Symbolic Parameter Estimation of Continuous-Time Markov Chains

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

Index Terms—Formal Verification, Parameter Estimation, Decision Diagram

1 Introduction

Markov models are a class of probabilistic models that are used to describe the evolution of a system over time. A Markov model has the Markov property, which states that the future behavior of the system depends only on its current state and not on its past history [1]. This property simplifies analysis by focusing only on the present state, making Markov models especially useful for systems where memory-less behavior is a reasonable assumption.

Markov models are widely used in various fields, such as biology, finance, and computer science, to model systems that exhibit stochastic behavior [2–5]. As such, their analysis has a wide range of applications.

An example of a Markov model, is a simple weather model, if today is sunny, there might be an 80% chance of sun tomorrow and a 20% chance of rain. Similarly, if today is rainy, there might be a 70% chance of rain tomorrow and a 30% chance of sun.

Model checking is a technique used to verify the correctness of Markov models by comparing the predictions of the model with observed data. Model checking is widely used in the verification of Markov models, where the model is analyzed to check if it satisfies certain properties [6]. It ensures reliability and correctness in critical systems, from traffic controls to industrial automation and communication protocols [6]. It is also used to check if the model satisfies certain properties, such as reachability, can we reach a desired state and safety properties, can we avoid going a specific sequence of states.

A real world example of model checking is the verification of a traffic light system, where the model is analyzed to check if the traffic lights are working correctly. For reachability, we can ask: *can a traffic light system always cycle back to green after being red?*. For safety properties we can ask, *can a traffic light system avoid having both lights green at the same time?*.

There exists several tools for model checking, such as PRISM [7] and Storm [8], which are widely used in the verification of Markov models. These tools use symbolic representations to represent the model and perform the operations required for model checking. The limitation of these tools is that they do not support parameter estimation, which makes them unsuitable for learning the parameters of the model from data.

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Parameter estimation is a crucial step in the analysis of Markov models, as the analysis of the model depends on the accuracy of the estimated parameters, particularly when in a timing and probabilistic behaviour [9]. Parameter estimation is the process of estimating the parameters of the model from observed data, which is used to make predictions about the system's behavior.

These parameters are used to ensure that the model accurately represents the system's behavior and dynamics and to make accurate predictions about the system's future behavior. Accurate parameter estimation is essential for making reliable predictions and validating model behavior, with applications ranging from healthcare diagnostics to network security [9].

The Baum-Welch algorithm is a widely used method for estimating the parameters of Markov models [10]. The algorithm uses the Expectation-Maximization (EM) framework to iteratively update the parameters of the model until convergence [11]. The Baum-Welch algorithm is computationally expensive for large models, as it uses matrices to represent the model, which has a space complexity that grows quadratically with the number of states in the model. This makes the algorithm computationally expensive for large models, as the memory requirements grow rapidly with the size of the model [12].

Addressing these challenges requires innovative techniques, such as symbolic representations, which reduce memory consumption while preserving accuracy.

1.1 Related Works

Jajapy [13] is a Python-based tool designed for estimating parameters in parametric models using the Baum-Welch algorithm. It employs a matrix representation of the model and implements the necessary operations for parameter estimation through standard matrix computations.

While accessible and straightforward, Jajapy is hindered by the space complexity inherent in its recursive-based calculation. This limitation makes it computationally expensive for large-scale models, as memory requirements grow quadratically with the number of states in the system.

SUDD [14] builds upon the limitations of Jajapy by introducing a symbolic representation for the forward-backward algorithm. Specifically, it leverages Algebraic Decision Diagrams (ADDs) to reduce memory consumption and improve the

runtime performance of the Baum-Welch algorithm. By employing ADD-based computations, SUDD provides a significant improvement in scalability, making it feasible to handle larger models.

However, the implementation is limited to a subset of the Baum-Welch algorithm, focusing primarily on forward-backward computations without addressing the full parameter estimation process.

In this paper, we extend the work of SUDD by utilizing ADDs to represent the full Baum-Welch algorithm. Our approach not only inherits the scalability benefits of ADDs but also implements the complete parameter estimation process. Additionally, we compare our implementation with both the original Jajapy, SUDD and an extended version of SUDD using the log-semiring framework, which improves numerical stability in computations.

PRISM [7] is a widely used probabilistic model checker designed to verify the correctness of Markov models. It employs symbolic representations such as ADDs to efficiently represent and manipulate large-scale models, enabling the verification of properties like reachability and safety.

For example, PRISM can determine whether a traffic light system will always cycle back to green after being red or verify that conflicting light signals are avoided. However, PRISM does not support parameter estimation, limiting its use to model verification rather than learning the parameters required for accurate system predictions.

Storm [8] is another state-of-the-art probabilistic model checker that shares many similarities with PRISM. Like PRISM, it uses symbolic representations to handle large models efficiently and focuses on verifying properties of Markov models. Storm has been optimized for scalability and flexibility, supporting a wide range of model types and verification tasks. Despite these strengths, Storm also lacks support for parameter estimation, making it unsuitable for tasks requiring the inference of model parameters from observed data.

Our work bridges the gap between parameter estimation tools (e.g. Jajapy and SUDD) and model checking tools (e.g. PRISM and Storm). By integrating scalable symbolic representations into the full Baum-Welch algorithm, we provide a method that not only estimates parameters efficiently but also enables the accurate modeling of complex systems. This integration of parameter learning with symbolic computation addresses a critical limitation in the current landscape of tools for Markov models.

2 Preliminaries

In this section, we introduce the necessary background concepts and definitions that are essential for understanding the subsequent sections. We begin by defining the key concepts of a Hidden Markov Model (HMM) and then describe how a HMM can be represented using matrices. We then introduce the Baum-Welch algorithm, which is used to estimate the parameters of a HMM from observed data. We describe all the steps involved in the Baum-Welch algorithm, including the forward-backward algorithm and the update algorithm. Finally, we discuss how the Baum-Welch algorithm can be implemented using matrix operations to efficiently compute the forward and backward variables, intermediate variables, and parameter updates.

2.1 Hidden Markov Models

HMMs were introduced by Baum and Petrie in 1966 [15]. HMM are a class of probabilistic graphical models that are widely used to model sequences of observations with underlying hidden states. These models consist of two main components: observations and hidden states. The observations are the visible data emitted by the model, while the hidden states represent the underlying process that generates these observations. The objective of an HMM is to infer the hidden states based on the observations. HMMs have applications in fields such as speech recognition [16], bioinformatics [17], and natural language processing [18]. HMMs was chosen as the model of choice for this project due to its versatility and ability to model complex systems.

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

- S is a finite set of states.
- $\mathcal{L}$ is a finite set of labels.
- $\ell : S \to D(\mathcal{L})$ is the emission function.
- $\tau : S \to D(S)$ is the transition function.
- $\pi : S \to \mathbb{R}$ is the initial distribution.

Here, $D()$ denotes the set of probability distributions over a finite set. The model emits a label l in state s with probability $\ell(s, l)$, transitions between states with probability $\tau(s, s')$, and starts in state s with probability $\pi(s)$.

HMMs can be further classified into discrete-time and continuous-time models based on the time scale of the underlying process. Discrete-time HMMs are the most common type of HMMs and are used to model sequences of observations that occur at discrete time intervals. Continuous-time HMMs are used to model sequences of observations that occur continuously over time. In this project, we focus on discrete-time HMMs.

2.2 Matrix Representation of HMMs

HMMs can be represented using matrices. The emission function ℓ can be represented as a matrix ω where $\omega_{s,l} = \ell(s, l)$. The matrix ω has the size $|S| \times |\mathcal{L}|$. The sum of each row in the matrix ω is equal to one, reflecting the total probability of emitting all labels from a given state.

$$\omega = \begin{bmatrix} \ell(s_1, l_1) & \cdots & \ell(s_1, l_{|\mathcal{L}|}) \\ \vdots & \ddots & \vdots \\ \ell(s_{|S|}, l_1) & \cdots & \ell(s_{|S|}, l_{|\mathcal{L}|}) \end{bmatrix}$$

The transition function τ can be represented as a matrix P where $P_{s,s'} = \tau(s, s')$. The matrix P has the size $|S| \times |S|$. The sum of each row in P is equal to one, reflecting the total probability of transitioning from a given state to all other states.

$$P = \begin{bmatrix} \tau(s_1, s_1) & \cdots & \tau(s_1, s_{|S|}) \\ \vdots & \ddots & \vdots \\ \tau(s_{|S|}, s_1) & \cdots & \tau(s_{|S|}, s_{|S|}) \end{bmatrix}$$

The initial distribution π can be represented as a vector π where $\pi_s = \pi(s)$. The vector π has the size $|S|$. The sum of all elements in π is equal to one, reflecting the total probability of starting in each state.

$$\pi = \begin{bmatrix} \pi(s_1) \\ \vdots \\ \pi(s_{|S|}) \end{bmatrix}$$

2.3 Observations and Hidden States

An HMM operates on sequences of observations, denoted as $O = O_1, O_2, \ldots, O_N$, where each O_i is a sequence of labels $o_1, o_2, \ldots, o_{|\mathbf{O}|-1}$. The task is to infer the sequence of hidden states $S = s_1, s_2, \ldots, s_{|\mathbf{O}|-1}$ that most likely generated these observations.

Given an observation sequence O, the goal is to maximize the probability of the hidden states conditioned on the observations.

This inference is commonly achieved using the Baum-Welch algorithm.

2.4 Baum-Welch Algorithm

The Baum-Welch algorithm is a key method for estimating the parameters of an HMM from observed data. It was chosen as the method of choice for this project due to its ability to estimate the parameters of a HMM without knowing the hidden states that generated the observations, and it is also the standard method for training HMMs. If looking at other Markov models such as Markov Chains (MCs), the Baum-Welch algorithm can be used to estimate the parameters of the model from observed data, therefore it is a suitable choice for this project, as this can be used to estimate the parameters of other Markov models. It leverages the Expectation-Maximization (EM) framework and consists of two iterative steps:

1) **Expectation Step (E-step)**: Compute the expected the forward and backward variables, for each state s and time t. of the latent variables, which are the unobserved state sequences corresponding to the observations. These variables represent the likelihood of being in state s at time t given the observed data up to time t and the likelihood of observing the remaining data from time t onwards given the state s at time t, respectivly.
2) **Maximization Step (M-step)**: Update the model parameters (emission matrix ω, transition matrix P, and initial distribution π) to maximize the likelihood of the observed data, using the expected values computed in the E-step.
3) Repeat the E-step and M-step until convergence.

The Baum-Welch algorithm is particularly useful for estimating the properbilities of the emission and transition matrices of a HMM, given a set of observations, without knowing the hidden states that generated the observations.

