the same label.

An example of a MC is a board game where a player moves between squares based on dice rolls. Each square corresponds to a state, the dice rolls determine the transition probabilities.

3.3 Conversion between MCs and HMMs

In this section, we will discuss the conversion between MCs and HMMs. This conversion is important because it allows us to use the same algorithms and techniques from the original CUPAAL implementation for both model types, even though they have different properties.

In our case, we're interested in trace-equivalent models. By trace-equivalent, we mean that the probability distribution over observed sequences is the same for both models. i.e. the labels emitted by moving through the probabilistic models follow the same distribution.

From the definition of a MC, we can see that it is a special case of an HMM where the emission function is deterministic, which makes this conversion very simple.

Definition 3 (Markov Chain to Hidden Markov Model). *For each MC $\mathcal{M} = (S, L, \omega, \tau, \pi)$, there exists a trace-equivalent HMM $\mathcal{M}' = (S', L', \omega', \tau', \pi')$, where:*

- $S' = S$.
- $L' = L$.
- $\omega'(s)(l) = \begin{cases} 1 & l = \omega(s) \\ 0 & \text{otherwise} \end{cases}$
- $\tau' = \tau$.
- $\pi' = \pi$.

The only difference in this case is the structure of the emission functions, thus preserving the probabilistic trace equivalence, i.e., for an arbitrary trace $O \in L^*$ we have $P[O | \mathcal{M}] = P[O | \mathcal{M}']$.

3.4 Baum-Welch Algorithm

The BW is a special case of the Expectation-Maximization (EM) framework used to estimate the parameters of a HMM given a set of observed sequences.

Since the underlying states are not directly observable, the algorithm iteratively refines the model parameters π , ω , and τ to maximize the likelihood of the observations. Each iteration of the algorithm consists of two steps:

- E-step Compute the expected values of the hidden variable given the current parameters.
- M-step Update the model parameters to maximize the expected complete-data log-likelihood.

Convergence is typically achieved when the change in the likelihood (or parameters) between iterations falls below a threshold [7].

We can represent the parameters of a HMM as matrices for computational efficiency.

They are defined as follows:

- π is the initial state distribution vector, where $\pi_i = \pi(s_i)$ is the probability of starting in state s_i , this is a column vector of size $|S|$.
- τ is the transition matrix, where $\tau_{ij} = \tau(s_i)(s_j)$ is the probability of transitioning from state s_i to state s_j , this is a square matrix of size $|S| \times |S|$.
- ω is the emission matrix, where $\omega_{ij} = \omega(s_i)(l_j)$ is the probability of emitting label l_j given state s_i , this is a matrix of size $|S| \times |L|$.

To illustrate our symbolic implementation, we describe a single Baum-Welch iteration in terms of matrix operations, assuming familiarity with the algorithm. For an introductory treatment, see [6, 11].

Let \mathcal{M} denote the current HMM hypothesis and let $O = o_1 \dots o_T$ be a sequence of observations, where each $o_t \in L$ and the observation sequence has the length T . Suppose \mathcal{M} has n states and m labels, i.e., $S = s_1, \dots, s_n$, with parameters represented as follows:

- $\pi \in [0, 1]^n$ is the initial state distribution column vector.
- $\tau \in [0, 1]^{n \times n}$ is the transition probability matrix.
- $\omega \in [0, 1]^{n \times m}$ is the emission probability matrix.

The forward and backward algorithms are implemented using dynamic programming, as shown in Listing 2. For a given time step t , let $\omega(t)$ be the column vector of emission probabilities for label o_t for each state, and \odot the Hadamard (element-wise) product.

FORWARD-ALGORITHM

```

1  $\alpha(1) = \omega(1) \odot \pi$ 
2 for  $t = 2$  to  $T$ 
3    $\alpha(t) = \omega(t) \odot (\tau^\top \alpha(t-1))$ 
```

BACKWARD-ALGORITHM

```

1  $\beta(T) = \mathbf{1}$ 
2 for  $t = T-1$  to 1
3    $\beta(t) = \tau (\beta(t+1) \odot \omega(t+1))$ 
```

Listing 2. Computation of the forward and backward coefficients

The above procedures compute the column vectors $\alpha(t)$ and $\beta(t) \in [0, 1]^n$ for $t = 1 \dots T$ which are later used to compute the coefficients $\gamma(t) \in [0, 1]^n$ and $\xi(t) \in [0, 1]^{n \times n}$ as follows:

$$\gamma(t) = \tau[O|\mathcal{M}]^{-1} \cdot \alpha(t) \odot \beta(t) \quad (1)$$

$$\xi(t) = (\tau[O|\mathcal{M}]^{-1} \cdot \tau) \odot (\alpha(t) \otimes (\beta(t+1) \odot \omega(t+1))^\top) \quad (2)$$

Here, \otimes is the Kronecker product and the probability $\tau[O|\mathcal{M}]$ to observe O in \mathcal{M} is computed as $\mathbf{1}^\top \alpha(T)$. We calculate $\gamma(t)$ from $t = 1$ to T and $\xi(t)$ from $t = 1$ to $T-1$.

Finally, the initial probability vector, the transition probability matrix and emission matrix are updated as follows:

$$\hat{\pi} = \gamma(1) \quad (3)$$

$$\hat{\omega} = (\mathbf{1} \oslash \gamma) \cdot \left(\sum_{t=1}^T \gamma(t) \otimes [[o_t]] \right) \quad (4)$$

$$\hat{\tau} = (\mathbf{1} \oslash \gamma) \cdot \xi \quad (5)$$

Where \cdot is the transposed Khatri-Rao product (i.e., row-by-row Kronecker product), and $[[o_t]] = ([[o_t = l]])_{l \in L}$ is the one-hot encoding of the observation o_t , meaning that it is a row vector of size $|L|$ with a 1 in the position corresponding to the observation o_t and 0 elsewhere. \oslash is the element-wise division, and \otimes is the Kronecker product. The γ and ξ are defined as follows:

$$\gamma = \sum_{t=1}^T \gamma(t) \quad (6)$$

$$\xi = \sum_{t=1}^{T-1} \xi(t) \quad (7)$$

These update rules form the standard BW for training HMMs on a single observation sequence. However, the approach can be naturally extended to multiple sequences.

