Extending Continuous Time Bayesian Networks for Parametric Distributions

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***Abstract*—The use of phase-type distributions has been suggested as a way to extend the representational power of the continuous time Bayesian network framework beyond exponentially-distributed state transitions. However, much of the discussion has focused on approximating a distribution that is learned from available data. This method is inadequate for applications where there is not sufficient data to represent a distribution. In this paper, we suggest a method for learning phase-type distributions from known parametric distributions. We find that by minimizing a modified KL-divergence value, we are able to obtain good phase-type approximations for a variety of parametric distributions. In addition, we investigate the effects of using varying numbers of phases. Finally, we propose and evaluate an extension that uses informed starting locations for the optimization process rather than random initialization.**

I. Introduction

A Markov process is a memoryless stochastic process, meaning that future states of the process are independent of previous states given the current state. A continuous time Markov process (CTMP) describes the evolution of a process in continuous time over a finite set of discrete states. A CTMP is represented as an initial distribution over the states, and a square transition intensity matrix Q with dimensions equal to the number of states in the process. An element q_{ij} in row i, column j of the matrix indicates the intensity with which the process transitions from state i to state j. More formally, the time it takes to transition between the states i and j is described by an exponential distribution with a rate that corresponds to the entry q_{ij}. The diagonal entries in Q are defined to be the negative sum of the remaining entries in the row, which ensures that every row in the matrix sums to zero. Any row with a nonzero entry represents a state that will eventually transition to another, and is therefore referred to as a transient state. If a row contains all zeros, there is no way to transition to another state and it is therefore considered an absorbing state. A Markov process will eventually transition into an absorbing state if one exists, and will remain in that state permanently.

A continuous time Bayesian network (CTBN) is a factored representation of a Markov process (Nodelman, Shelton, & Koller, 2002). This representation has two components: an initial distribution over the variables in the model, and a set of conditional intensity matrices (CIMs) for each variable. The factorization is achieved by taking advantage of conditional independences, which are encoded using a directed graph whose node's represent the variables in the process. Each CIM is an intensity matrix conditioned on an instantiation of the node's parents. The CTBN formulation provides a framework that can model time directly in a way that other temporal models, such as dynamic Bayesian networks, cannot.

Although CTBNs have been successfully used to model system change over time, the framework does have practical limitations. In particular, the computational efficiency achieved by CTBNs is rooted in its exploitation of the Markov property, and these efficiency gains are reliant on the use of exponential distributions. As a consequence, CTBNs in their original form can only describe processes with exponentially distributed duration times. This restriction can be very limiting when it comes to modeling real-world domains. The desire to retain the computational advantages afforded by CTBNs while simultaneously expanding their scope to describe more complex distributions has motivated the use of phase-type distributions as an extension to the CTBN framework.

Phase-type distributions, represented by the time until absorption in a Markov process, can be used to closely approximate any positive parametric distribution. This versatility, combined with their adherence to the Markov property, makes phase-type distributions especially valuable in the context of CTBNs. Recent work has shown that phase-type distributions can be used to extend the expressive power of CTBNs by transforming each state within the CIM into multiple phases, and using the absorbing phase to define an exit distribution to another state in the system (Gopalratnam, Kautz, & Weld, 2005). This allows the CTBN to retain the Markov property and the related efficiency gains, while also providing a more expressive model that can approximate a greater number of distributions. A more formal treatment of phase-type distributions can be found in Section II-C of this paper. To date, work on extending CTBNs through the use of phase-type distributions has focused on the problem of approximating a distribution that describes available data. This is achieved by applying expectation maximization algorithms to learn a model that optimizes the log-likelihood of the data. While this approach works well in the presence of abundant data, in many practical applications there is not enough data available to describe a distribution sufficiently. Fitting a distribution to data requires a minimum amount of data points to measure goodness of fit (Banks, 1998). In cases where there is not sufficient data, a viable alternative is to rely on domain knowledge to indicate transition rates with a well-defined probability distribution. These distributions are known to describe the behavior of a system accurately and as such we will refer to these well-defined probability distributions as “true” distributions.

A true distribution, unlike an unknown distribution described by available data, is specified entirely by its parameters.

Using true distributions as a means to describe system behavior is a well-established practice when performing tasks such as failure rate analysis (Farewell & Prentice, 1977). Learning phase-type distributions from true distributions provides information about transition times for a variable while avoiding the need for significant amounts of data. To this end, we propose minimizing the KL-divergence of a learned phase-type distribution from the true distribution, which is equivalent to maximizing the closeness of the approximation.