Given a multiset of observations $\mathcal{O}$ and initial parameters $\mathbf{x}_0$, the Baum-Welch algorithm estimates the parameters of a HMM $\mathcal{P}$ by iteratively improving the current hypothesis $\mathbf{x}_n$ using the previous estimate $\mathbf{x}_{n-1}$ until a convergence criterion is met. A hypothesis refers to a specific set of values for the parameters $\mathbf{x}$.

Each iteration of the algorithm produces a new hypothesis, denoted as $\mathbf{x}_n$, which is the algorithm's current best guess for the parameter values based on the observed data. The algorithm consists of three main steps: the forward-backward procedure, the update step, and the convergence criterion. The Baum-Welch algorithm iteratively refines the parameters until the improvement between successive iterations falls below a predefined threshold. This is typically evaluated using a convergence criterion such as:

$$||l(\mathbf{x}_n) - l(\mathbf{x}_{n-1})|| < \epsilon \tag{1}$$

where $\epsilon > 0$ is a small threshold, and $l(\mathbf{x}_n)$ denotes the likelihood of the observed data given the parameter values at the n-th iteration.

The algorithm stops when the change in parameters is sufficiently small, indicating that the model has converged to a local maximum of the likelihood function. The parameter estimation procedure is outlined in Algorithm 1.

ESTIMATE-PARAMETERS($\mathcal{P}, \mathbf{x}_0, \mathcal{O}$)
1 $\mathbf{x} \leftarrow \mathbf{x}0$
2 **while** ¬CRITERION($\mathbf{x}_{n-1}, \mathbf{x}_n$)
3 $\quad \mathbf{x}_{n-1} \leftarrow \mathbf{x}_n$
4 $\quad (\alpha, \beta) =$ FORWARD-BACKWARD($\mathcal{P}(\mathbf{x}_n), \mathcal{O}$)
5 $\quad \mathbf{x}_n =$ UPDATE($\mathcal{P}(\mathbf{x}_n), \mathcal{O}, \alpha, \beta$)
6 **return** $\mathbf{x}_n$

Algorithm 1. Parameter estimation procedure [14].

Starting with initial parameters $\mathbf{x}_0$, the parameter estimation procedure iteratively improves the current hypothesis $\mathbf{x}_n$ using the previous estimate $\mathbf{x}_{n-1}$ until a specified criterion for convergence is met, the algorithm returns the final estimate $\mathbf{x}_n$. The specifics of the FORWARD-BACKWARD and UPDATE procedures are detailed in subsection 2.5 and subsection 2.6 from [19].

2.5 Forward-Backward Algorithm

For a given HMM $\mathcal{M}$, the forward-backward algorithm computes the forward and backward variables, $\alpha_s(t)$ and $\beta_s(t)$, for each observation sequence $o_0, o_1, \ldots, o_{|\mathbf{o}|-1} = \mathbf{o} \in \mathcal{O}$. The forward variable $\alpha_s(t)$ represents the likelihood of observing the partial sequence $o_0, o_1, \ldots, o_t$ and being in state s at time t, given the model $\mathcal{M}$. The backward variable $\beta_s(t)$ represents the likelihood of observing the partial sequence $o_{t+1}, o_{t+2}, \ldots, o_{|\mathbf{o}|-1}$ given state s at time t and the model $\mathcal{M}$.

The forward variable $\alpha_s(t)$ and backward variable $\beta_s(t)$ can be computed recursively as follows:

$$\alpha_s(t) = \begin{cases} \omega_s(0)\, \pi_s & \text{if } t = 0 \\ \omega_s(t) \sum_{s' \in S} P_{s's} \alpha_{s'}(t-1) & \text{if } 0 < t \leq |\mathbf{o}| - 1 \end{cases} \tag{2}$$

$$\beta_s(t) = \begin{cases} \mathbb{1} & \text{if } t = |\mathbf{o}| - 1 \\ \sum_{s' \in S} P_{ss'} \omega_{s'}(t+1) \beta_{s'}(t+1) & \text{if } 0 \leq t < |\mathbf{o}| - 1 \end{cases} \tag{3}$$

Here, $\omega_s(t)$ is the likelihood of observing o_t given that the state at time t is s and the model $\mathcal{M}$, formally $\omega_s(t) = l(o_t \mid S_t = s, \mathcal{M})$. Meaning that $\omega_s(t)$ is the probability of observing the label o_t in state s.

The forward-backward algorithm computes the forward and backward variables for each state s and time t in the observation sequence $\mathbf{o}$, providing a comprehensive view of the likelihood of the observed data under the model.

In preparation for later discussions we would like to draw the attention to the fact that the above recurrences can be solved using dynamic programming requiring one to use $\Theta(|S| \times |(|\mathbf{o}| - 1)|)$ space.

2.6 Update Algorithm

The update algorithm refines the parameter values of the HMM model based on the observed data and the forward and backward variables computed in the forward-backward procedure. Given the forward and backward variables $\alpha_s(t)$ and $\beta_s(t)$, the update algorithm aims to maximize the likelihood of the observed data by adjusting the parameter values.

The update step is based on the expected sufficient statistics of the latent variables, which are the unobserved state sequences corresponding to the observations.

2.6.1 Intermediate Variables

We need to calculate the intermediate variables $\gamma_s(t)$ and $\xi_{ss'}(t)$, $\gamma_s(t)$ represent the expected number of times the model is in state s at time t and $\xi_{ss'}(t)$ represent the expected number of transitions from state s to state s' at time t. For a given HMM $\mathcal{M}$, the intermediate variables, $\gamma_s(t)$ and $\xi_{ss'}(t)$, are computed for each observation sequence $o_0, o_1, \ldots, o_{|\mathbf{o}|-1} = \mathbf{o} \in \mathcal{O}$. These variables are computed as follows:

$$\gamma_s(t) = \frac{\alpha_s(t)\beta_s(t)}{\sum_{s' \in S} \alpha_{s'}(t)\beta_{s'}(t)} \tag{4}$$

In Equation 4, the numerator is the product of the forward variable $\alpha_s(t)$ and the backward variable $\beta_s(t)$, representing the joint likelihood of observing the enire sequence and the model given that the model passed by state s at time t. The denominator represents the likelihood of the observation sequence.

$$\xi_{ss'}(t) = \frac{\alpha_s(t)P_{ss'}\omega_{s'}(t+1)\beta_{s'}(t+1)}{\sum_{s''} \alpha_{s''}(t)\beta_{s''}(t)} \tag{5}$$

In Equation 5, the numerator is the joint likelihood of observing the sequence given that the model transitions from state s to state s' at time t. The denominator represents the likelihood of the observation sequence.

The terms $\gamma_s(t)$ and $\xi_{ss'}(t)$ are normalized to ensure they represent probabilities. For $\gamma_s(t)$, this involves dividing by the total likelihood across all states at time t, while for $\xi_{ss'}(t)$, normalization occurs over all possible transitions at time t.

2.6.2 Parameter Update

The parameter update step refines the parameter values of the model based on the earlier computed intermediate variables $\gamma_s(t)$ and $\xi_{ss'}(t)$. The update algorithm aims to maximize the expected likelihood of the observed data under the model by adjusting the parameter values.

Once $\gamma_s(t)$ and $\xi_{ss'}(t)$ are computed for all states s, s' and all time steps t for every observation sequence, the model parameters can be updated to maximize the expected log-likelihood.

Transition Probabilities (P): We update the transition probabilities based on the expected number of transitions between states:

$$P_{s \to s'} = \frac{\sum_{t=1}^{|\mathbf{o}|-1} \xi_{ss'}(t)}{\sum_{t=1}^{|\mathbf{o}|-1} \gamma_s(t)} \tag{6}$$

The numerator sums the expected number of transitions from state s to state s' over all time steps. The denominator sums the expected number of times the model is in state s over all time steps, ensuring $P_{ss'}$ is normalized across all s'.

Emission Probabilities (ω): We update the emission probabilities based on the expected occupancy of state s and the corresponding observations, meaning the likelihood of observing the specific label o in state s. The update is given by:

$$\omega_s(o) = \frac{\sum_{t=1}^{|\mathbf{o}|-1} \gamma_s(t)[\![o_t = o]\!]}{\sum_{t=1}^{|\mathbf{o}|-1} \gamma_s(t)} \tag{7}$$

The numerator sums $\gamma_s(t)$ for all time steps t where the observed value $o_t = o.$, meaning the model is in state s and emits the observation o. The denominator sums $\gamma_s(t)$ for all time steps t where the model is in a given state s.

Initial Probabilities (π): We update the initial probabilities based on the expected occupancy of state s at $t = 1$:

$$\pi_s = \gamma_s(1) \tag{8}$$

We can then update the parameters $\mathbf{x}$ by maximizing the expected log-likelihood of the observed data under the model. The update algorithm iteratively refines the parameter values until convergence is reached.

2.7 Matrix Operations

The Baum-Welch algorithm can be implemented using matrix operations to efficiently compute the forward and backward variables, intermediate variables, and parameter updates.

Given a HMM $\mathcal{M}$ with parameters ω, P, and π, and an observation sequence $\mathbf{o}$, the forward and backward variables α_t and β_t can be computed using matrix operations as follows:

$$\alpha_t = \begin{cases} \omega_0 \circ \pi & \text{if } t = 0 \\ \omega_t \circ \left(P^\top \alpha_{t-1}\right) & \text{if } 0 < t \leq |\mathbf{o}| - 1 \end{cases} \tag{9}$$

$$\beta_t = \begin{cases} \mathbb{1} & \text{if } t = |\mathbf{o}| - 1 \\ P\left(\beta_{t+1} \circ \omega_{t+1}\right) & \text{if } 0 \leq t < |\mathbf{o}| - 1 \end{cases} \tag{10}$$

Here $\circ$ represents the Hadamard (point-wise) matrix multiplication, $P^\top$ denotes the transpose of the matrix P, and $\mathbb{1}$ is a column vector of ones. The resulting vectors α_t and β_t for each time step t are then related to $\alpha_s(t)$ and $\beta_s(t)$ for some s by:

$$\alpha_t = \begin{bmatrix} \alpha_{s_0}(t) \\ \vdots \\ \alpha_{s_{|S|-1}}(t) \end{bmatrix}, \ \beta_t = \begin{bmatrix} \beta_{s_0}(t) \\ \vdots \\ \beta_{s_{|S|-1}}(t) \end{bmatrix} \tag{11}$$

γ and ξ can be expressed in terms of matrix operations as follows:

$$\gamma_t = \left(\sum_{i=1}^{|\mathbf{o}|-1} (\alpha_{ti}\, \beta_{ti})\right)^{-1} \cdot \alpha_t \circ \beta_t \tag{12}$$

$$\xi_t = \left(\left(\sum_{i=1}^{|\mathbf{o}|-1} (\alpha_{ti}\, \beta_{ti})\right)^{-1} \cdot\ P\right) \circ \left(\alpha_t \otimes \left(\beta_{t+1} \circ \omega_{t+1}\right)\right) \tag{13}$$

Here $\otimes$ represents the Kronecker (block) matrix multiplication, $\cdot$ denotes the scalar product and $^{-1}$ denotes the elementwise inverse of a matrix.