The BW algorithm runs until convergence, in this case until the difference in log-likelihood between iterations is less than $\ell(\mathcal{M}; O) - \ell(\hat{\mathcal{M}}; O) < \epsilon$. The log-likelihood of an iteration can be calculated using the α probabilities in this way:

$$\ell(\mathcal{M}; O) = \sum_{s=1}^S \log(\alpha(T)_s) \quad (8)$$

3.5 Multiple Observation Sequences

Suppose we are given a multiset of independently identically distributed (i.i.d.) observation sequences $\mathcal{O} = O_1, O_2, \dots, O_{|\mathcal{O}|}$, where each $O_i = (o_{i1}, o_{i2}, \dots, o_{iT})$ is of length T . The E-step remains unchanged: for each sequence, we compute the corresponding $\alpha_i(t)$, $\beta_i(t)$, $\gamma_i(t)$, and $\xi_i(t)$ values independently.

In the M-step, we aggregate statistics across all sequences to update the parameters. Specifically, we define:

$$\gamma = \sum_{i=1}^{|\mathcal{O}|} \sum_{t=1}^T \gamma_i(t) \quad (9)$$

$$\xi = \sum_{i=1}^{|\mathcal{O}|} \sum_{t=1}^{T-1} \xi_i(t) \quad (10)$$

With these aggregate quantities, the update rules for the initial distribution (see Equation 3) and transition matrix (see Equation 5) remain unchanged, because they are already defined in terms of the sum over all sequences. However, the emission matrix update needs to account for all sequences.

The emission matrix is updated as follows:

$$\omega_s(o) = (\mathbf{1} \oslash \gamma) \cdot \left(\sum_{i=1}^N \sum_{t=1}^T \gamma_i(t) \otimes [[o_{it}]] \right) \quad (11)$$

This mirrors the single-sequence case (see Equation 4) but extends the summation in the left side of the Kronecker

product to cover all sequences and all time steps. This allows us to compute the emission probabilities for each state across all sequences, ensuring that the model captures the overall distribution of observations.

3.6 Baum-Welch Algorithm for Markov Chains

Since MCs can be seen as HMMs with deterministic emissions, where each state emits a unique observation with probability 1, the BW simplifies accordingly when applied to MCs.

In this case:

- The forward and backward algorithms are computed identically to the HMM case, but without weighting by emission probabilities, as these are implicitly handled by the observation sequence.
- The **E-step** computations for $\gamma(t)$ and $\xi(t)$ remain structurally the same, though emission terms are omitted due to determinism.
- The **M-step** updates for the initial distribution π and the transition matrix τ are unchanged.
- The emission matrix ω is not updated, as it is fixed by the model's structure and need not be learned.

This simplification avoids unnecessary computation and reflects the reduced uncertainty in the model: there is no need to marginalize over emissions, as each state deterministically produces a known label. Consequently, the BW becomes more efficient when applied to MCs.

3.7 Decision Diagrams

Binary Decision Diagrams (BDDs) are data structures for efficiently representing and manipulating Boolean functions. They are a compressed representation of truth tables, capturing the logical structure of a function in a graph-based format by eliminating redundancy, reducing memory usage, and improving computational efficiency [12].

A Binary Decision Diagram (BDD) is a directed acyclic graph derived from a decision tree, where each non-terminal node represents a Boolean variable, edges correspond to binary assignments (0 or 1), and terminal nodes store function values (0 or 1). To reduce the size of the decision tree, BDDs exploit redundancy by merging equivalent substructures, resulting in a canonical form (when reduced and ordered) that allows for efficient operations such as function evaluation, equivalence checking, and Boolean operations [12].

BDDs have been widely used in formal verification, model checking, and logic synthesis due to their ability to compactly represent large Boolean functions while maintaining efficient computational properties. However, in rare cases BDDs can suffer from exponential blowup. This can occur particularly when dealing with functions that lack inherent structure or when representing numerical computations that go beyond Boolean logic.

3.8 ADDs

Algebraic Decision Diagrams (ADDs) generalize the concept of BDDs by allowing terminal nodes to take values beyond Boolean constants (0 and 1). Instead of restricting values to true/false, ADDs can store arbitrary numerical values, making them useful for representing and manipulating functions

over discrete domains [13]. This generalization enables the efficient representation of functions such as cost functions [14], probabilities [15], and other numerical relationships that arise in probabilistic reasoning.

The fundamental structure of an ADD remains similar to a BDD, where a decision tree is compacted by merging redundant substructures. However, instead of performing Boolean operations, ADDs allow for arithmetic operations such as addition and multiplication, making them well-suited for representing matrices [13].

4 IMPLEMENTATION

This section will provide an overview of the implementation of Cupaal. This will include the Baum-Welch algorithm, and how CUPAAL is integrated into JAJAPY, creating JAJAPY 2.

4.1 Motivation for CuPAAL

The motivation for CUPAAL is to provide a more efficient and scalable implementation of the Baum-Welch algorithm for parameter estimation. Specifically, we aim to improve the performance of the algorithm when dealing with large and complex models, and improve upon the existing limitations of the Baum-Welch algorithm in JAJAPY.

4.1.1 Recursive vs. Matrix vs. ADD-based Approaches

When working with the Baum-Welch algorithm, different approaches can be taken to optimize computational efficiency. Three common strategies are recursive, matrix-based, and ADD-based approaches, each with distinct advantages and limitations.