II. Parametric Distributions

Our work is primarily motivated by a desire to model system failures. For this reason, we focus our discussion specifically on a subset of distributions that are commonly used to model time-to-failure (TTF); specifically, the Weibull and lognormal distributions (Kalbfleisch & Prentice, 2011). Exponential distributions are also sometimes used to model failure rates, but CTBNs are already naturally suited to model these distributions. We note that although we limit the scope of our discussion to Weibull and lognormal, the framework we propose allows for the approximation of any positive true distribution.

A. *Weibull Distribution*

Weibull is a flexible distribution parameterized by a rate parameter λ and a shape parameter k (Pinder, Wiener, & Smith, 1978). Consider the case where the input x to the distribution is interpreted as the TTF. When $k < 1$, the Weibull distribution represents a decreasing failure rate, and an increasing failure rate when $k > 1$. In the special case where $k = 1$, the Weibull distribution reduces to an exponential distribution with a rate of λ. When x is positive, the probability density function (PDF) for the Weibull distribution is defined below.

$$f(x;\lambda,k) = \frac{k}{\lambda}\left(\frac{x}{\lambda}\right)^{k-1}\exp\left(-\left(\frac{x}{\lambda}\right)^{k}\right)$$

Since the failure rate for a Weibull distribution can be increasing, decreasing, or constant, it can be used to model the “infant mortality” stage (where $k < 1$), the “useful life” stage (for $k = 1$), and the “end of life” stage (where $k > 1$) of an object. When spliced together in this order, these three piece-wise segments form what is often called the “bathtub” curve. This is considered an appropriate model for the failure rate of many objects, as it reflects a higher rate of failure surrounding the birth and death of an object, and a relatively small constant rate of failure during the rest of the object’s lifespan. Additionally, it has been suggested that this composite approach may prove to be a more realistic model for TTF than monotone failure rate models (Rajarshi & Rajarshi, 1988). The plot for this function using several different parameterizations is shown in Figure 1.

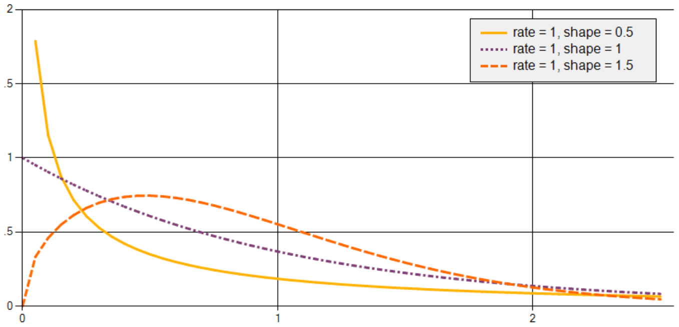


Fig. 1: PDFs for various parameterizations of Weibull distributions.

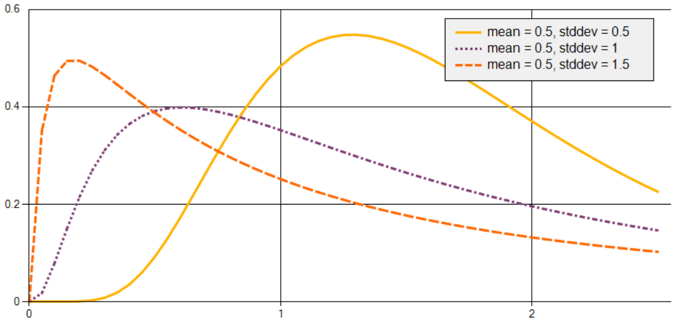


Fig. 2: PDFs for various parameterizations of lognormal distributions.

B. *Lognormal Distribution*

Another frequently used TTF curve is the lognormal distribution, which indicates that the log of a random variable follows a normal distribution. Due to its dependence on the normal distribution, the only necessary parameters for the lognormal distribution are the mean parameter μ and the variance parameter σ. The lognormal distribution is well suited for instances where failure occurs due to an accumulation of causes that have a multiplicative effect, a phenomenon known as multiplicative degradation (Srinivasan, Adve, Bose, & Rivers, 2005). When the input x is positive, the PDF for the lognormal distribution is as follows.

$$f(x;\mu,\sigma) = \frac{1}{x\sigma\sqrt{2\pi}}\exp\left(-\frac{(\ln x-\mu)^2}{2\sigma^2}\right)$$

Figure 2 provides a plot of various parameterizations for this function.

C. *Phase-Type Distributions*

Phase-type distributions are a semi-parametric class of distributions that use exponential distributions as a means to approximate general positive distributions, including (but not limited to) both Weibull and lognormal. Formally, phase-type distributions represent the time until absorption in a Markov process with n transient states and one absorbing state (Aalen, 1995). The transient states in the Markov process are also referred to as the phases of the phase-type distribution. A variable will move through each of these phases according to the exponential distributions defined for each phase by the rates in the Markov process, until the variable eventually reaches the absorbing state. The phase-type distribution is defined as the distribution of the entire time it takes the process to move through these phases.