We can simplify $\sum_{i=1}^{|\mathbf{o}|-1} (\alpha_{ti}\beta_{ti})$ as, the sum does not depend on t:

$$\sum_{i=1}^{|\mathbf{o}|-1} (\alpha_{ti}\ \beta_{ti}) = \sum_{i=1}^{|\mathbf{o}|-1} \alpha_{|\mathbf{o}|-1i} \tag{14}$$

$$= \mathbb{1}^T\ \alpha_{|\mathbf{o}|-1} \tag{15}$$

Here $\mathbb{1}^T$ is a row vector of ones, and $\alpha_{|\mathbf{o}|-1}$ is the last column of the matrix $\alpha_{t_T \in 0\ldots|\mathbf{o}|-1}$.

So we get:

$$\gamma_t = (\mathbb{1}^T\ \alpha_{|\mathbf{o}|-1})^{-1} \cdot \alpha_t \circ \beta_t \tag{16}$$

$$\xi_t = ((\mathbb{1}^T\ \alpha_{|\mathbf{o}|-1})^{-1} \cdot\ P) \circ (\alpha_t \otimes (\beta_{t+1} \circ \omega_{t+1})) \tag{17}$$

The resulting vectors γ_t and ξ_t for each time step t are then related to $\gamma_s(t)$ and $\xi_{ss'}(t)$ for some s, s' by:

$$\gamma_t = \begin{bmatrix} \gamma_{s_0}(t) \\ \vdots \\ \gamma_{s_{|S|-1}}(t) \end{bmatrix},\ \xi_t = \begin{bmatrix} \xi_{s_0 s_0}(t) & \cdots & \xi_{s_0 s_{|S|-1}}(t) \\ \vdots & \ddots & \vdots \\ \xi_{s_{|S|-1} s_0}(t) & \cdots & \xi_{s_{|S|-1} s_{|S|-1}}(t) \end{bmatrix} \tag{18}$$

We can update the parameters with matrix operations as follows:

$$P = (\mathbb{1} \oslash \gamma) \bullet \xi \tag{19}$$

$$\omega_s(o) = (\mathbb{1} \oslash \gamma) \bullet (\sum_{t=1}^{|\mathbf{o}|-1} \gamma_t \otimes \mathbb{1}_{yt}^{|\mathbf{o}|-1}) \tag{20}$$

$$\pi = \gamma_1 \tag{21}$$

Where $\oslash$ denotes Hadamard division (elementwise division) product and $\bullet$ denotes the Katri-Rao product (column-wise Kronecker product). In the formulas above, $\mathbb{1}$ denotes a column vector of ones, $\mathbb{1}_{yt}$ denotes a row vector of ones, γ and ξ are the sum of the respective vectors over all time steps t:

$$\gamma = \sum_{t=1}^{|\mathbf{o}|-1} \gamma_t,\ \xi = \sum_{t=1}^{|\mathbf{o}|-1} \xi_t \tag{22}$$

3 Implementation

In this section, we will discuss the implementation of the project. We will start by discussing the tools used in the implementation, followed by the transition from matrices to ADDs. Finally, we will discuss the implementation of the matrix operations using ADDs.

3.1 CUDD

The Colorado University Decision Diagram (CUDD) library [20] is a powerful tool for implementing and manipulating decision diagrams, including Binary Decision Diagrams (BDDs) and ADDs. ADDs are compact representations of functions, often used to handle large state spaces symbolically and efficiently.

In this project, the CUDD library stores ADDs and performs operations on them. Its optimized algorithms and efficient memory management allow us to handle large and complex matrices symbolically, leading to significant performance improvements over traditional methods.

The CUDD library is implemented in C, ensuring high-performance execution, but it also ensures it can be used in C++ programs.

3.2 Storm

Storm is a versatile, open-source probabilistic model checking tool designed to verify the correctness and properties of stochastic models [8]. It supports a wide range of probabilistic models, including HMMs,MCs and Markov Decision Processs (MDPs). Storm allows users to analyze models efficiently by computing various quantitative properties, such as probabilities, expected rewards, or long-run averages.

A key feature of Storm is its ability to represent models symbolically, leveraging data structures like BDDs and ADDs. These symbolic representations compactly encode the model's state space and transition structure, enabling efficient manipulation and analysis even for large-scale systems. Storm achieves this by interfacing with the CUDD library, mentioned earlier.

In our implementation, Storm serves as a parser for loading the input models. Specifically, we utilize Storm to convert the model into its ADD representation. This ADD representation provides a compact and hierarchical encoding of the underlying matrices, which can then be used to perform symbolic matrix operations using the CUDD library.

The reason for using Storm lies in it is open-source, which makes it easy to integrate into our project. Storm is designed to handle large and complex models efficiently for model checking. Therefore the next step in Storm is to calculate the parameters of interest, such as transition probabilities, rewards, or other metrics derived from the model. By performing these computations symbolically within the ADD framework, we achieve a scalable and efficient approach to analyzing stochastic models.

3.3 Transition to ADDs

The first step in the implementation is to transition from vectors and matrices to ADDs. This conversion leverages the compact and efficient representation of ADDs to perform operations symbolically.

To convert a vector into an ADD, the vector must first be interpreted as a square matrix. This step ensures compatibility with the ADD representation, which organizes data hierarchically. When a matrix is represented as an ADD, the matrix also has to be square, as the ADD representation requires a square matrix, if the matrix is not square, it has to be padded with zeros to make it square.

Consider the following vector:

$$V = \begin{bmatrix} 1 & 2 & 3 & 4 \end{bmatrix}$$

This vector corresponds to a matrix of size 4×4.

$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

In an ADD, each layer corresponds to one binary variable (or bit) in the encoding of an index. For a matrix of size $n \times n$, where $n = 2^k$, the binary representation of the row and column indices requires k bits each. By interleaving these bits (e.g., alternating between row and column bits), we construct a balanced and regular structure that preserves the matrix's two-dimensional nature. In the case of the vector V, the vector has 4 elements, so it requires $4 = 2^2$ bits to represent the indices.

TABLE 1
Binary encoding of a vector V of size 4

Vector Index	Value	Binary Encoding
1	1	0000
2	2	0001
3	3	0010
4	4	0011

The binary representation of the vector entries is shown in Table 1, the rest of the matrix indices is filled with zeros.

The ADD representation of this vector is shown in Figure 1. The binary encodings determine the structure of the decision diagram, where each entry in the vector is stored as a terminal node. The paths to these nodes are dictated by the binary representation of their indices.

The conversion of a matrix to an ADD is similar to that of a vector, but with an additional layer of nodes to represent the rows. The ADD can however be reduced as shown in Figure 2. This reduction is done by removing the duplicated terminal nodes, removing the redundant nodes and merging the nodes with the same children. The techniques for reducing ADDs is the standard reduction techniques used for BDDs. The reduction of the ADD is done to reduce the size of the ADD and to make the operations on the ADD more efficient. CUDD has built-in functions for reducing the ADD, that follows the standard reduction techniques.

3.4 Matrix operations using ADDs

The matrix operations are implemented using ADDs. The matrix operations implemented are matrix transpose, matrix addition, matrix multiplication, Hadamard product, Hadamard division, Kronecker product and Khatri-Rao product.

$$A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$$

and

$$B = \begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix}$$

are used as examples in the following subsections.

3.4.1 Matrix Transpose

The matrix transpose is implemented by swapping the row and column variables in the ADD. Specifically, for each path in the ADD representing an entry (i, j), the roles of the row index i and column index j are exchanged. The terminal nodes (values of the matrix entries) remain unchanged. The transpose of matrix A is:

$$A^T = \begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix}$$

3.4.2 Matrix addition

Matrix addition is implemented by adding the terminal nodes of two ADDs while keeping the structure of the row and column indices consistent. The process involves:

1) Traversing the paths of both ADDs simultaneously.
2) Summing the values at the terminal nodes where the row and column indices match.

The resulting ADD represents the element-wise sum of the two matrices. The sum of matrices A and B is:

$$A + B = \begin{bmatrix} 6 & 8 \\ 10 & 12 \end{bmatrix}$$

3.4.3 Matrix multiplication

Matrix multiplication is implemented symbolically using the dot product of the row and column indices. In the ADD:

1) For each pair of rows in the first matrix and columns in the second matrix, the corresponding elements are multiplied.
2) The products are summed along the shared index, combining them into the final terminal nodes of the resulting ADD.

The hierarchical structure of the ADD ensures that only relevant paths are explored, making the operation efficient. The product of matrices A and B is

$$A \times B = \begin{bmatrix} 19 & 22 \\ 43 & 50 \end{bmatrix}$$

3.4.4 Hadamard product

The Hadamard product is implemented by pairwise multiplication of corresponding terminal nodes in the two ADDs. For each matching row-column index pair (i, j):

1) The values from both ADDs are multiplied.
2) The resulting product is stored in the terminal node of the new ADD.

The structure of the indices remains unchanged. The Hadamard product of matrices A and B is:

$$A \circ B = \begin{bmatrix} 5 & 12 \\ 21 & 32 \end{bmatrix}$$

3.4.5 Hadamard division

The Hadamard division is implemented as Hadamard product, but with division instead of multiplication. See subsubsection 3.4.4 for more details. The Hadamard division of matrices A and B is

$$A \oslash B = \begin{bmatrix} 0.2 & 0.3333 \\ 0.4286 & 0.5 \end{bmatrix}$$

3.4.6 Kronecker product

The Kronecker product is implemented by expanding the indices and terminal nodes of the two matrices symbolically, with the resulting ADD having the dimensions of the sum of the dimensions of the two matrices. The Kronecker product is a generalization of the outer product, where each element of the first matrix is multiplied by the second matrix as a whole. For each entry (i, j) in the first matrix with value a, the second matrix B is multiplied by a, and the indices are adjusted:

1) The row and column indices of B are shifted based on i and j of A.
2) The resulting values are stored in a new ADD.