- **Recursive Approach:** Conceptually simple, recursion follows a divide-and-conquer strategy, and makes use of a dynamic programming approach. Previous calculations are used to build upon future calculations. These results are stored in a list or a map, so that they can be accessed when needed [16, Chapter 4].
- **Matrix Representation:** Reformulating algorithms using matrix operations leverages algebraic properties for parallel computation and efficient processing. By building upon the recursive approach, matrices provide an efficient method of accessing the stored results leading the faster computations overall [16, Chapter 4, 15 & 28].
- **ADD-based Approach:** ADDs provide a compact representation that eliminates redundancy in recursive computations. By reusing previously computed substructures, they improve efficiency and reduce memory overhead [13]. Compared to matrices, ADDs can offer a more space-efficient alternative for structured data while extending BDD techniques to handle both Boolean and numerical computations.

In this work we explore the benefits of ADD-based approaches for solving complex problems, focusing on parameter estimation in Discrete Time Markov Chains (DTMCs) and Continuous Time Markov Chains (CTMCs). We compare the performance of ADD-based algorithms against recursive-based implementations, highlighting the advantages of using ADDs for efficient computation and memory management.

4.2 What is CuPAAL

CUPAAL is a C++ library that implements the Baum-Welch algorithm for parameter estimation, and has evolved over time.

The initial version of CUPAAL was written in C and called *SUDD*, which was a partial implementation of the Baum-Welch algorithm, using ADDs. This version was mainly focused on displaying the efficiency of ADDs for parameter estimation problems, and was not fully functional. The next iteration was called CUPAAL, which was a complete implementation of the Baum-Welch algorithm, using ADDs, however it only supported HMMs, and was only designed to make use of a single observation.

The current version of CUPAAL has been extended to support DTMCs and can handle multiple observations. This version of CUPAAL is designed to be used in conjunction with JAJAPY, allowing for easy integration and use in parameter estimation problems.

The following sections will provide an overview of what CUPAAL is, and what it can do.

4.2.1 What Does Cupaal Contain

Throughout all its iterations, CUPAAL has made use of Colorado University Decision Diagram (CuDD). Colorado University Decision Diagram (CuDD) is a library for implementing and manipulating BDDs and ADDs developed at the University of Colorado. The CuDD library [17] is a powerful library for implementing and manipulating various types of decision diagrams, including BDDs and ADDs.

Implemented in C, the CuDD library ensures high-performance execution and can be seamlessly integrated into C++ programs, which we utilize in CUPAAL. By leveraging the CuDD library, we demonstrate the benefits of ADD-based approaches for solving parameter estimation problems in DTMCs.

The CuDD library is used to store ADDs and perform operations on them. Its optimized algorithms and efficient memory management enable symbolic handling of large and complex matrices, significantly improving performance compared to traditional methods.

We have not modified or extended the CUDD library. All functionality used in our implementation is available through the standard CUDD library.

4.2.2 From Prism to Cupaal

In the current iteration of CUPAAL, it is possible to use Prism models as input to the Baum-Welch algorithm.

The models are encoded from Prism models to CUPAAL models. This is done by parsing the Prism model to JAJAPY, using Stormpy.

The Jajapy model contains a matrix for its transitions, a matrix for its labels, and a vector for the initial state. The model is passed to CUPAAL where these matrices and vectors are encoded into ADDs, as a function $f : \{0, 1\}^n \times \{0, 1\}^n \rightarrow R$.

The Transition matrix is a $S \times S$ matrix, where $S = States$, and is encoded to an ADD, by each row and column with a binary value. This value is determined based on the size of the matrix, $n = \lceil \log_2(S) \rceil$.

The label matrix is a $S \times L$ matrix, where $L = Labels$ and since there is no guarantee that $S = L$, the encoding is handled differently. The matrix is instead treated as a list of vectors.

Each vector is encoded as square matrices, where each row or column (depending on the vector type) is duplicated, which is then encoded to a list of ADDs. Knowing the exact dimensions of matrices and that they are square helps to simplify some of the symbolic operations. An example of this will be displayed in subsubsection 4.2.3.

The Initial state vector is encoded similarly to the label matrix, but only as a single ADD.

4.2.3 Kronecker Product Implementation

The Kronecker product is implemented in CUPAAL, using the row and column duplication method mentioned in subsubsection 4.2.2.

The structure of Decision Diagrams in CUPAAL, where keeping track of all the new binary values used for encoding from a matrix to an ADD can add a layer of complexity for calculation. Especially when computing operations that translate matrices to new dimensions, such as the Kronecker product. This matrix-based approach enables efficient symbolic operations, as the Kronecker product can be calculated by taking the Hadamard product between a column matrix ADD and a row matrix ADD, simplifying what would otherwise be a more complex operation.

An example of this can be seen with the two vectors \hat{A} and \hat{B}

$$\text{Let } \hat{A} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \text{ and } \hat{B} = \begin{bmatrix} 3 & 4 \end{bmatrix}.$$

The Kronecker product of these two vectors is computed as follows:

$$\hat{A} \otimes \hat{B} = \begin{bmatrix} 1 \cdot 3 & 1 \cdot 4 \\ 2 \cdot 3 & 2 \cdot 4 \end{bmatrix} = \begin{bmatrix} 3 & 4 \\ 6 & 8 \end{bmatrix}. \quad (12)$$

Another way to calculate the Kronecker product is to expand the vectors into matrices. \hat{A} and \hat{B} are expanded to be matrices, similar to how the matrix was treated as a list of vectors and then expanded to square matrices, as seen with the Label matrix.

$$\text{Let } \mathbf{A} = \begin{bmatrix} 1 & 1 \\ 2 & 2 \end{bmatrix} \text{ and } \mathbf{B} = \begin{bmatrix} 3 & 4 \\ 3 & 4 \end{bmatrix}.$$

The Kronecker product of \hat{A} and \hat{B} can also be calculated, by using the Hadamard product of \mathbf{A} and \mathbf{B} . This is done as follows:

$$\mathbf{A} \circ \mathbf{B} = \begin{bmatrix} 1 \cdot 3 & 1 \cdot 4 \\ 2 \cdot 3 & 2 \cdot 4 \end{bmatrix} = \begin{bmatrix} 3 & 4 \\ 6 & 8 \end{bmatrix}. \quad (13)$$

Hereby showing that the Hadamard product can be used to compute the Kronecker product between two matrices, by using the row and column duplication method. This is a technique that only works for Kronecker products between vectors, specifically one row and one column vector, as it relies on the structure of the vectors being expanded into square matrices.