Since a phase-type distribution depends only on a Markov process, its parameters are specified fully by the initial distribution and transition intensity matrix for the Markov process. It is generally assumed that the probability of starting in the absorbing state is zero, and in many cases it is further restricted to ensure that the process starts in the first transient state. The movement of a variable through the transient states of the Markov process can be directed in a variety of ways. In the most general case, all transient states are capable of transitioning to any other state, including the absorbing state. Specific classes of phase-type distributions restrict the movement of a variable between the transient states. Several types of restricted phase-type distributions are discussed in the review of related literature.

The PDF for a phase-type distribution is given as

$$f(x) = \alpha \exp(\mathbf{S}x)\mathbf{S^0} \tag{1}$$

where α is a vector corresponding to the probability of starting in each state, $\mathbf{S^0}$ is a vector of intensities for transitioning to the absorbing state from each of the other states, and $\mathbf{S}$ is a square matrix of intensities for transitioning between non-absorbing states. The matrix exponential operation, $\exp(\mathbf{S})$, is defined by the Taylor series as shown.

$$\exp(\mathbf{S}) = \sum_{k=0}^{\infty} \frac{1}{k!}\mathbf{S}^k \tag{2}$$

Calculating the matrix exponential is generally intractable. Fortunately, there exists a variety of methods for calculating an approximate matrix exponential (Moler & Van Loan, 2003). We chose to utilize the most commonly used method for calculating approximate matrix exponentials, known as the scaling and squaring method (Higham, 2005).

The idea behind scaling and squaring is to scale the matrix by a power of two to reduce the norm to order one, and then compute a Padé approximant [1] for the matrix exponential on the scaled matrix. Repeatedly squaring the resulting matrix undoes the scaling. By using the scaling and squaring method to calculate the matrix exponential, calculating the PDF of a phase-type distribution becomes tractable. The ability to calculate this PDF becomes important when evaluating the quality of a phase-type approximation for a true distribution.

Work has been done to demonstrate that a phase-type distribution can be directly embedded into a CIM for a CTBN without significantly changing the usage of the CTBN (Nodelman & Horvitz, 2003). Essentially, a single row in a CIM can be replaced by entries calculated using the phase-type distribution and the original multinomial distribution defined by the row. When performing inference over the CTBN, a node is interpreted as being in a particular state if it is currently in any of the phases that have been inserted for the state. The underlying mechanics remain unchanged, since phase-type distributions are built using exponential distributions, which adhere to the Markov assumption.

III. Related Work

The use of phase-type distributions for CTBNs was first proposed by Nodelman and Horvitz (Nodelman & Horvitz, 2003). They demonstrated that phase-type distributions can be inserted as subsystems in a CTBN without altering the underlying mechanics of the model. Their work was restricted to Erlang distributions, a subclass of phase-type distributions where loops are not permitted and each phase is required to have the same rate parameter and must be visited in order before transitioning to the absorbing state. The use of an Erlang distribution was shown to improve the performance of the CTBN model when the underlying distribution was non-exponential. The primary contribution made by the authors is the notion that phase-type distributions can be inserted into a CTBN without changing the framework as a whole. The specific details of how to parameterize the phase-type distributions were omitted.

The work by Nodelman and Horvitz was later extended from Erlang distributions to Erlang-Coxian distributions, which are another more expressive subclass of phase-type distributions (Gopalratnam et al., 2005). A Coxian distribution is similar to an Erlang distribution in that it does not permit cycles in the phases. In contrast, however, a Coxian distribution may be uniquely parameterized at each phase, and any of the phases may transition to the absorbing state. An Erlang-Coxian distribution combines these two ideas by forcing sequential progression through the Erlang phases until the Coxian phases are reached, at which point the phase may either transition to the next phase, or go to the absorbing state directly.

The addition of the Coxian phases increases the expressiveness of the model, but at the cost of added complexity through an increase in the required number of parameters. Instead of requiring a single rate parameter λ, two additional parameters are required for each phase in the Coxian distribution. This additional complexity can be managed by restricting the Coxian distribution to only two phases. Gopalratnam *et al.* propose a method for learning these parameters from data based on expectation maximization (EM). Unlike the method we propose here, their technique attempts to parameterize the distribution such that the log-likelihood between the data and the model is maximized.