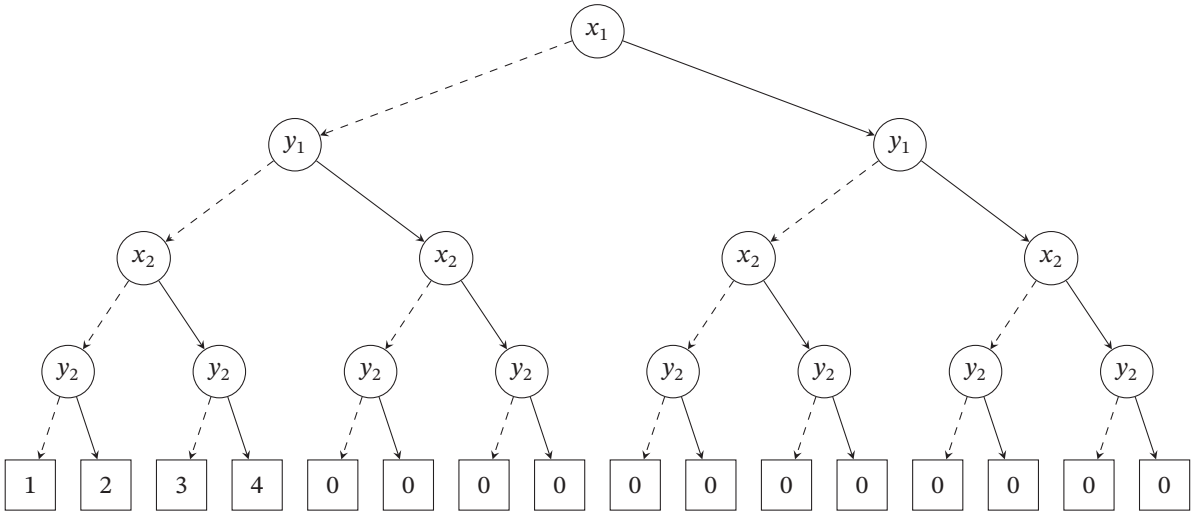

Fig. 1. Vector V represented as an ADD

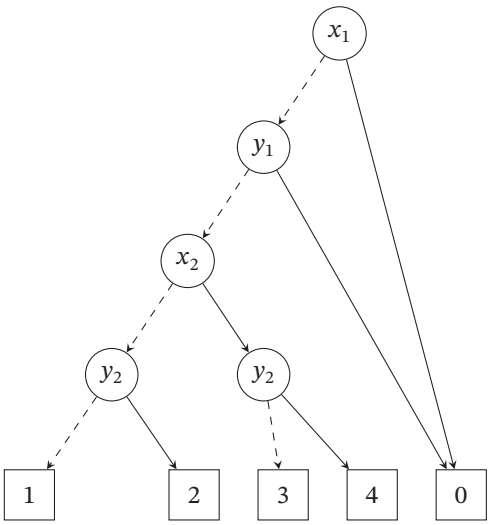

Fig. 2. Reduced ADD of matrix V

The Kronecker product of matrices A and B is

$$A \otimes B = \begin{bmatrix} 5 & 6 & 10 & 12 \\ 7 & 8 & 14 & 16 \\ 15 & 18 & 20 & 24 \\ 21 & 24 & 28 & 32 \end{bmatrix}$$

3.4.7 Khatri-Rao product

The Khatri-Rao product is implemented by combining rows of the first matrix with corresponding rows of the second matrix. For each row index i:

1) The elements of row i in the first matrix are multiplied element-wise with the entire row i in the second matrix.
2) The resulting row is constructed symbolically within the ADD.

The Khatri-Rao product of matrices A and B is

$$A \bullet B = \begin{bmatrix} 5 & 6 & 10 & 12 \\ 21 & 24 & 28 & 32 \end{bmatrix}$$

The resulting ADD has the dimensions of sum of the dimensions of the two matrices, as in the Kronecker product.

4 Definitions

Definition 2 (Markov Chain). A Markov chain is a tuple $\mathcal{M} = (S, \mathcal{L}, \ell, \tau, \pi)$, where:

- S is a finite set of states.
- $\mathcal{L}$ is a finite set of labels.
- $\ell : S \to \mathcal{L}$ is a labeling function, which assigns a label to each state.
- $\tau : S \to \mathcal{D}(S)$ is a transition function. The model moves from state s to state s' with probability $\tau(s, s')$.
- π: is the initial distribution, the model starts in state s with probability $\pi(s)$.

Intuitively, a Markov chain is a model that starts in a state s with probability $\pi(s)$, and then transitions to a new state s' with probability $\tau(s, s')$. The model continues to transition between states according to the transition function.

Definition 3 (Hidden Markov Model). A Hidden Markov Model (HMM) is a tuple $\mathcal{M} = (S, \mathcal{L}, \ell, \tau, \pi)$, where $S, \mathcal{L}, \tau, \pi$ are defined as above, and:

- $\ell : S \to D(\mathcal{L})$ is the emission function. The model emits a label l in state s with probability $\ell(s, l)$.

Intuitively, an HMM is a model that starts in a state s with probability $\pi(s)$, then emits a label l with probability $\ell(s, l)$, and transitions to a new state s' with probability $\tau(s, s')$. The model continues to emit labels and transition between states according to the emission and transition functions.

Definition 4 (Markov Decision Process). A Markov Decision Process (MDP) is a tuple $\mathcal{M} = (S, \mathcal{L}, \ell, A, \{\tau_a\}_{a \in A}, \pi)$ where $S, \mathcal{L}, \ell, \pi$ are defined as above, and:

- A is a finite nonempty set of actions.
- $\tau_a : S \to \mathcal{D}(S)$ is a transition function for each action $a \in A$. The model moves from state s to state s' with probability $\tau_a(s, s')$ when action a is taken.

Intuitively, an MDP is a model that starts in a state s with probability $\pi(s)$, then emits a label $\ell(s)$ and, it can recieve an action $a \in A$ and transition to a new state s' with probability $\tau_a(s, s')$.

4.1 Continuous-Time

In the previous definitions, the models are discrete-time models, where time advances in fixed, regular steps. For example, in a discrete-time Markov chain, the system transitions between states at each step or tick of a clock, and the probability of moving from one state to another is governed by the transition function $\tau(s, s')$. This means that transitions can only happen at specific time intervals (e.g., after every second, every minute, etc.).

In contrast, continuous-time models allow transitions to occur at any time, rather than at fixed intervals. The time between transitions is variable and follows a continuous distribution. This introduces the concept of transition rates rather than discrete transition probabilities.

Definition 5 (Continuous-Time Markov Chain). A Continuous-Time Markov Chain (CTMC) is a tuple $\mathcal{M} = (S, \mathcal{L}, \ell, R, \pi)$, where $S, \mathcal{L}, \ell, \pi$ are defined as above, and:

- $R : S \times S \to \mathbb{R}_{\geq 0}$ is the rate function. The model transitions from state s to state s' with rate $R(s, s')$.

For two states s and s', $R(s, s')$ gives the rate at which the system moves from state s to state s'. A higher rate means a faster transition.

A Continuous-Time Markov Chain (CTMC) is a type of Markov model where the time between transitions is not fixed but is governed by exponential distributions. If there are more then one outgoing transition from a state, we get race-conditions, the first transition to occur is the one that will be taken. The time spent in a state before transitioning to a new state is called $dwell - time$. This is exponentially distributed with a rate $E(s) = \sum_{s' \in S} R(s, s')$. The probability of transitioning from state s to state s' is $R(s, s')/E(s)$, the time spent in s is independent from the properbility of transitioning to s'.

4.2 Matrix Representation

The transition function τ can be represented as a matrix, where each element $\tau(s, s')$ is the probability of transitioning from state s to state s'. The matrix representation of τ is called the transition matrix. The transition matrix is a square matrix with dimensions $|S| \times |S|$, where $|S|$ is the number of states in the model. The transition matrix is a stochastic matrix, meaning that the sum of each row is equal to 1, meaning all the probabilities of transitioning from state s to all other states sum to 1.

If we take an example of a model with two states $S = \{s_1, s_2\}$, the transition matrix τ is defined as:

$$\tau = \begin{bmatrix} \tau(s_1, s_1) & \tau(s_1, s_2) \\ \tau(s_2, s_1) & \tau(s_2, s_2) \end{bmatrix} \tag{23}$$

We can give an example of a transition matrix for a model with two states, where the model transitions from state s_1 to state s_2 with probability 0.4 and transitions from state s_2 to state s_1 with probability 0.5:

$$\tau = \begin{bmatrix} 0.6 & 0.4 \\ 0.5 & 0.5 \end{bmatrix} \tag{24}$$

The initial distribution π is a vector that represents the probability of starting in each state. The initial distribution is a stochastic vector, meaning that the sum of all probabilities is equal to 1. The initial distribution π is a vector with dimensions $|S|$, where $|S|$ is the number of states in the model. Each element $\pi(s)$ is the probability of starting in state s.

$$\pi = \begin{bmatrix} 0.6 \\ 0.5 \end{bmatrix} \tag{25}$$

The labeling function ℓ can be represented as a matrix, where each element $\ell(s, l)$ is the probability of emitting label l in state s. The matrix representation of ℓ is called the emission matrix. The emission matrix is a matrix with dimensions $|S| \times |\mathcal{L}|$, where $|\mathcal{L}|$ is the number of labels in the model. The emission matrix is a stochastic matrix, meaning that the sum of each row is equal to 1, meaning all the probabilities of emitting a label in state s sum to 1.

If we take an example of a model with two states $S = \{s_1, s_2\}$ and two labels $\mathcal{L} = \{l_1, l_2\}$, the emission matrix ℓ is defined as:

$$\ell = \begin{bmatrix} \ell(s_1, l_1) & \ell(s_1, l_2) \\ \ell(s_2, l_1) & \ell(s_2, l_2) \end{bmatrix} \tag{26}$$

We can give an example of an emission matrix for a model with two states and two labels, where the model emits label l_1 in state s_1 with probability 0.7 and emits label l_2 in state s_2 with probability 0.6:

$$\ell = \begin{bmatrix} 0.7 & 0.3 \\ 0.4 & 0.6 \end{bmatrix} \tag{27}$$

The rate function R can be represented as a matrix, where each element $R(s, s')$ is the rate of transitioning from state s to state s'. The matrix representation of R is called the rate matrix. The rate matrix is a square matrix with dimensions $|S| \times |S|$, where $|S|$ is the number of states in the model. The rate matrix is a non-negative matrix, meaning that all elements are greater than or equal to 0.

$$R = \begin{bmatrix} R(s_1, s_1) & R(s_1, s_2) \\ R(s_2, s_1) & R(s_2, s_2) \end{bmatrix} \tag{28}$$

If we take an example of a model with two states $S = \{s_1, s_2\}$, the rate matrix R is defined as:

$$R = \begin{bmatrix} 0.5 & 0.3 \\ 0.2 & 0.4 \end{bmatrix} \tag{29}$$

5 HMM Example

5.1 Setup

We have a simple HMM with, two hidden states S_1 and S_2, two observation symbols: O_1 and O_2 and an observation sequence $O = \{O_1, O_2, O_1\}$.

The HMM parameters are:

Transition matrix A (probability of moving from one state to another):

$$A = \begin{bmatrix} 0.6 & 0.4 \\ 0.5 & 0.5 \end{bmatrix}$$

Emission matrix B (probability of emitting observation given a state):

$$B = \begin{bmatrix} 0.7 & 0.3 \\ 0.4 & 0.6 \end{bmatrix}$$

Initial state probability vector π (probability of starting in each state):

$$\pi = \begin{bmatrix} 0.8 & 0.2 \end{bmatrix}$$

5.2 Expectation step

In the expectation step we calculate α and β.