4.3 Implementation to Jajapy

This section will give an overview of how CUPAAL is implemented into JAJAPY, using bindings between C++ and Python. Figure 2 shows the overall architecture of the implementation.

CUPAAL consists of two main components, the main function and the BW library. Both of these are compiled to an executable program, called `cupaal.exe`, which can be used to run the Baum-Welch algorithm on a given model.

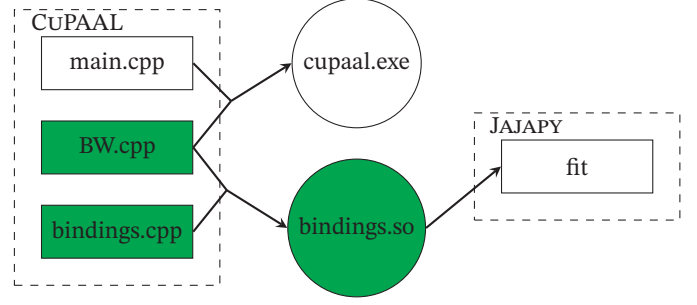


Fig. 2. Architecture of CUPAAL combined with JAJAPY.

4.3.1 Bindings

To implement CUPAAL into JAJAPY, we create bindings between C++ and Python using the `pybind11` library [18]. This allows us to call C++ functions from Python, enabling us to use CUPAAL in JAJAPY.

In the code examples, some parts have been removed for brevity and clarity.

```

1 // Some parameters have been removed for brevity
2 cupaal_markov_model
3   ↳ cupaal_bw_symbolic(vector<string>& states,
4   ↳ vector<string>& labels,
5   ↳ vector<vector<string>>& observations,
6   ↳ vector<double>& initial_distribution,
7   ↳ vector<double>& transitions, vector<double>&
8   ↳ emissions, int max_iterations = 100, double
9   ↳ epsilon = 1e-2){
10  MarkovModel model(states, labels,
11  ↳ initial_distribution, transitions,
12  ↳ emissions, observations);
13  cupaal_markov_model model_data;
14  chrono::seconds time = chrono::seconds(3600);
15  model.baum_welch_multiple_observations(
16  ↳ max_iterations, epsilon, time);
17
18 // Removed output and result path for brevity
19 model_data.initial_distribution =
20 ↳ model.initial_distribution;
21 model_data.transitions = model.transitions;
22 model_data.emissions = model.emissions;
23
24 Cudd_Quit(model.manager);
25 return model_data;
26 }
  
```

Listing 3. C++ bindings file for CuPAAL

We create a C++ bindings file, that uses the BW library from CUPAAL and define the function we want to expose to Python, we call this function `cupaal_bw_symbolic`, seen in Listing 3. This function takes model parameters from a JAJAPY model as input, and transforms them to be used in CUPAAL. The transformation is done at line 3, where all the parameters are inputted to create a Markov Model object, which is then used to run the Baum-Welch algorithm at line 6. Each of the values that are relevant from the BW algorithm are then passed into the `model_data` object, which is then returned to JAJAPY, seen in lines 10 through 15.

These being the initial distribution, the transitions and the emissions.

The C++ bindings file is then compiled to a shared library, which can be imported in JAJAPY. JAJAPY can call

```

1 void baum_welch_multiple_observations(unsigned int
   ↳ max_iterations = 100, double epsilon = 1e-6,
   ↳ chrono::seconds time = chrono::seconds(3600));

```

Listing 4. Prototype of the function used to run the Baum-Welch algorithm on multiple observations in CuPAAL.

the `cupaal_bw_symbolic` function, which will then call the CUPAAL implementation of the Baum-Welch algorithm.

We create a new function in JAJAPY, called `_bw_symbolic`, which is used to call the CUPAAL implementation of the Baum-Welch algorithm, as seen in Listing 5. This function is used to prepare the model parameters from JAJAPY, so they are in the correct format for CUPAAL. The preparation is done at lines 7 through 20, after this the CUPAAL implementation is called at line 22, where the `cupaal_bw_symbolic` function is called with the prepared parameters, giving the CUPAAL model as a return value.

The values are then extracted from the CUPAAL model and assigned to the JAJAPY model, seen in lines 23 through 25, where they are reshaped to be in line with JAJAPY.

The fit function in JAJAPY is modified to call the `_bw_symbolic` function when a new parameter called `symbolic` is set to true, as seen in Listing 6.

A check is made to see if the `symbolic` parameter is set to true at line 4, and when the parameter is true, the JAJAPY model will call the Listing 5 function, which will then call the CUPAAL implementation of the Baum-Welch algorithm.

4.4 Integration Discussion

The integration of CUPAAL into JAJAPY has been successful, allowing us to leverage the Baum-Welch algorithm for parameter estimation for HMMs and DTMCs.

The decision to use pybind11 for creating bindings between C++ and Python has proven to be effective, as it allows us to call C++ functions from Python, but further considerations should be made for the future if this is the best approach.

The exact implementation of the symbolic fit function in JAJAPY is shown in Listing 6, is to be discussed with the JAJAPY creator and some changes are expected to be made.

5 EXPERIMENTS

In this section, we present an evaluation comparing the performance of two implementations of the BW algorithm: the original version from JAJAPY and the new symbolic implementation introduced in JAJAPY 2.