After demonstrating the utility of Erlang distributions as subsystems in CTBNs, in subsequent work Nodelman *et al.* discuss a method for performing EM and structural EM (SEM) to learn the parameters and structure of a CTBN model from partially observed data (Nodelman, Shelton, & Koller, 2012). This EM algorithm further relaxes the restrictions on which subclasses of phase-type distributions are applicable, such that any phase-type distribution can be used. This allows phases to occur within a loop, significantly improving the expressiveness of the model. The experiments again showed a marked improvement over a CTBN model that did not use phase-type distributions. Nodelman *et al.* demonstrate the utility of this approach, but we explore a different angle with our contributions. While Nodelman learns phase-type distributions from data, we learn the parameters for a phase-type distribution to fit a known distribution.

[1] An [n,m] Padé approximant is a rational function consisting of a polynomial of degree m divided by a polynomial of degree n, useful for providing an approximation of the power series of another function (Baker Jr & Gammel, 1970).

IV. Approach

The primary goal of our research is to provide a method for learning a phase-type distribution that accurately approximates a given true distribution. To achieve this, we first cast the parameterization of the model distribution as an optimization problem. We then solve the optimization problem such that the result is a parameterization of a phase-type distribution that accurately approximates the specified true distribution.

As an example, consider a Weibull distribution with a rate parameter of 1.0 and a shape parameter of 1.5. The learned initial distribution and transition matrix for a phase-type distribution that approximates this Weibull distribution are shown below.

$$P(X) = (0.98 \quad 0.02 \quad 0.00)$$

$$Q = \begin{pmatrix} -2.09 & 1.98 & 0.11 \\ 0.00 & -1.99 & 1.99 \\ 0.00 & 0.00 & 0.00 \end{pmatrix}$$

A plot of the PDFs for both the Weibull distribution and the approximating phase-type distribution is shown in Figure 3. For reference, the goodness of fit for this approximation is quantified by a KL-divergence value of 0.0361.

A. Kullback-Leibler Divergence

In this work, we utilize the Kullback-Leibler divergence measure, often referred to simply as KL-divergence. The KL-divergence of distribution Q from distribution P is denoted as $D_{KL}(P||Q)$. For the case when P and Q are continuous, KL-divergence is defined by Equation 3. In practice, a discrete approximation can be used that evaluates the PDF for each distribution at specified intervals. In this work, we use the equation specified by equation 4. Note that in addition to evaluating the distributions at discrete intervals, we restrict the upper bound of the summation to be a finite value less than infinity. We have manually specified an upper bound of 2.5 since it has been deemed the area of interest for the distribution, but a more automated approach could be taken that chooses the upper bound based on the percentage of the distribution covered, as determined by the cumulative distribution function (CDF). Furthermore, notice that we have introduced an absolute value to the log term, which is a modification to the standard KL-divergence equation. This is done to avoid situations where underestimation in one section of the approximate PDF might mask overestimation in another, which may occur due to the fact that the log term can be positive or negative.

$$D_{KL}(P||Q) = \int_0^\infty p(x) \log \frac{p(x)}{q(x)} \, \mathrm{d}x \tag{3}$$

$$\approx D_{KL}(P||Q) = \sum_{i=1}^{n} P(i) \left| \log \frac{P(i)}{Q(i)} \right| \tag{4}$$

KL-divergence serves as a measure of the information lost when approximating a true distribution with an approximating distribution and is equal to zero if the two distributions are identical. Using this principle, we are able to construct an accurate approximation by choosing phase-type parameters that minimize the KL-divergence of the phase-type distribution from the true distribution.

We use Equation 4 to calculate the KL-divergence of the phase-type distribution Q from the true distribution P. This calculation requires knowledge of the PDFs of both distributions. The PDF for the true distribution is unique to each distribution, but it is generally a trivial calculation. We use an approximation of the PDF for a phase-type distribution, along with the PDF for the true distribution, to compute the KL-divergence as described in Equation 4.

B. Optimization

Selecting parameters for the phase-type approximation of a true distribution is an optimization problem that seeks to minimize KL-divergence. There are many possible approaches to such a problem. In this study, we take a soft-computing approach and use a genetic algorithm (GA), and particle swarm optimization (PSO). For a baseline comparison, we compare against a simple hill-climbing algorithm that uses simulated annealing.

1) Hill-Climbing with Simulated Annealing: The first method we utilized to select parameters that minimize KL-divergence is hill climbing using simulated annealing. The heart of this procedure lies in using simulated annealing, a numerical analogue to the process of slowly cooling metals so that they crystallize at their minimum energy state, to improve upon the basic hill climbing search (Press, Flannery, Teukolsky, & Vettering, 1986).