5.2.1 Forward step α

We first compute the forward probabilities $\alpha_t(i)$, which represent the probability of being in state i at time t after observing the first t symbols.

5.2.1.1 Initialization at ($t = 1$):

$$\alpha_1 = \pi \circ B_{y1}$$

Where B_{y1} is the first column of the emission matrix, corresponding to observation O_1

(i.e., $B_{y1} = \begin{bmatrix} 0.7 \\ 0.4 \end{bmatrix}$) and $\circ$ represents the Hadamard product.

So, we get:

$$\alpha_1 = \begin{bmatrix} 0.8 \\ 0.2 \end{bmatrix} \circ \begin{bmatrix} 0.7 \\ 0.4 \end{bmatrix} = \begin{bmatrix} 0.56 \\ 0.08 \end{bmatrix}$$

5.2.1.2 Induction (for $t = 2, 3, \dots, T$): For subsequent timesteps, we compute:

$$\alpha_{t+1} = B_{yt+1} \circ (A^T \alpha_t)$$

Where A^T is the transpose of the transition matrix. Let's apply this to compute the forward probabilities for $t = 2$ and $t = 3$:

At $t = 2$ **(observation** O_2**)**:

$$\alpha_2 = B_{y2} \circ (A^T \alpha_1)$$

We have:

$$B(y2) = \begin{bmatrix} 0.3 \\ 0.6 \end{bmatrix}$$

and

$$A^T = \begin{bmatrix} 0.6 & 0.5 \\ 0.4 & 0.5 \end{bmatrix}$$

We get:

$$\alpha_2 = \begin{bmatrix} 0.3 \\ 0.6 \end{bmatrix} \circ \left(\begin{bmatrix} 0.6 & 0.5 \\ 0.4 & 0.5 \end{bmatrix} \cdot \begin{bmatrix} 0.56 \\ 0.08 \end{bmatrix} \right) = \begin{bmatrix} 0.1128 \\ 0.1584 \end{bmatrix}$$

At $t = 3$ **(observation** O_1**)**:

$$\alpha_2 = B_{y1} \circ (A^T \alpha_2)$$

We get:

$$\alpha_3 = \begin{bmatrix} 0.7 \\ 0.4 \end{bmatrix} \circ \left(\begin{bmatrix} 0.6 & 0.5 \\ 0.4 & 0.5 \end{bmatrix} \cdot \begin{bmatrix} 0.1 \\ 0.1584 \end{bmatrix} \right) = \begin{bmatrix} 0.102816 \\ 0.049728 \end{bmatrix}$$

5.2.2 Backward step β

The backward probabilities $\beta_t(i)$ represent the probability of observing the rest of the sequence starting from time $t+1$, given that the system is in state i at time t.

Initialization (at $t = T = 3$**)**

$$\beta_T = \mathbf{1} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

5.2.2.1 Induction (for $t = T-1, T-2, \dots, 1$): For earlier timesteps, we compute:

$$\beta_t = A(\beta_{t+1} \circ B_{yt+1})$$

At $t = 2$ **(observation** O_1**)**:

$$\beta_2 = A(\beta_3 \circ B_{y1})$$

$$B_{y1} = \begin{bmatrix} 0.7 \\ 0.4 \end{bmatrix}, \quad \beta_3 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

We get:

$$\beta_2 = \begin{bmatrix} 0.6 & 0.4 \\ 0.5 & 0.5 \end{bmatrix} \cdot \left(\begin{bmatrix} 1 \\ 1 \end{bmatrix} \circ \begin{bmatrix} 0.7 \\ 0.4 \end{bmatrix} \right)$$

$$\beta_2 = \begin{bmatrix} 0.6 & 0.4 \\ 0.5 & 0.5 \end{bmatrix} \cdot \begin{bmatrix} 0.7 \\ 0.4 \end{bmatrix} = \begin{bmatrix} 0.58 \\ 0.55 \end{bmatrix}$$

At $t = 1$ **(observation** O_2**)**:

$$\beta_1 = A(\beta_2 \circ B_{y2})$$

We have:

$$B_{y2} = \begin{bmatrix} 0.3 \\ 0.6 \end{bmatrix}, \quad \beta_2 = \begin{bmatrix} 0.58 \\ 0.55 \end{bmatrix}$$

$$\beta_1 = \begin{bmatrix} 0.6 & 0.4 \\ 0.5 & 0.5 \end{bmatrix} \cdot \left(\begin{bmatrix} 0.3 \\ 0.6 \end{bmatrix} \circ \begin{bmatrix} 0.58 \\ 0.55 \end{bmatrix} \right)$$

$$\beta_1 = \begin{bmatrix} 0.6 & 0.4 \\ 0.5 & 0.5 \end{bmatrix} \cdot \begin{bmatrix} 0.174 \\ 0.33 \end{bmatrix} = \begin{bmatrix} 0.2364 \\ 0.252 \end{bmatrix}$$

5.3 Step 3: Compute γ and ξ

5.3.1 Compute γ

We can compute γ by

$$\gamma_t = (\mathbb{1}^T \cdot \alpha_T)^{-1} \cdot (\alpha_t \circ \beta_t)$$

$$\alpha_T = \begin{bmatrix} 0.089628 \\ 0.053328 \end{bmatrix}$$

$$\mathbb{1}^T \cdot \alpha_T = 0.089628 + 0.053328 = 0.152544$$

This is the total probability of oberserving our sequence $O = \{O_1, O_2, O_1\}$

Now we can compute γ_t for each time stamp.

At t=1: We have

$$\alpha_1 = \begin{bmatrix} 0.56 \\ 0.08 \end{bmatrix}, \quad \beta_1 = \begin{bmatrix} 0.2364 \\ 0.252 \end{bmatrix}$$

We take the Hadamard product of this.

$$\alpha_1 \circ \beta_1 = \begin{bmatrix} 0.56 \cdot 0.2364 \\ 0.08 \cdot 0.252 \end{bmatrix} = \begin{bmatrix} 0.132384 \\ 0.02016 \end{bmatrix}$$

We normalize the first part and take the scalar product.

$$\gamma_1 = \frac{1}{0.152544} \cdot \begin{bmatrix} 0.132384 \\ 0.02016 \end{bmatrix} = \begin{bmatrix} 0.8678414 \\ 0.1321589 \end{bmatrix}$$

At t = 2:

We have:

$$\alpha_2 = \begin{bmatrix} 0.1074 \\ 0.1584 \end{bmatrix}, \quad \beta_2 = \begin{bmatrix} 0.58 \\ 0.55 \end{bmatrix}$$

The Hadamard product is:

$$\alpha_2 \circ \beta_2 = \begin{bmatrix} 0.1074 \cdot 0.58 \\ 0.1584 \cdot 0.55 \end{bmatrix} = \begin{bmatrix} 0.062292 \\ 0.08712 \end{bmatrix}$$

We normalize the first part and take the scalar product.

$$\gamma_2 = \frac{1}{0.152544} \cdot \begin{bmatrix} 0.062292 \\ 0.08712 \end{bmatrix} = \begin{bmatrix} 0.42888609 \\ 0.57111391 \end{bmatrix}$$

At t = 3
We have:

$$\alpha_3 = \begin{bmatrix} 0.089628 \\ 0.053328 \end{bmatrix}, \quad \beta_3 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

The Hadamard product is:

$$\alpha_3 \circ \beta_3 = \begin{bmatrix} 0.089628 \\ 0.053328 \end{bmatrix}$$

We normalize the first part and take the scalar product.

$$\gamma_3 = \frac{1}{0.152544} \cdot \begin{bmatrix} 0.089628 \\ 0.053328 \end{bmatrix} = \begin{bmatrix} 0.67400881 \\ 0.32599119 \end{bmatrix}$$

5.3.2 Calculating ξ

We calculate ξ by

$$\xi_t = ((\mathbb{1}^T \alpha_T)^{-1} \cdot A) \circ (\alpha_t \otimes (\beta_{t+1} \circ B_{yt+1})^T)$$

We start by calculating $((\mathbb{1}^T \alpha_T)^{-1} \cdot A)$: From before, we have

$$(\mathbb{1}^T \alpha_T)^{-1} = \frac{1}{0.152544} = 6.996$$

We have:

$$A = \begin{bmatrix} 0.6 & 0.4 \\ 0.5 & 0.5 \end{bmatrix}$$

We get:

$$8.996 \cdot A = \begin{bmatrix} 6.996 \cdot 0.6 & 6.996 \cdot 0.4 \\ 6.996 \cdot 0.5 & 6.996 \cdot 0.5 \end{bmatrix} = \begin{bmatrix} 4.198 & 2.798 \\ 3.498 & 3.498 \end{bmatrix}$$

We can now calculate $\alpha_1 \otimes (\beta_2 \circ B_{y2})^T$. We have :

$$\alpha_1 = \begin{bmatrix} 0.56 \\ 0.08 \end{bmatrix}, \quad \beta_2 = \begin{bmatrix} 0.58 \\ 0.55 \end{bmatrix}, \quad B_{y2} = \begin{bmatrix} 0.3 \\ 0.6 \end{bmatrix}$$

We calculate $\beta_2 \circ B_{y2}$:

$$\beta_2 \circ B_{y2} = \begin{bmatrix} 0.58 \\ 0.55 \end{bmatrix} \circ \begin{bmatrix} 0.3 \\ 0.6 \end{bmatrix} = \begin{bmatrix} 0.174 \\ 0.33 \end{bmatrix}$$

Outer product:

$$\alpha_1 \otimes (\beta_2 \circ B_{y2})^T = \begin{bmatrix} 0.56 \\ 0.08 \end{bmatrix} \otimes \begin{bmatrix} 0.174 & 0.33 \end{bmatrix}$$

$$= \begin{bmatrix} 0.09744 & 0.1848 \\ 0.01392 & 0.0264 \end{bmatrix}$$

We can now calculate ξ_1

$$\xi_1 = \begin{bmatrix} 4.198 & 2.798 \\ 3.498 & 3.498 \end{bmatrix} \circ \begin{bmatrix} 0.09744 & 0.1848 \\ 0.01392 & 0.0264 \end{bmatrix}$$

$$\xi_1 = \begin{bmatrix} 0.38325991 & 0.03650094 \\ 0.60572687 & 0.08653241 \end{bmatrix}$$

At t=2:
We have:

$$B_{y1} = \begin{bmatrix} 0.7 \\ 0.4 \end{bmatrix}, \quad \alpha_2 = \begin{bmatrix} 0.1074 \\ 0.1584 \end{bmatrix}, \quad \beta_3 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