For this comparison, we use a MC model, taken from the QComp benchmark set [19], which is a collection of models used for quantitative verification and learning tasks. The goal is to assess scalability of the symbolic implementation and its performance in terms of runtime and accuracy.

We designed three experiments to evaluate the performance of the symbolic implementation of the BW algorithm in JAJAPY 2:

- **Scalability** — Evaluating how the symbolic implementation scales with increasing model size.
- **Accuracy** — Comparing the accuracy of the symbolic implementation against the original recursive implementation.

- **Extra Scalability** — Evaluating the scalability of the symbolic implementation when adjusting the initialization of the model hypothesis.

The experiments are designed to answer the following research questions:

- **Question 1:** How does runtime scale as model size increases for JAJAPY 2 vs JAJAPY?
- **Question 2:** What is the relative estimation accuracy of the symbolic implementation in JAJAPY 2 compared to the original recursive implementation in JAJAPY?
- **Question 3:** How much does an informed initialization accelerate JAJAPY 2?

The experiments are designed to provide insights into the performance and scalability of the symbolic implementation of the BW algorithm in JAJAPY 2, and to compare it with the original recursive implementation in JAJAPY.

5.1 Model

The model used in the experiments is "leader_sync", which is a DTMC model from the QComp benchmark set [19]. The model is from the PRISM case study [20], which is a collection of models used for quantitative verification and learning tasks.

The "leader_sync" model is a distributed system model that simulates the behavior of a group of processors that need to choose a leader among themselves. The model's size ranges from 26 to 1050 states, depending on the number of processors in the system, the states increase {26, 69, 147, 61, 274, 812, 141, 1050}.

The non-linear progression in model size arises because the QComp benchmark defines model variants using two parameters: the number of processors and the maximum number a leader can select to be elected.

The model is chosen because of its scalability, making it suitable for evaluating the performance of the symbolic implementation of the BW algorithm in JAJAPY 2. The model was also simple to understand and analyze, allowing us to add more labels to the model to make it suitable for the experiments.

The labels added to the model are shown in Listing 7.

5.2 Experimental Setup

All experiments were conducted on the same machine, see Appendix A for full specs and the python environment.

The following steps were taken to set up the experiments:

- 1) Load the PRISM model
- 2) Generate $N_{\text{seq}} \in \{25, 50, 100\}$ observation sequences of length 20.
- 3) Create a random initial MC using `MC_random`.
- 4) Run BW for up to 4 hours or until the log-likelihood difference converges to a threshold of 0.01.
- 5) Record runtime and save the model.

We save both the initial models and observations in files, to ensure both implementations use inputs by default. The generation of the training set and the randomization of the model is done using JAJAPY, which provides a convenient way to generate random models and training sets. The training set is generated by creating a set of observation sequences from the original model, which is then used to train the randomized model.

```

1 def _bw_symbolic(self, max_iteration = 100, epsilon = 1e-2, outputPath = "", resultPath = ""):
2     try:
3         import libcupaal_bindings
4     except ModuleNotFoundError:
5         print("Cannot find module")
6
7     states = [str(i) for i in range (self.h.nb_states)]
8     labels = list(set(self.h.labelling))
9     observations = []
10    for times, sequences in zip(self.training_set.times, self.training_set.sequences):
11        for i in range(times):
12            observations.append(list(sequences))
13    initial_state = self.h.initial_state.tolist()
14    transitions = self.h.matrix.flatten().tolist()
15    emissions = zeros((len(labels), self.h.nb_states))
16    for row in range(len(labels)):
17        for col in range(self.h.nb_states):
18            if self.h.labelling[col] == labels[row]:
19                emissions[row][col] = 1
20    emissions = emissions.flatten().tolist()
21
22    cupaal_model = libcupaal_bindings.cupaal_bw_symbolic( states, labels, observations, initial_state,
23        ↳ transitions, emissions, max_iteration, epsilon, outputPath, resultPath)
24    self.h.initial_state = array(cupaal_model.initial_distribution)
25    self.h.matrix = array(cupaal_model.transitions).reshape( self.h.nb_states, self.h.nb_states)
26    self.h.emissions = array(cupaal_model.emissions).reshape( len(labels), self.h.nb_states)
27    return self.h

```

Listing 5. Jajapy's implementation of the Baum-Welch algorithm using CuPAAL.

```

1 # Some parameters have been removed for brevity
2 def fit(self, output_file: str, output_file_prism:
3     ↳ str, epsilon: float, max_it: int, symbolic:
4     ↳ bool):
5     # Removed preparation and settings number of
6     ↳ processes, for brevity
7     if symbolic :
8         return self._bw_symbolic(max_it, epsilon,
9             ↳ output_file, output_file_prism)
10    else:
11        return self._bw(max_it, pp, epsilon,
12            ↳ output_file, output_file_prism,
13            ↳ verbose, stormpy_output, return_data)

```

Listing 6. Jajapy's fit function, which calls the CuPAAL implementation of the Baum-Welch algorithm when symbolic is set to true.

```

1 label "reading" = s1=1&s2=1&s3=1;
2 label "deciding" = s1=2&s2=2&s3=2;
3 label "elected" = s1=3&s2=3&s3=3;

```

Listing 7. Labels added to the "leader_sync" model.

We then run the BW algorithm on the randomized model and the training set for both the original recursive implementation in JAJAPY and the symbolic implementation in JAJAPY 2. We run each implementation for each model size and number of observation sequences ten times to obtain average results.

The results of the experiments are recorded, including the runtime, number of iterations, log-likelihood, and error of the estimated transition probabilities.

We do not measure memory usage, as the symbolic implementation is implemented in C++ using Python bindings making it difficult to measure memory usage accurately, therefore we focus on runtime and accuracy.

5.3 Experiment 1: Scalability

The first experiment evaluates the scalability of the symbolic implementation of the BW algorithm in JAJAPY 2. The goal is

to measure the runtime performance of the symbolic implementation as the size of the model increases. The experiment measures the average runtime of the BW algorithm for each model size and number of observation sequences.