The original hill-climbing algorithm is relatively simple. The candidate solution, which for our purposes is a parameterization of the model, is initialized at a random state in the search space. Then, at each iteration, a random neighbor state is considered. If the neighboring state is found to have a better fitness value than the current state, the neighbor is accepted and becomes the current state. For the implementation described here, a better fitness value is defined as a lower KL-divergence from the true distribution. Simulated annealing introduces an extra step at each iteration to avoid becoming stuck in local optima. Once a neighbor state is selected, it is accepted or rejected based on the acceptance probability.

$$P(accept) = \exp\left(\frac{\text{energy}(current) - \text{energy}(neighbor)}{kT}\right) \tag{5}$$

where the energy of a given parameterization is its KL-divergence from the true distribution and T is a value known as the *temperature*, which is initialized to some positive number and slightly decreased each iteration. A better neighbor state will still always be accepted, but now a worse solution may also be accepted based both on how much worse it is and on the temperature at that iteration.

The gradual lowering of the temperature parameter produces the desired annealing effect: the likelihood of accepting a worse solution is initially high but decreases as a function of

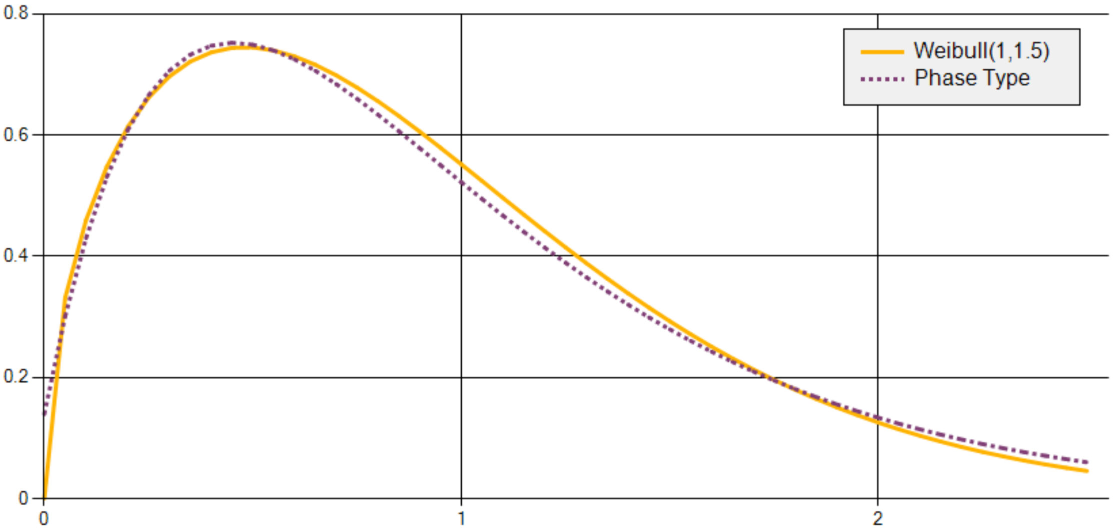


Fig. 3: Example of a phase-type distribution fitted to a Weibull distribution with a rate of 1.0 and a shape of 1.5.

time. This enables the algorithm to avoid becoming stuck in local optima early in the search process while still converging on a close-to-optimal solution in the later iterations of the search.

2) Genetic Algorithm: Genetic algorithms, as their name suggests, are an attempt to bring the advantages of Darwinian evolution to optimization algorithms (Mitchell, 1998). The idea behind a genetic algorithm is to start with a population of randomly generated solutions, which are in this case assignments of values to the parameters of a phase-type distribution. Each solution in the population is called an *individual* or *chromosome*, and the fitness for these solutions are calculated as their KL-divergence from the true distribution. Iteratively, a new "offspring" population is created from the existing population as follows.

First, two parent chromosomes are chosen such that assignments with lower KL-divergence are more likely to be selected. In our genetic algorithm implementation, we used tournament selection. This compares a small pool of candidate parents uniformly selected from the population and probabilistically chooses the fittest to become a parent. The parent is then returned to the population and another selected in the same manner; thus, it is possible to have the same chromosome as both parents.

Once the parents have been selected, crossover takes place. We utilized five-point multi-point crossover, which involves randomly selecting sections of parameters and swapping them between the parents to create two offspring chromosomes. These offspring are then mutated, a process that randomly changes the values of some of their parameters by a small amount.

This process repeats until a desired number, n of new offspring have been created, at which point the generation is completed and is used to replace the old population. The algorithm is repeated for a specified number of generations, after which the fittest individual in the population is returned as the solution.