Hadamard product for $\beta_3 \circ B_{y1}$

$$\beta_3 \circ B_{y1} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \circ \begin{bmatrix} 0.7 \\ 0.4 \end{bmatrix} = \begin{bmatrix} 0.7 \\ 0.4 \end{bmatrix}$$

Outer product:

$$\alpha_2 \otimes \begin{bmatrix} 0.7 & 0.4 \end{bmatrix} = \begin{bmatrix} 0.07518 & 0.04296 \\ 0.11088 & 0.06336 \end{bmatrix}$$

We can now calculate ξ_2:

$$\xi_2 = \begin{bmatrix} 4.198 & 2.798 \\ 3.498 & 3.498 \end{bmatrix} \circ \begin{bmatrix} 0.07518 & 0.04296 \\ 0.11088 & 0.06336 \end{bmatrix}$$

$$\xi_2 = \begin{bmatrix} 0.07341938 & 0.06873304 \\ 0.03726872 & 0.0523348 \end{bmatrix}$$

At t=3:
We have:

$$B_{y1} = \begin{bmatrix} 0.7 \\ 0.4 \end{bmatrix}, \quad \alpha_3 = \begin{bmatrix} 0.089628 \\ 0.053328 \end{bmatrix}, \quad \beta_3 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

Hadamard product for $\beta_3 \circ B_{y1}$

$$\beta_3 \circ B_{y1} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \circ \begin{bmatrix} 0.7 \\ 0.4 \end{bmatrix} = \begin{bmatrix} 0.7 \\ 0.4 \end{bmatrix}$$

Outer product:

$$\alpha_3 \otimes \begin{bmatrix} 0.7 & 0.4 \end{bmatrix} = \begin{bmatrix} 0.062740 & 0.035852 \\ 0.037329 & 0.021331 \end{bmatrix}$$

We can now calculate ξ_3:

$$\xi_2 = \begin{bmatrix} 4.198 & 2.798 \\ 3.498 & 3.498 \end{bmatrix} \circ \begin{bmatrix} 0.062740 & 0.035852 \\ 0.037329 & 0.021331 \end{bmatrix}$$

$$\xi_3 = \begin{bmatrix} 0.2839837 & 0.09127753 \\ 0.13480176 & 0.06519824 \end{bmatrix}$$

5.4 Update values

$$\hat{\pi} = \gamma_1 = \begin{bmatrix} 0.86784141 \\ 0.1321589 \end{bmatrix}$$

$$\hat{A} = (\mathbb{1} \oslash \gamma) \bullet \xi$$

$$\hat{B} = (\mathbb{1} \oslash \gamma) \bullet (\sum_{t=1}^{T} \gamma_t \otimes \mathbb{1}_{yt}^T)$$

When referring to γ, we use the sum of the probabilities:

$$\gamma = \sum_{t=1}^{T} \gamma_t$$

and ξ:

$$\xi = \sum_{t=1}^{T} \xi_t$$

We therefore calculate:

$$\gamma = \begin{bmatrix} 0.86784141 \\ 0.1321589 \end{bmatrix} + \begin{bmatrix} 0.42888609 \\ 0.57111391 \end{bmatrix} + \begin{bmatrix} 0.67400881 \\ 0.32599119 \end{bmatrix} = \begin{bmatrix} 1.97073631 \\ 1.02926369 \end{bmatrix}$$

And

$$\xi = \begin{bmatrix} 0.38325991 & 0.03650094 \\ 0.60572687 & 0.08653241 \end{bmatrix} + \begin{bmatrix} 0.07341938 & 0.06873304 \\ 0.03726872 & 0.0523348 \end{bmatrix}$$

$$+ \begin{bmatrix} 0.2830837 & 0.09127753 \\ 0.13480176 & 0.06519824 \end{bmatrix} = \begin{bmatrix} 0.739763 & 0.19651152 \\ 0.77779736 & 0.20406545 \end{bmatrix}$$

We can now calculate

$$\mathbb{1} \oslash \gamma = \begin{bmatrix} \frac{1}{2.0923} \\ \frac{1}{1.1352} \end{bmatrix}$$

We can now calculate $\hat{A}$

$$\hat{A} = \begin{bmatrix} \frac{1}{2.0923} \\ \frac{1}{1.1352} \end{bmatrix} \bullet \begin{bmatrix} 0.9897 & 0.7370 \\ 0.5670 & 0.3888 \end{bmatrix} = \begin{bmatrix} 0.37537391 & 0.19092437 \\ 0.39467348 & 0.198226353 \end{bmatrix}$$

We calculate $\hat{B}$ We first calculate the sum of the outer products:

$$\sum_{t=1}^{T} \gamma_t \otimes \mathbb{1}_{yt}^{T}$$

At t = 1:

$$\gamma_1 \otimes \begin{bmatrix} 1 & 0 \end{bmatrix} = \begin{bmatrix} 0.86784141 \\ 0.1321589 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \end{bmatrix} = \begin{bmatrix} 0.86784141 & 0.13215859 \\ 0 & 0 \end{bmatrix}$$

At t = 2:

$$\gamma_2 \otimes \begin{bmatrix} 0 & 1 \end{bmatrix} = \begin{bmatrix} 0.42888609 \\ 0.57111391 \end{bmatrix} \otimes \begin{bmatrix} 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0.42888609 & 0.57111391 \end{bmatrix}$$

At t = 3:

$$\gamma_3 \otimes \begin{bmatrix} 1 & 0 \end{bmatrix} = \begin{bmatrix} 0.67400881 \\ 0.32599119 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \end{bmatrix} = \begin{bmatrix} 0.67400881 & 0.32599119 \\ 0 & 0 \end{bmatrix}$$

We summearize these to get:

$$\begin{bmatrix} 0.86784141 & 0.13215859 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0.42888609 & 0.57111391 \end{bmatrix} +$$

$$\begin{bmatrix} 0.67400881 & 0.32599119 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 1.54185022 & 0.45814978 \\ 0.42888609 & 0.57111391 \end{bmatrix}$$

$$\hat{b} = \begin{bmatrix} \frac{1}{2.0923} \\ \frac{1}{1.1352} \end{bmatrix} \bullet \begin{bmatrix} 1.54185022 & 0.45814978 \\ 0.42888609 & 0.57111391 \end{bmatrix}$$

$$= \begin{bmatrix} 0.78237266 & 0.23247645 \\ 0.41669214 & 0.55487618 \end{bmatrix}$$

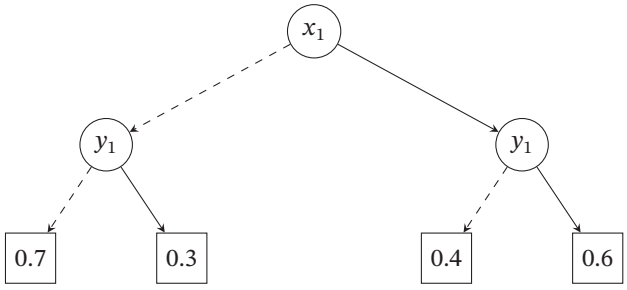

Fig. 3. B-matrix representation in ADD

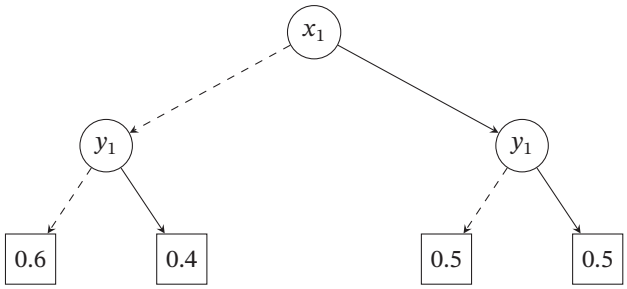

Fig. 4. A-matrix representation in ADD

5.5 ADD representation

As we only need one bit to represent the the rows and columns with one bit, we only need one variable for the them, as x_1 is the variable for rows and y_1 is the variable for column.

We first make the matrices into ADD representation.

We can now use the ADD representation to calculate α and β.

When using ADD's it is important to remember, if we need take a row from a matrix, we fix the input to the ADD by tting the x-variables to the desired row. An example is taking the third row of a matrix with 8 rows, we set, $x_1 = 1, x_2 = 1, x_3 = 0$ and $x_4 = 0$. if we need to take the second column, set $y_1 = 1, y_2 = 0$ and $y_3 = 0, y_4 = 0$. Hadamard product row-wise multiplication of the matrices. So to calculate the

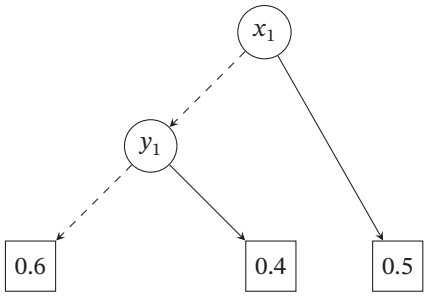

Fig. 5. A-matrix representation in ADD caption reduced

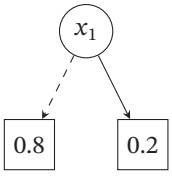

Fig. 6. π-matrix representation in ADD

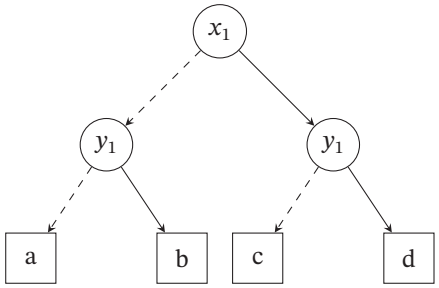

Fig. 7. Matrix A in ADD

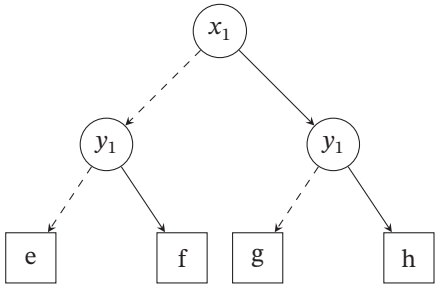

Fig. 8. Matrix B in ADD

Hadamard product of two matrices, we set the x-variables to the same row in both matrices and multiply the corresponding nodes in the ADDs. To calculate a Hadamard product in ADD, we multiply the corresponding nodes in the ADDs, as shown in the following figure.

Matrix multiplication is done by fixing the input to the first matrix and the output to the second matrix. We then sum the result of the Hadamard product of the rows of the first matrix and the columns of the second matrix. This is shown in the following figure.