5.4 Experiment 2: Accuracy

The second experiment evaluates the accuracy of JAJAPY 2 compared to the original JAJAPY. The goal is to measure the accuracy of the symbolic implementation in terms of log-likelihood and absolute error of the estimated transition probabilities. The absolute error is defined as:

$$\text{Error} = |e - r|,$$

where e is the estimated transition probability and r is the reference value from the original model. We use the results from the first experiment, and compare the log-likelihood and absolute error of the properties estimated by the symbolic implementation against the original recursive implementation.

The properties used in this experiment are shown in Listing 8, the properties are taken from the QComp benchmark set [19].

```

1 P>=1 [ F "elected" ]
2 R{ "num_rounds" }=? [ F "elected" ]

```

Listing 8. Properties used in the "leader_sync" model.

5.5 Experiment 3: Extra Scalability

The third experiment evaluates the scalability of the symbolic implementation in JAJAPY 2 when adjusting the initialization of the model hypothesis.

This experiment aims to measure the scalability of JAJAPY 2 under circumstances that are theoretically good for the symbolic implementation. The more repeated values the transition

matrix contains, the sparser the ADD representing it will be. By initializing the transition matrix with a reduced amount of different values, we hope that the symbolic approach might benefit.

For the first experiment, the transition matrix was initialized randomly. For this experiment instead, we only use $|S|$ different values in the transition matrix. It is expected that this improves the speed of each iteration of the BW algorithm, as it reduces the number of unique computations necessary for the symbolic implementation.

6 RESULTS

In this section, we present the results of our experiments, which are divided into two main parts: the first part focuses on the scalability of JAJAPY and CUPAAL in terms of time and scalability, while the second part evaluates the accuracy of both tools.

The experiments were conducted on a machine with the specifications and environment listed in section A.

6.1 Scalability

These results are the time taken to train a model, based on two parameters: the number of states, and the length of the observations in the model increasing.

TABLE 1
Leader Sync model variations in training time in seconds.

model	states	length	jajapy (s)	cupaal (s)
3.2	26	25	1.38	0.26
3.2	26	50	1.95	0.14
3.2	26	100	4.09	0.23
3.3	69	25	7.95	2.46
3.3	69	50	11.20	1.59
3.3	69	100	19.65	1.75
3.4	147	25	27.10	8.54
3.4	147	50	42.57	9.20
3.4	147	100	84.02	9.90
4.2	61	25	15.68	11.18
4.2	61	50	24.87	13.56
4.2	61	100	52.11	11.24
4.3	274	25	194.88	231.28
4.3	274	50	414.30	379.21
4.3	274	100	447.83	117.78
4.4	812	25	1846.68	3324.83
4.4	812	50	2290.28	1848.44
4.4	812	100	5652.14	3447.56
5.2	141	25	95.59	104.71
5.2	141	50	342.05	553.66
5.2	141	100	798.73	982.97
5.3	1050	25	4586.86	10906.91
5.3	1050	50	7791.95	10405.75
5.3	1050	100	9821.74	5992.51

The results for the leader sync model are displayed in Table 1 and Figure 3, and show the time it takes to train a model, given the number of states and observation length. Only the training time is considered; the initialization of the programs is not a factor in these numbers.

In Figure 3, simple planes are fit with linear regression from the data in Table 1. This is not an attempt to say anything definitive about the degrees of the scaling, but instead to show the generally observable trend.

Contrary to our expectations, the data does not show a clear difference in the time taken to train the leader sync model between JAJAPY and CUPAAL for DTMCs.

For very small models, the running time does not matter too much, but we observe an initial overhead related to JAJAPY. This is likely related to the general consensus that Python is a slower language than C in general.

Generally, more states mean longer running time, but interestingly, variations with similar number of states may have very different training times. The most obvious example is the 3.4 and 5.2 models, with 147 and 141 states respectively. The 5.2 model is much slower, especially in CUPAAL, showing a ~ 10 times increase in training time, despite having slightly fewer states.

Initially, we only had data for observations of length 25, and the data under those conditions suggested that JAJAPY scaled quite a bit better than CUPAAL.

To explore this behaviour, we extended the experiment to contain data for observations of different lengths, and now our observations are more in line with our expectations. JAJAPY gets slower at a pace roughly linear with the length of the observations; doubling the observation length doubles the run time of JAJAPY. This is not the case for CUPAAL, where we do not see any particular increase in running time as the observation length increases.

In fact, looking at Figure 4 and Figure 5, the CUPAAL runtimes look a little strange.

From Figure 3

6.2 Accuracy

7 IMPROVEMENTS

This section outlines the improvements gained by transitioning from the recursive implementation in Jajapy to the symbolic approach in CuPAAL.

As discussed in (Ref to previous section talking about Jajapy), Jajapy uses a recursive implementation of the Baum-Welch algorithm to learn HMMs. In contrast, CuPAAL implements the Baum-Welch algorithm using ADDs. By leveraging ADDs, CuPAAL demonstrates significant improvements over the recursive approach used in Jajapy. The discussion of these improvements is based on the experimental results presented in Section 5.

7.1 Run Time

One of the most notable advantages of CuPAAL over Jajapy is the reduction in run time, particularly for models with a large number of states.

The use of ADDs minimizes redundant computations by merging identical values within the structure. This optimization significantly reduces the computational needs, compared to a recursive implementation. As a result, the run time gap between CuPAAL and Jajapy increases as the number of states grows, making CuPAAL a more scalable solution for large HMMs.

The number of iterations of CuPAAL for each model is also slightly reduced compared to Jajapy.

This advantage is particularly beneficial in scenarios where handling large probability matrices would otherwise lead to excessive computational costs.