3) Particle Swarm Optimization: PSO begins by initializing a population of particles, each of which has a position in the search space that represents a possible candidate solution (Kennedy, 2010). The quality of each particle's position can be evaluated using a fitness function that is problem specific. Particles move through the search space as defined by their velocity, which is updated during each iteration of the algorithm according to the velocity update shown in the following equation.

$$v_i = \omega v_i + U(0, \phi_1) \otimes (p_i - x_i) + U(0, \phi_2) \otimes (p_g - x_i) \quad (6)$$

Here, v_i is the velocity for particle i, x_i is the position of the particle, p_i is the particle's current best solution, and p_g is the best position seen by any particle in the population. For our purposes, the "best" solution is defined to be the solution with the lowest KL-divergence.

The entire population is collectively referred to as a swarm, and the behavior of a particle is intended to mimic the social behavior of animals, such as flocking birds or schooling fish. The effect of the velocity update equation is that an individual particle is drawn toward three locations: the direction it was previously heading ("momentum"), the best position it has ever found ("cognitive component"), and the best position any particle in the swarm has ever found ("social component"). This social component achieves the desired flocking behavior.

V. Experiments

In addition to comparing optimization algorithms, we explored the effects of several other factors on the ability to learn phase-type approximations. Specifically, we were also interested in how much an increase in the number of phases in the model added to its expressive power. We also proposed and evaluated alternatives to strictly random initialization of solutions during optimization. The relevant experiments are detailed in the remainder of this section.

A. *Optimization Methods*

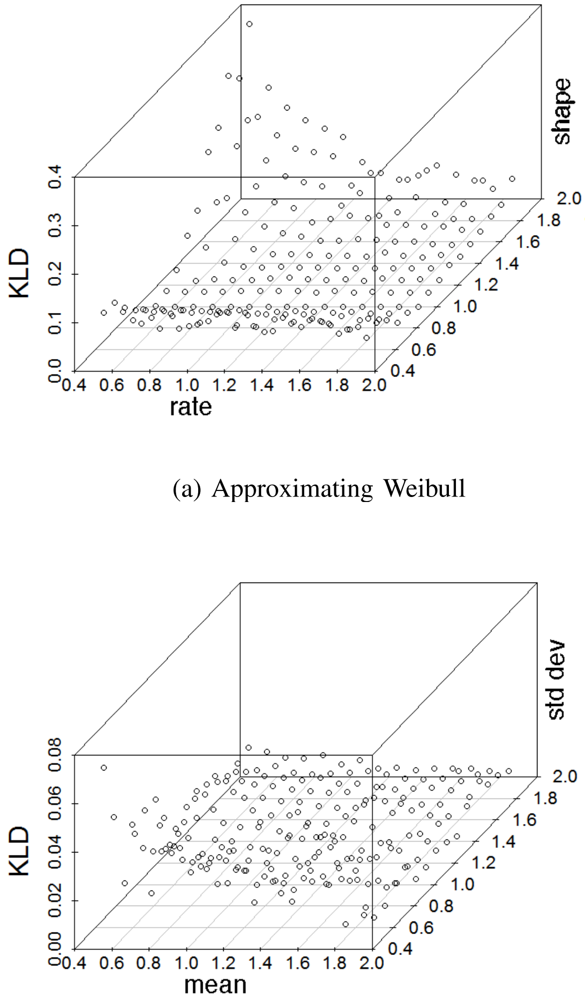
We ran the hill-climbing with simulated annealing (HC), genetic algorithm (GA), and PSO optimization algorithms on various parameterizations of Weibull and lognormal distributions. For Weibull we varied both the rate and shape parameters from 0.5 to 2.0 by increments of 0.1 for a total of 225 instances. The same values were used with the lognormal distribution for the mean and standard deviation parameters.

For this initial experiment, we fixed the size of the learned distribution to three phases. We used general phase-type distributions, which have no structural restrictions. The intensity matrix and initial distribution for each phase-type distribution was serialized so that they conformed to the optimization algorithm frameworks. This is done by extracting all non-diagonal entries from the intensity matrix excluding the last row, since the diagonal entries for each row of the intensity matrices can be computed as the negative sum of the rest of the row, and the last row will always be set to 0 since it is absorbing. We also included all but the last value of the initial distribution in the serialization, since the last value is the complement of the remaining values, such that the initial distribution sums to one. The result is a vector of size n^2, where n is the number of phases. We bound the valid search space for the optimization such that the initial distribution values are smaller than one, while the entries for the intensity matrix are bounded by some positive user-specified value which we set to 2.00 for all experiments. The deserialization process reverses the described procedure to produce a phase-type distribution that can be used to evaluate candidate solutions for the optimization algorithms.