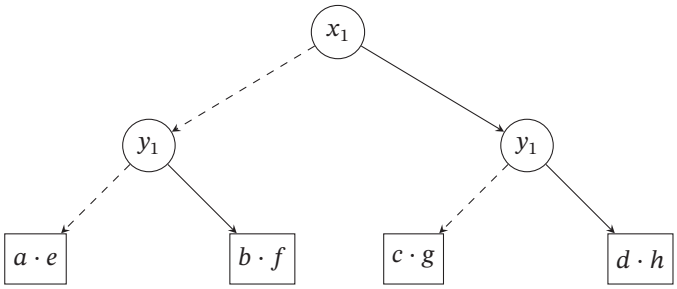

Fig. 9. Hadamard product of A and B in ADD

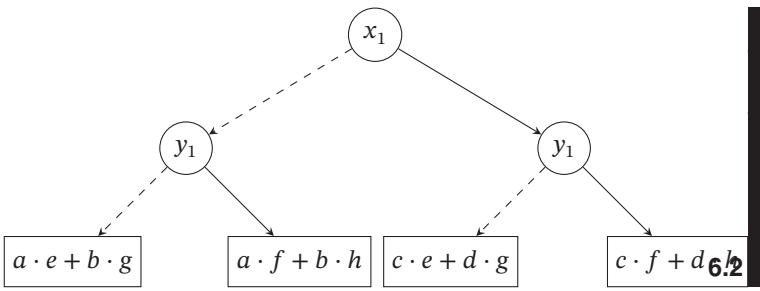

Fig. 10. Matrix multiplication of A and B in ADD

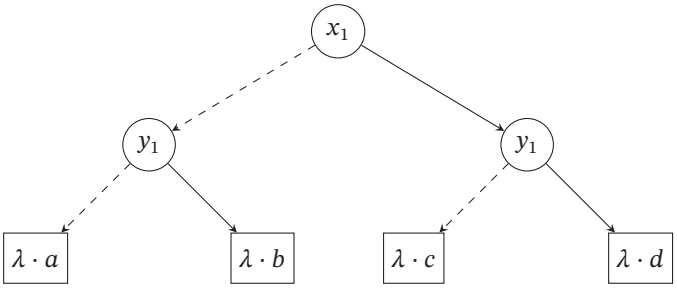

Fig. 11. Scalar product in ADD

6 Class Diagram

The class diagram in Figure 16 shows the relationships between the different classes in the system. The `Model` class represents the underlying model of the system, which can be a CTMC, DTMC, HMM and MDP. The `Model` class has a aggregation relationship with the `Algorithm` class, which represents the functions used in the Baum-Welch algorithm, with and without ussing log-semiring. The `Algorithm` class has a dependency relationship with the `CUDD` class, which is a wrapper for the CUDD library. The `CUDD` class is used to perform the matrix operations as ADD's required by the Baum-Welch algorithm. The `Model` class also has a aggregation relationship with the `CUDD` class, as the `Model` class uses the `CUDD` class to perform the ADD operations.

6.1 `Model` Class

The `Model` class serves as the foundation for representing various probabilistic models like CTMC, MDP, and DTMC. It holds fields needed to describe these models, such as the transition matrices, emission probabilities, and initial states, all represented using Algebraic Decision Diagrams (ADDs). The `Model` class also provides methods for training models, such as the Baum-Welch algorithm.

Attributes:

- `Type_model`: Defines the type of model (e.g., CTMC, MDP, DTMC).
- `transfer`: A list of ADD structures representing state transition probabilities.
- `Emission`: An ADD for the emission probabilities (relevant in Hidden Markov Models).
- `pi`: The initial state distribution, also stored as an ADD.
- `training_set`: A collection of observed data.

Methods:

- `Instantiate_with_parameters(prismfile, parameters: Dictionary)`: Instantiates a model with specified parameters.
- `Instantiate_without_parameters(prismfile)`: Creates a model without additional parameters.
- `Baum-welsh(log, Model)`: This method implements the Baum-Welch algorithm for training Hidden Markov Models, utilizing various operations from the `Algorithm` class.

6.2 `CUDD` Class

The `CUDD` class (CUDD Manager) is responsible for managing ADDs. These ADDs are crucial in representing the probabilistic

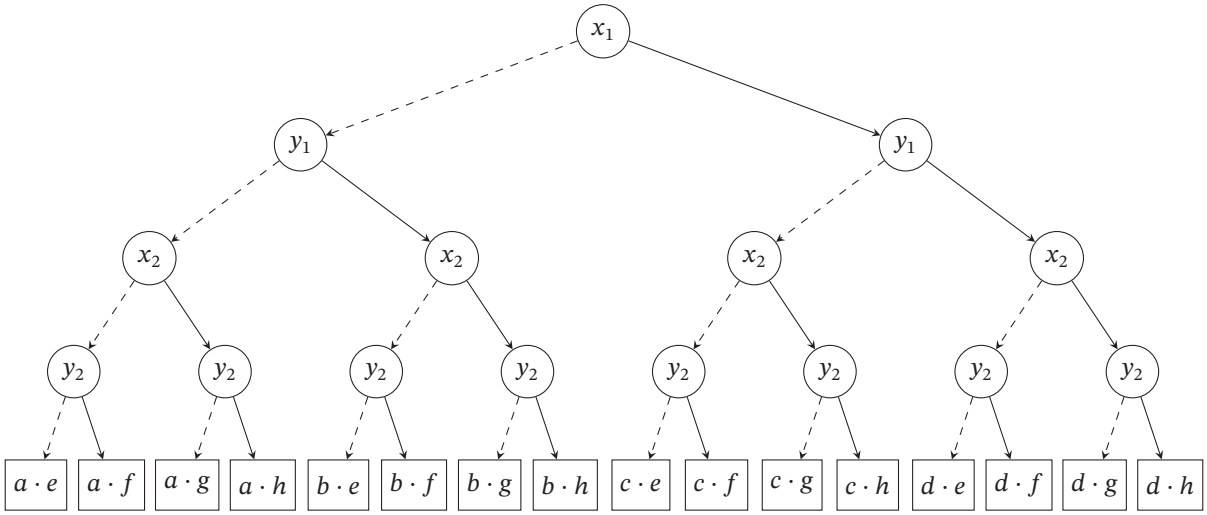

Fig. 12. Kroneker product in ADD

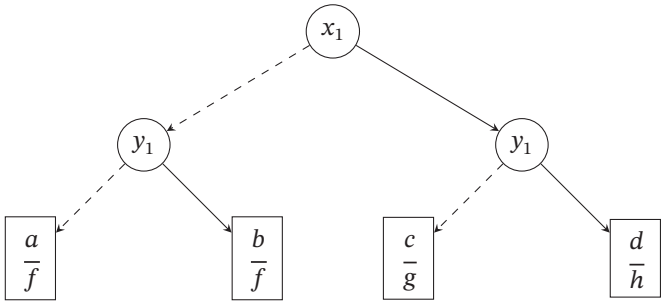

Fig. 13. Hadamard division of A and B in ADD

data structures used in the `Model` class. `CUDD` provides a set of operations that allow mathematical and logical manipulation of these diagrams.

Attributes:

- `rowvars, colvars`: Representing variables used in the ADD structures.
- `ADD`: The main data structure for storing probabilities or logical expressions.
- `Manager`: A control structure that coordinates operations on ADDs.

Methods:

- `Hadamard(), Log_Hadamard()`: Perform element-wise operations on ADDs.
- `Matrix_mul(), Log_matrix_mul()`: For matrix multiplications.
- `Sum(), Transpose()`: Additional helper methods for summing and transposing ADDs.

6.3 `Algorithm` Class

The `Algorithm` class encapsulates various methods for performing probabilistic calculations. These methods are mainly used for inference in models such as Hidden Markov Models (HMM) and Markov Chains.

Methods:

- `calculate_alpha(), calculate_beta()`: Compute the forward (alpha) and backward (beta) probabilities, respectively.
- `calculate_gamma(), calculate_xi()`: Intermediate probability calculations needed for parameter estimation and model training.

Each method operates on the ADD structures created and managed by the `CUDD` class, ensuring efficient computation of the probabilities.

6.4 Relationships Between Classes

6.4.1 `Model` to `Algorithm`: Association Relationship

The `Model` class uses the `Algorithm` class to compute the forward-backward probabilities and other values necessary for inference. The Baum-welsh(log, Model) method in `Model` invokes the relevant methods from `Algorithm` (calculate_alpha(), calculate_beta(), etc.) during the training process of HMMs. These methods, while called collectively in Baum-Welch, can also be used independently to perform specific calculations.

6.4.2 `Model` to `CUDD`: Aggregation Relationship

The `Model` class contains several attributes (transfer, Emission, pi) that are represented as ADDs, managed by the `CUDD` class. This relationship is best represented as an aggregation, where the `Model` holds instances of ADD but does not directly manage their internal workings. Instead, `CUDD` provides the operations required to manipulate and operate on these diagrams, such as matrix multiplication or element-wise functions (Hadamard products). The `Model` depends on `CUDD` for these operations, making it an integral part of the system's backend.

6.4.3 `Algorithm` to `CUDD`: Dependency Relationship

The `Algorithm` class depends on the `CUDD` class for all its operations on ADDs. Every method in `Algorithm` (e.g., calculate_alpha(), calculate_gamma()) relies on ADD operations provided by `CUDD`, such as Matrix_mul() and Hadamard(). This is represented by a dependency relationship, where `Algorithm` calls `CUDD`'s methods to perform its computations.