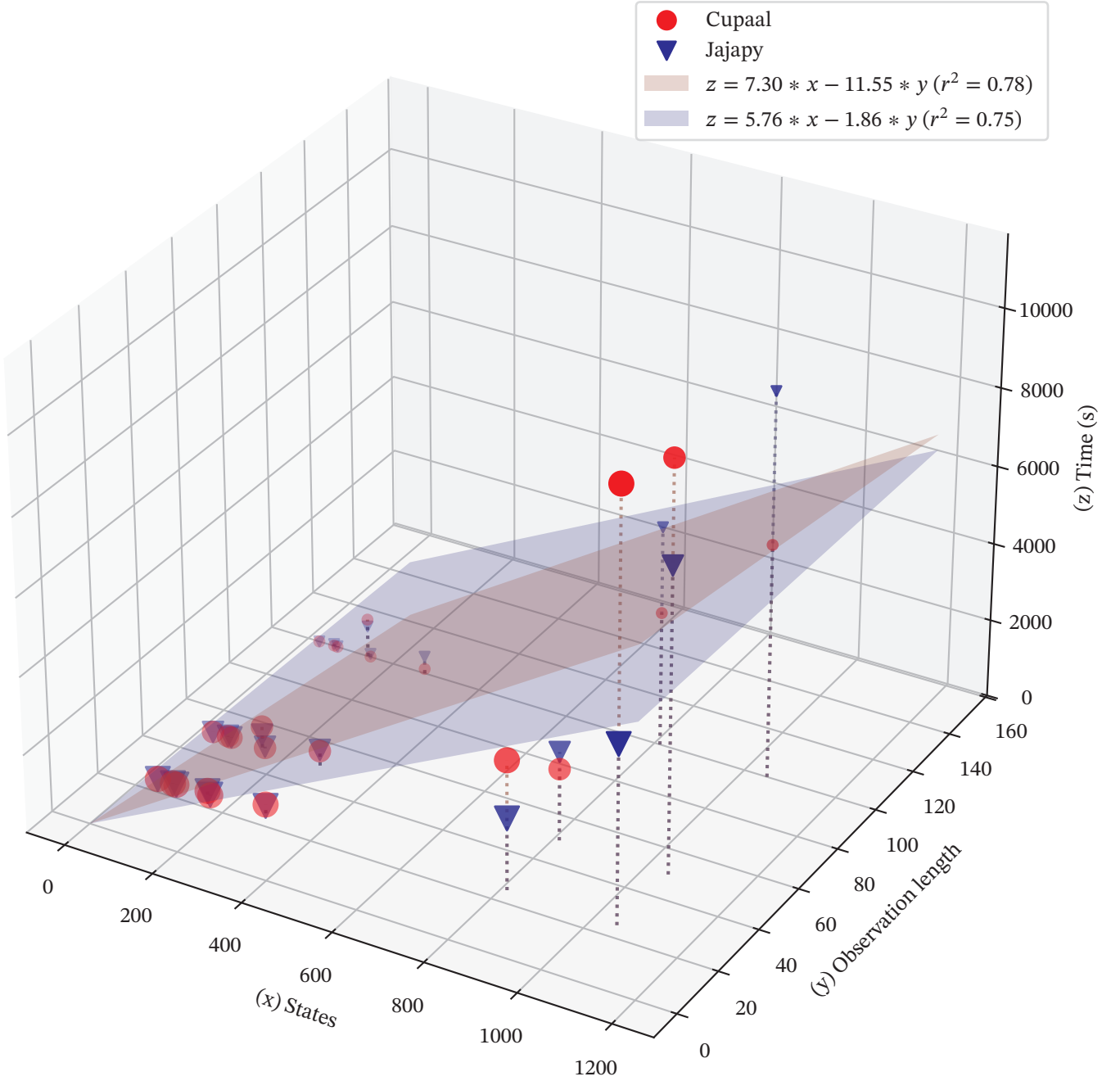


Fig. 3. Plot of the run time of JAJAPY and CuPAAL for the leader sync models, given the number of states and the length of the observations. The planes are linear regression fits to indicate the directions of the trends for the datapoints of similar color.

7.2 Accuracy

While run time is a key advantage of CuPAAL, it is equally important to assess whether these performance gains come at the cost of accuracy. Since both approaches implement the Baum-Welch algorithm, they are expected to converge to similar model parameters when learning HMMs.

As shown in Section 5, CuPAAL achieves accuracy comparable to Jajapy across various models. These results can be seen in the values of avg delta and the log-likelihood, where the closer the value is to 0 the better. Displaying that a symbolic implementation does not introduce significant numerical errors,

ensuring that the learned transition and emission probabilities remain consistent with those obtained using the recursive approach.

Furthermore, by eliminating redundant calculations, CuPAAL may reduce floating-point errors that typically accumulate in recursive implementations. Importantly, CuPAAL maintains accuracy even as the number of states increases, showcasing that its efficiency improvements do not compromise learning quality. This makes it particularly well-suited for handling large-scale HMMs.

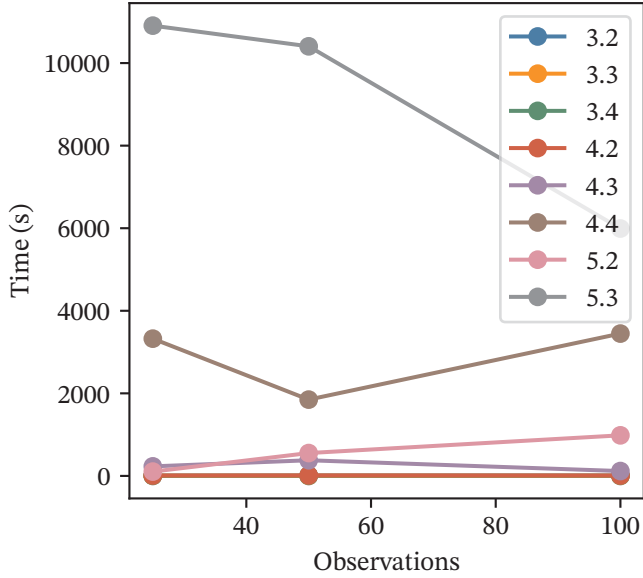


Fig. 4. CuPAAL runtimes with increasing observation length.