Algorithms were compared on the KL-divergence between the final learned phase-type distribution and the true distribution. The parameters for each algorithm were manually tuned. Hill-climbing used an initial temperature of 100 and decreased this value by a factor of 0.05 at each iteration. For the genetic algorithm, we used 100 individuals, five-point crossover, and two-parent tournament selection with a 75% chance of choosing the fittest parent. PSO used five particles that moved according to a velocity equation with a momentum of 0.9, a personal learning rate of 1.0, and a social learning rate of 1.5. Each of the algorithms were run for 1000 iterations, which in all cases appear to be sufficient for convergence.

Algorithms were compared with the Wilcoxon signed-rank test, a nonparametric test chosen because the datapoints originate from different distributions. Based on our statistical analysis, PSO significantly outperforms the GA, which in turn significantly outperforms HC. For this reason, we focus the rest of our experiments on how well PSO performs under varying conditions and omit any further results for GA and HC.

We also investigate PSO's ability to approximate distributions over different regions of the parameter space. As specified above, we use the 225 parameterizations for Weibull and lognormal and plot the KL-divergence values obtained using PSO in Figure 4. We see in Figure 4a that relatively low KL-divergence values are obtained for the majority of the search space, with the exception of those cases when the rate is low and the shape is high. Similarly, we find from Figure 4b that most parameterizations of the lognormal distribution can be approximated well, but performance degrades when both the mean and standard deviation are low.



(a) Approximating Weibull

(b) Approximating lognormal

Fig. 4: KL-divergence values for approximating various parameterizations of Weibull and lognormal distributions using PSO.

B. *Number of Phases*

The next experiment investigated the effect of varying the number of phases in the phase-type distribution. Phase-type distributions with more states have more representational power, and therefore allow for a more accurate approximation. However, more states implies more parameters in the resulting CTBN and therefore increased model complexity.

For this experiment, we used five representative parameterizations each for the Weibull and lognormal distributions. For Weibull, these values included $(0.8, 1.7)$, $(1.0, 1.5)$, $(1.3, 1.7)$, $(0.7, 0.7)$ and $(1.0, 0.5)$, where the first value in each pair is the rate and the second value of the pair corresponds to the shape. In the case of lognormal, we used $(0.8, 1.2), (1.0, 1.2), (1.0, 1.0), (1.2, 1.0)$ and $(0.95, 1.0)$, where the first values are the means and the second values are the standard deviations.

For each of these ten true distributions, we used PSO to learn phase-type distributions with varying numbers of phases. Specifically, we started with a a single phase (which is equivalent to the exponential distribution) and increased incrementally to ten phases. Our analysis of these results consisted of a series of Wilcoxon signed-rank tests. The single-phase distribution was significantly outperformed by every other case. We also found that the use of only two phases was significantly worse than using three, four, five, or six phases. In addition, using six phases was significantly better than using seven and eight, as well as one and two.

C. Informed Initialization

Our final experiment tests an extension to our proposed algorithm which we call informed initialization. The idea is that, rather than initializing particles randomly, we can use a more intelligent starting solution. This is accomplished by first approximating a variety of distributions using random initialization and saving the resulting parameters for the phase-type distributions. When learning a new distribution, the algorithm can then initialize using a similar cached solution by calculating the sum of the differences between parameters and sorting the list.

For this experiment, the set of saved solutions was generated using the experiments run in Section V-A, resulting in 225 potential starting positions for each distribution. For the true distributions, we used the ten distributions discussed in Section V-B and the parameters for each were perturbed by $+0.05$ so that they cannot be found exactly in the set of saved solutions. We varied the number of particles that were initialized using the set of saved solutions from zero (equivalent to random initialization) to all five. When multiple particles use informed initialization, solutions were drawn from the saved set in order of similarity.

The performance of the algorithm as a function of the number of iterations for the cases when 0, 1, and 5 particles use informed initialization is shown in Figure 5. Using more particles that are initialized with informed starting positions results in faster convergence to lower KL-divergence values. We omit 2, 3, and 4 initialized particles from the graph for clarity, but we note that there is an incremental decrease in the KL-divergence for each case. We also used a Wilcoxon signed-rank test to compare the results of 0 initialized particles to 5 initialized particles after every 200 iterations. The results of these tests are shown in Table **??**. Results indicate that, at several stages in the algorithm, the informed initialization performs significantly better than random initialization.

VI. Discussion and Conclusions

The experiment from Section V-A showed that, of the optimization methods considered, PSO performed best. In addition, Figure 4 gives a sense of how well phase-type distributions are able to approximate various parameterizations of Weibull and lognormal distributions. KL-divergence values were higher when the true distribution had harsher peaks in its PDF. This indicates that phase-type distributions are better at approximating smooth distributions. Intuitively, using a larger number of phases should combat this problem.