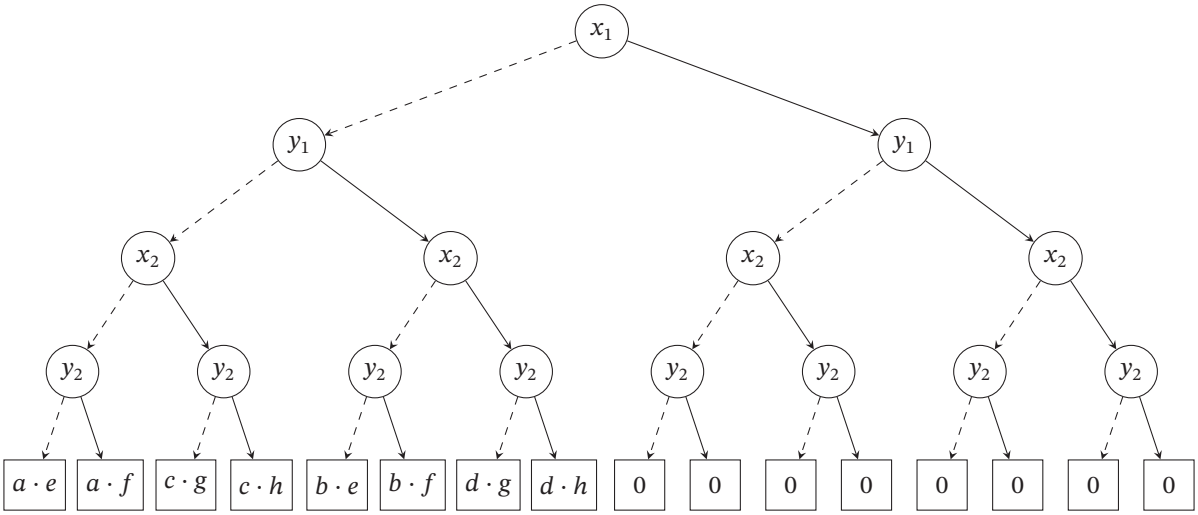

Fig. 14. Katri-Rao in ADD

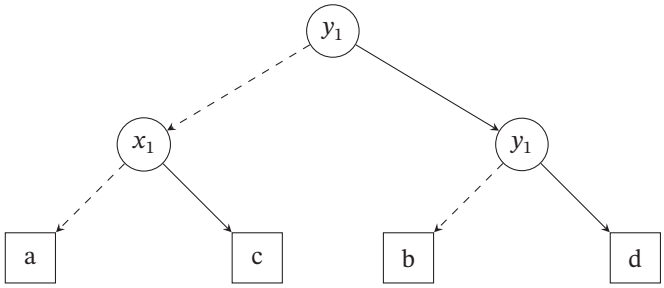

Fig. 15. transpose in ADD

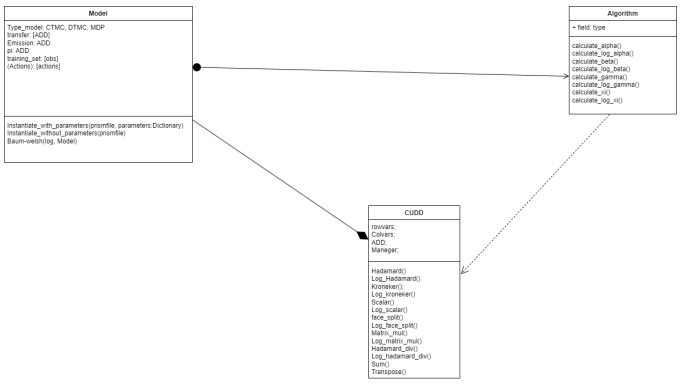

Fig. 16. Class diagram of the system

7 Experiment

The purpose of the experiments is to evaluate the performance of different implementations of the Baum-Welch algorithm when applied to various CTMC models. Specifically, we compare our implementation that utilize ADDs with and without the log semiring to other implementations from Jajapy, namely the original Jajapy implementation of the Baum-Welch algorithm and the improved SUDD implementation. By analyzing both parameter estimation accuracy and runtime, we aim to determine the efficiency and reliability of each implementation across multiple model types. We also investigate the scalability of the Baum-Welch algorithm by increasing the number of states in the model and comparing the runtime of each implementation.

We use 5 different models to test the performance of the Baum-Welch algorithm. Each model provides a different structure and complexity level for testing the Baum-Welch algorithm. The models are derived from CTMCs and include:

- **Polling**: A model representing a server polling multiple queues, often used in network communication scenarios.
- **Cluster**: Simulates clusters of entities competing for shared resources.
- **Tandem**: A series of interconnected queues where entities move sequentially from one queue to the next.
- **Philosophers(I) and Philosophers(II)**: Models representing the classic synchronization problem where entities (philosophers) compete for limited resources (e.g., forks), with Philosophers2 containing one additional parameter.

In every model, we have a number of parameters we want to estimate. The number of parameters to estimate in each model is shown in Table 2. The polling model is the smallest model with 2 parameters to estimate, while philosophers(II) is the largest model, with 4 parameters to estimate.'

TABLE 2
Number of parameters to estimate in each model

Model	Num of parameters
Polling	2
Cluster	3
Tandem	3
Philosophers(I)	3
Philosophers(II)	4

7.1 Parameter Estimation Accuracy

The first experiment measures the time and accuracy of the Baum-Welch algorithm for each implementation. We generate observation sequences from each model and use the Baum-Welch algorithm to estimate the parameters of the model. We compare the estimated parameters with the true parameters of the model to evaluate the accuracy of the estimation.

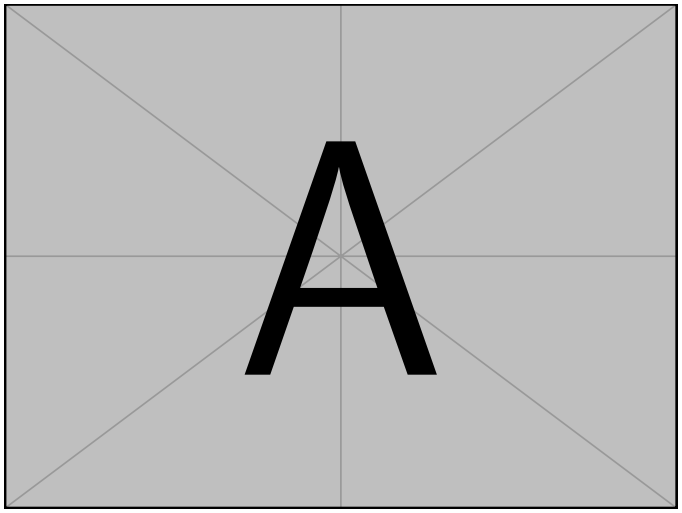

Fig. 17. Scalability of Baum-Welch implementations for the Tandem model

The experiment is made with the following steps:

1) We load the model.
2) Generate an observation sequence from the model with untimed steps.
3) Calculate the model's parameters using each variant of the Baum-Welch algorithm, recording both the parameter estimates and runtime.
4) Repeat steps 2 and 3 ten times without changing the model, the sequence length, or whether the sequence is timed or untimed. The results are averaged to account for any variance in runtime and estimation accuracy.
5) Repeat with timed steps to observe the effects of timing information on estimation accuracy and runtime.
6) Compare the estimated parameters with the true parameters and record the runtime for each implementation.
7) Move to the next model and repeat the entire process.

Following the experiment, the estimated parameters for each implementation are compared with the true parameters for accuracy assessment. Additionally, runtime for each Baum-Welch implementation is recorded. These results are presented in tables and plots to facilitate a direct comparison of performance across models and between implementations.

Table 3, 4, 5, 6 and 7 show detailed results for each model in terms of runtime and estimation accuracy (relative formula error and relave parameter error).

7.2 Scalability experiment

We also test the scalability of the Baum-Welch algorithm by increasing the number of states in a model. We use the Tandem model and increase the number of states from 28 to 1225. We then compare the runtime of the Baum-Welch algorithm for each implementation. We run the experiment 10 times for each number of states and compare the runtime of the Baum-Welch algorithm for each implementation.

We use plots to illustrate the scalability by showing runtime across an increasing number of states for the Tandem model, highlighting each implementation's computational efficiency.

7.3 Results

The comparison of the Baum-Welch implementations is based on the following criteria:

- **Parameter estimation accuracy**: The accuracy of the estimated parameters compared to the true parameters.
- **Runtime**: The time it takes to estimate the parameters.
- **Scalability**: How the runtime scales with the number of states in the model.

The results are displayed as tables and plots to facilitate a direct comparison of performance across models and between implementations.

Acronyms

AAU Aalborg University. 1
ADD Algebraic Decision Diagram. 2, 5–7

BDD Binary Decision Diagram. 5, 6

HMM Hidden Markov Model. 2–5

MC Markov Chain. 3, 5
MDP Markov Decision Process. 5

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TABLE 3
Comparison of Baum-Welch implementations for Polling

Implementation	Timed Observations				Untimed Observations			
	Time(s)	Iteration	avg δ	avg ϕ	Time(s)	Iteration	avg δ	avg ϕ
CuPAAL	132.5	3.5	0.1	0.1	132.5	3.5	0.1	0.1
CuPAAL_log	132.5	3.5	0.1	0.1	132.5	3.5	0.1	0.1
SUDD	23.5	3.5	0.1	0.1	23.5	3.5	0.1	0.1
SUDD_log	0.5	3.5	0.1	0.1	0.5	3.5	0.1	0.1
Jajapy	9.5	3.5	0.1	0.1	9.5	3.5	0.1	0.1

TABLE 4
Comparison of Baum-Welch implementations for Cluster

Implementation	Timed Observations				Untimed Observations			
	Time(s)	Iteration	avg δ	avg ϕ	Time(s)	Iteration	avg δ	avg ϕ
CuPAAL	132.5	3.5	0.1	0.1	132.5	3.5	0.1	0.1
CuPAAL_log	132.5	3.5	0.1	0.1	132.5	3.5	0.1	0.1
SUDD	23.5	3.5	0.1	0.1	23.5	3.5	0.1	0.1
SUDD_log	0.5	3.5	0.1	0.1	0.5	3.5	0.1	0.1
Jajapy	9.5	3.5	0.1	0.1	9.5	3.5	0.1	0.1

TABLE 5
Comparison of Baum-Welch implementations for Tandem

Implementation	Timed Observations				Untimed Observations			
	Time(s)	Iteration	avg δ	avg ϕ	Time(s)	Iteration	avg δ	avg ϕ
CuPAAL	132.5	3.5	0.1	0.1	132.5	3.5	0.1	0.1
CuPAAL_log	132.5	3.5	0.1	0.1	132.5	3.5	0.1	0.1
SUDD	23.5	3.5	0.1	0.1	23.5	3.5	0.1	0.1
SUDD_log	0.5	3.5	0.1	0.1	0.5	3.5	0.1	0.1
Jajapy	9.5	3.5	0.1	0.1	9.5	3.5	0.1	0.1

TABLE 6
Comparison of Baum-Welch implementations for Philosophers(I)

Implementation	Timed Observations				Untimed Observations			
	Time(s)	Iteration	avg δ	avg ϕ	Time(s)	Iteration	avg δ	avg ϕ
CuPAAL	132.5	3.5	0.1	0.1	132.5	3.5	0.1	0.1
CuPAAL_log	132.5	3.5	0.1	0.1	132.5	3.5	0.1	0.1
SUDD	23.5	3.5	0.1	0.1	23.5	3.5	0.1	0.1
SUDD_log	0.5	3.5	0.1	0.1	0.5	3.5	0.1	0.1
Jajapy	9.5	3.5	0.1	0.1	9.5	3.5	0.1	0.1

TABLE 7
Comparison of Baum-Welch implementations for Philosophers(II)

Implementation	Timed Observations				Untimed Observations			
	Time(s)	Iteration	avg δ	avg ϕ	Time(s)	Iteration	avg δ	avg ϕ
CuPAAL	132.5	3.5	0.1	0.1	132.5	3.5	0.1	0.1
CuPAAL_log	132.5	3.5	0.1	0.1	132.5	3.5	0.1	0.1
SUDD	23.5	3.5	0.1	0.1	23.5	3.5	0.1	0.1
SUDD_log	0.5	3.5	0.1	0.1	0.5	3.5	0.1	0.1
Jajapy	9.5	3.5	0.1	0.1	9.5	3.5	0.1	0.1

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Appendix A
Compiling in draft

You can also compile the document in draft mode. This shows todos, and increases the space between lines to make space for your supervisors feedback.