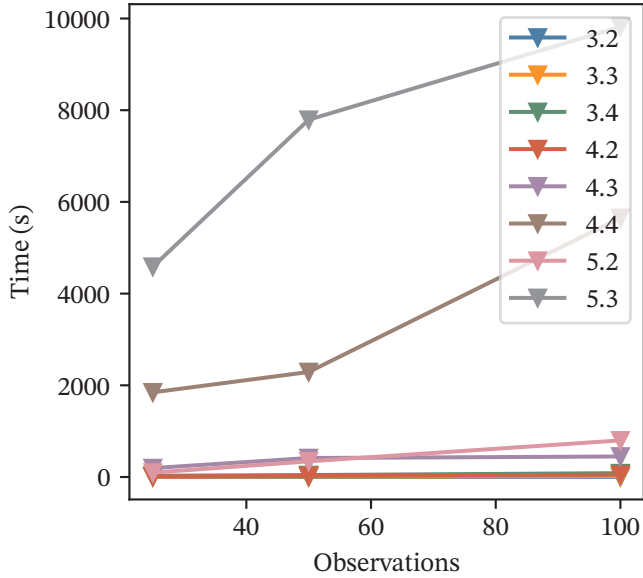


Fig. 5. JAJAPY runtimes with increasing observation length.

7.3 Implementation

The implementation of CuPAAL has been done in c++, compared to Jajapy which is implemented in Python. This could also be a factor aiding the performance improvement of CuPAAL, as C++ is generally faster at computation compared to Python. This choice of implementation not only improves speed but also ensures that CuPAAL can efficiently handle large models that would be infeasible in Python.

7.4 Final improvement overview

The improvements introduced by CuPAAL stem from multiple factors: the adoption of ADDs, optimized run time and a high-performance C++ implementation. These enhancements make CuPAAL a powerful alternative to recursive approaches like

Jajapy, particularly when working with large, redundant, and complex HMMs.

8 DISCUSSION

The accuracy of the models learned with the BW algorithm strongly depends on selecting an appropriate size for the output model. However, increasing this size substantially raises the computational cost of each update iteration, both in terms of time and space complexity.

This is because each iteration requires running the forward-backward algorithm on every trace in the training set. In the original implementation, this step was performed using Jajapy models, incurring a cost of $O(n^2 \cdot K)$ in time and $O(n \cdot K)$ in space per iteration, where n is the number of states in the output model and K is the total number of label occurrences in the training set. Moreover, computing the updated transition probabilities from the forward and backward coefficients added an extra $O(n^2 \cdot K)$ overhead in both time and space.

Unsurprisingly, this had a significant impact on the performance of the BW algorithm as the number of states increased.

To address this limitation, CuPAAL introduces a symbolic engine that efficiently handles both the forward-backward computation and the parameter updates.

ACRONYMS

AAU	Aalborg University. 1
ADD	Algebraic Decision Diagram. 1, 2, 4–6, 9, 11
BDD	Binary Decision Diagram. 4, 5
BW	Baum-Welch. 1–4, 6–9
CTMC	Continuous Time Markov Chain. 5
CuDD	Colorado University Decision Diagram. 5
DTMC	Discrete Time Markov Chain. 5, 7, 9
HMM	Hidden Markov Model. 1–5, 7, 9–11
i.i.d.	independently identically distributed. 4
MC	Markov Chain. 1–4, 7

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APPENDIX A MACHINE SPECIFICATIONS

The specifications of the machine used for the experiments are listed in Table 2. The image used for the experiments is based on the movesrwth/stormpy image (version 1.9.0), which is a Docker image that contains the necessary dependencies for running JAJAPY¹. We add the dependencies for CuPAAL to the image, which are listed in Table 3. For full details see the github repository for CuPAAL.

TABLE 2
Machine specifications

Specification	Value
CPU	AMD Ryzen 5 3600
RAM	64 GB DDR4
OS	Windows 11 Pro
Docker	4.40.0

A.1 Python Environment

This section describes the Python environment used for the experiments. The Python version and the versions of the libraries used are listed in Table 3.

TABLE 3
Python environment

Requirement	Version
Python	3.12.3
Jajapy	0.10.8
CuPAAL	0.1.0
numpy	1.26.0
pandas	2.2.3
scipy	1.11.2
sympy	1.12.0
matplotlib	3.8.1
alive-progress	3.1.4
pybind11 global	2.13.6

APPENDIX B CHEATSHEET

If something is represented with a greek letter, it is something we calculate.

1. <https://hub.docker.com/r/movesrwth/stormpy>

TABLE 4
Symbol table.

Symbol	Meaning
\mathbb{R}	Real numbers
\mathbb{B}	Boolean domain
\mathbb{Q}	Rational numbers
\mathbb{N}	Natural numbers
\mathcal{M}	Markov Model
$s \in S$	States
$l \in L$	Labels
$o \in O \in \mathcal{O}$	Observations
$t \in T$	Time steps
$\mathbf{1}$	Column vector of ones
π	Initial distribution
τ	Transition function
ω	Emission function
α	Forward probabilities
β	Backward probabilities
γ	State probabilities given O
ξ	Transition probabilities given O
$\lambda = (\pi, \tau, \omega)$	Model Parameters
μ	Mean
σ	Standard deviation
$\theta = (\mu, \sigma^2)$	Parameters of a distribution
$P(\mathcal{O}; \lambda)$	Probability of \mathcal{O} given λ
$\ell(\lambda; \mathcal{O})$	Log likelihood of λ under \mathcal{O}
\cdot	Scalar product
\odot	Hadamard product
\otimes	Kronecker product
\oslash	Hadamard division
\bullet	Transposed Khatri-Rao product