The conclusion of the experiment in Section V-B is that a phase-type distribution with a single phase or few phases may lead to unsatisfactory approximations. Six phases seems optimal, as further increasing the number of phases does indeed increase expressiveness, but also makes optimization more difficult. Since the search space increases quadratically with the number of phases, adding more phases greatly expands the parameter space the optimization method must search. Note that this is not necessarily a concern, in that we seek to find good approximations while using as few parameters as possible. We found that three phases is likely sufficient to get a reasonable approximation, and two phases may also work when model complexity is a concern.

As discussed in Section V-C, informed initialization does appear to improve the approximations. Initializing all particles in PSO produced significantly better results at intermediate stages of the optimization process. In addition, Figure 5 shows that the solution converges much faster when informed initialization is used, which could be important in applications where learning time is important.

The goal of this work was to develop a method for approximating known parametric distributions using phase-type distributions. We demonstrated that this can be accomplished by minimizing a modified KL-divergence value. We investigated several optimization algorithms and found that PSO produced the best approximations. We explored how well this procedure works in relation to the specified parameters for both Weibull and lognormal distributions, and also tested how the number of phases impacts the quality of the approximation. Finally, we propose an extension that uses informed initialization to improve convergence speed of the optimization algorithm. Experiments in these areas have shown promising results, paving the way for additional improvements.

A. Future Work

One possible area for future work involves alternate approximations of the matrix exponential. The scaling and squaring method, while accurate, is also computationally expensive. A potential improvement to our approach could be to use a faster approximation initially, and later switch back to the more accurate scaling and squaring. The threshold at which this switch is most effective, along with the specific alternate method used, is left to future work.

We would also like to experiment with approximating distributions beyond Weibull and lognormal. The same framework can be used for any positive distribution, so long as the PDF can be calculated at the specified intervals for the KL-divergence calculation. While we expect our results will generalize, it is possible that features unique to other distributions may influence the ability to find satisfactory phase-type approximations.

Finally, we plan to provide a more formal treatment of the process required to embed phase-type distributions into a conditional intensity matrix. Although it has been discussed briefly by Nodelman and Horvitz, as well as in later works, there has been no mathematically rigorous explanation has

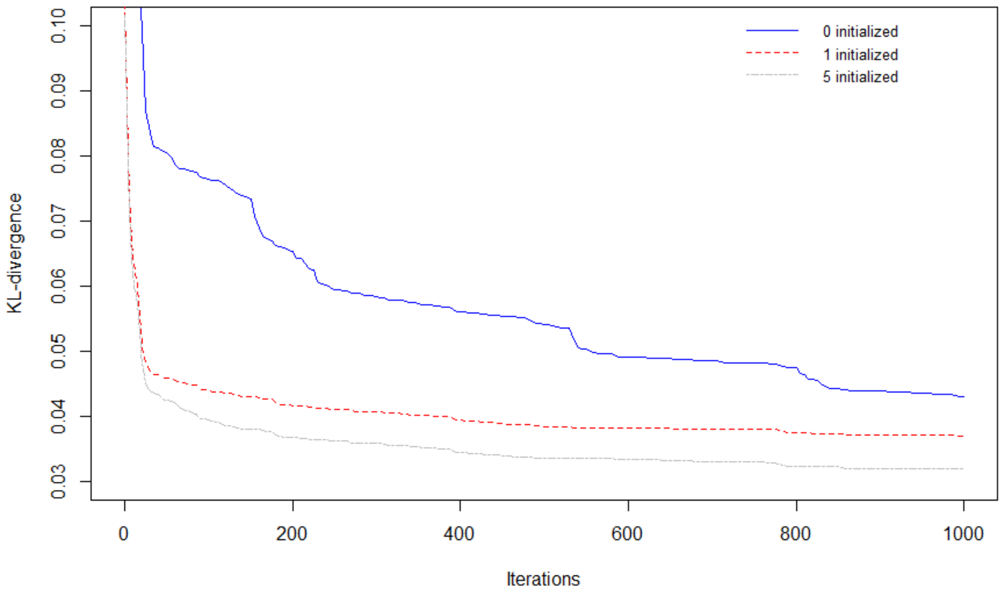


Fig. 5: Effect of informed initialization on KL-divergence.

been given that describes the embedding process. Furthermore, discussion of the embedding process typically assumes features of the phase-type distribution, such as an initial distribution that deterministically starts in the first phase. We intend to present a formal description of how to construct a CIM via block matrices, each of which can be generated using the learned phase-type distribution and the multinomial distribution defined by the row of the CIM.

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